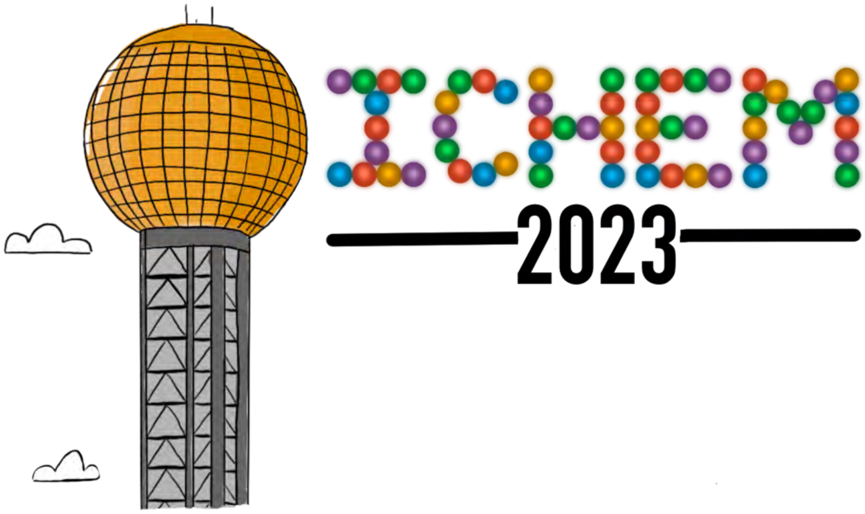

INTERNATIONAL CONFERENCE
ON
HIGH-ENTROPY MATERIALS

Knoxville, TN

June 18-22, 2023

We gratefully acknowledge sponsorship from

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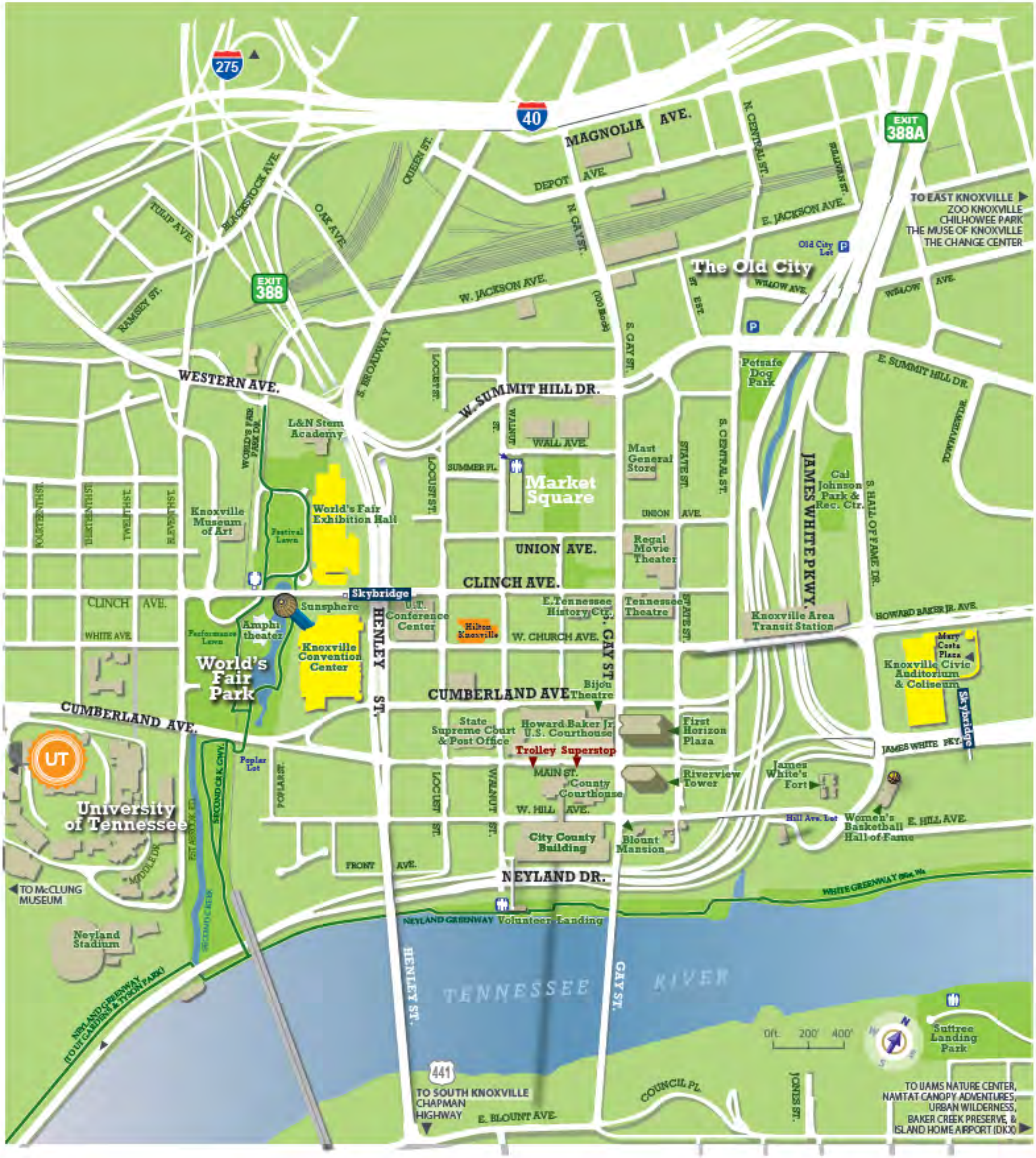
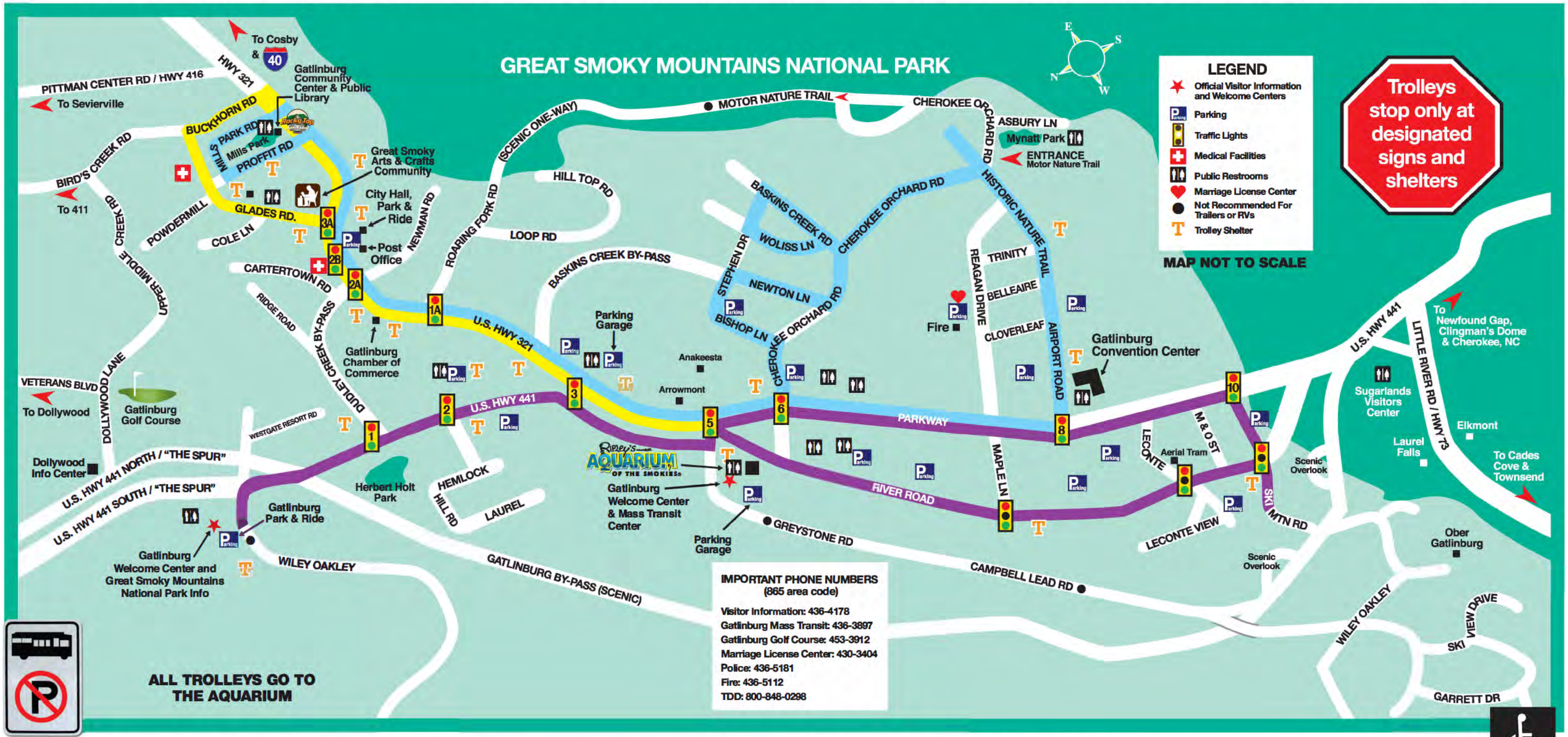


275
40
EXIT 388
EXIT 388A
MAGNOLIA AVE.
DEPOT AVE.
N. GAY ST.
N. CENTRAL ST.
SULLIVAN ST.
E. JACKSON AVE.
TO EAST KNOXVILLE
ZOO KNOXVILLE
CHILHOWEE PARK
THE MUSE OF KNOXVILLE
THE CHANGE CENTER
Old City Lot
The Old City
WILLOW AVE.
WILLOW AVE.
QUEEN ST.
OAK AVE.
BLACKSTOCK AVE.
TULIP AVE.
RAMSEY ST.
W. JACKSON AVE.
(100 Block)
S. GAY ST.
S. BROADWAY
LOCUST ST.
WESTERN AVE.
W. SUMMIT HILL DR.
E. SUMMIT HILL DR.
Petsafe Dog Park
L&N Stem Academy
WORLD'S FAIR PARK DR.
WALNUT ST.
WALL AVE.
SUMMER PL.
Market Square
Mast General Store
STATE ST.
S. CENTRAL ST.
JAMES WHITE PKWY.
Cal Johnson Park & Rec. Ctr.
S. HALL OF FAME DR.
McCALLIE DR.
FOURTEENTH ST.
THIRTEENTH ST.
TWELFTH ST.
ELEVENTH ST.
Knoxville Museum of Art
Festival Lawn
World's Fair Exhibition Hall
UNION AVE.
UNION AVE.
Regal Movie Theater
CLINCH AVE.
CLINCH AVE.
Skybridge
Sunsphere
U.T. Conference Center
E. Tennessee History Ctr.
Tennessee Theatre
Knoxville Area Transit Station
HOWARD BAKER JR. AVE.
WHITE AVE.
Performance Lawn
Amphitheater
Hilton Knoxville
W. CHURCH AVE.
Mary Costa Plaza
Knoxville Civic Auditorium & Coliseum
Skybridge
World's Fair Park
Knoxville Convention Center
HENLEY ST.
GAY ST.
Bijou Theatre
CUMBERLAND AVE.
CUMBERLAND AVE.
State Supreme Court & Post Office
Howard Baker Jr. U.S. Courthouse
First Horizon Plaza
JAMES WHITE PKY.
UT
Poplar Lot
POPLAR ST.
Trolley Superstop
MAIN ST.
Riverview Tower
James White's Fort
County Courthouse
W. HILL AVE.
Hill Ave. Lot
Women's Basketball Hall of Fame
E. HILL AVE.
University of Tennessee
1ST ASSEMBLY ST.
SECOND CREEK GWY.
MIDDLE DR.
City County Building
Blount Mansion
FRONT AVE.
NEYLAND DR.
TO McCLUNG MUSEUM
WHITE GREENWAY (Riv. Wk.)
NEYLAND GREENWAY
Volunteer Landing
Neyland Stadium
SECOND CREEK
NEYLAND GREENWAY (TO UT GARDENS & TYSON PARK)
HENLEY ST.
TENNESSEE RIVER
GAY ST.
0ft. 200' 400'
Suttree Landing Park
441
TO SOUTH KNOXVILLE
CHAPMAN HIGHWAY
E. BLOUNT AVE.
COUNCIL PL.
JONES ST.
TO IJAMS NATURE CENTER,
NAVITAT CANOPY ADVENTURES,
URBAN WILDERNESS,
BAKER CREEK PRESERVE, &
ISLAND HOME AIRPORT (DKX)

GATLINBURG TROLLEY ROUTES



LEGEND

★	Official Visitor Information and Welcome Centers
P	Parking
🚦	Traffic Lights
✚	Medical Facilities
🚻	Public Restrooms
♥	Marriage License Center
●	Not Recommended For Trailers or RVs
T	Trolley Shelter

Trolleys stop only at designated signs and shelters

IMPORTANT PHONE NUMBERS
(865 area code)

Visitor Information: 436-4178
Gatlinburg Mass Transit: 436-3897
Gatlinburg Golf Course: 453-3912
Marriage License Center: 430-3404
Police: 436-5181
Fire: 436-5112
TDD: 800-848-0298

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BLUE
East Parkway, Community Center, Rocky Top Sports World, Library, Ripley's Aquarium of the Smokies, Convention Center

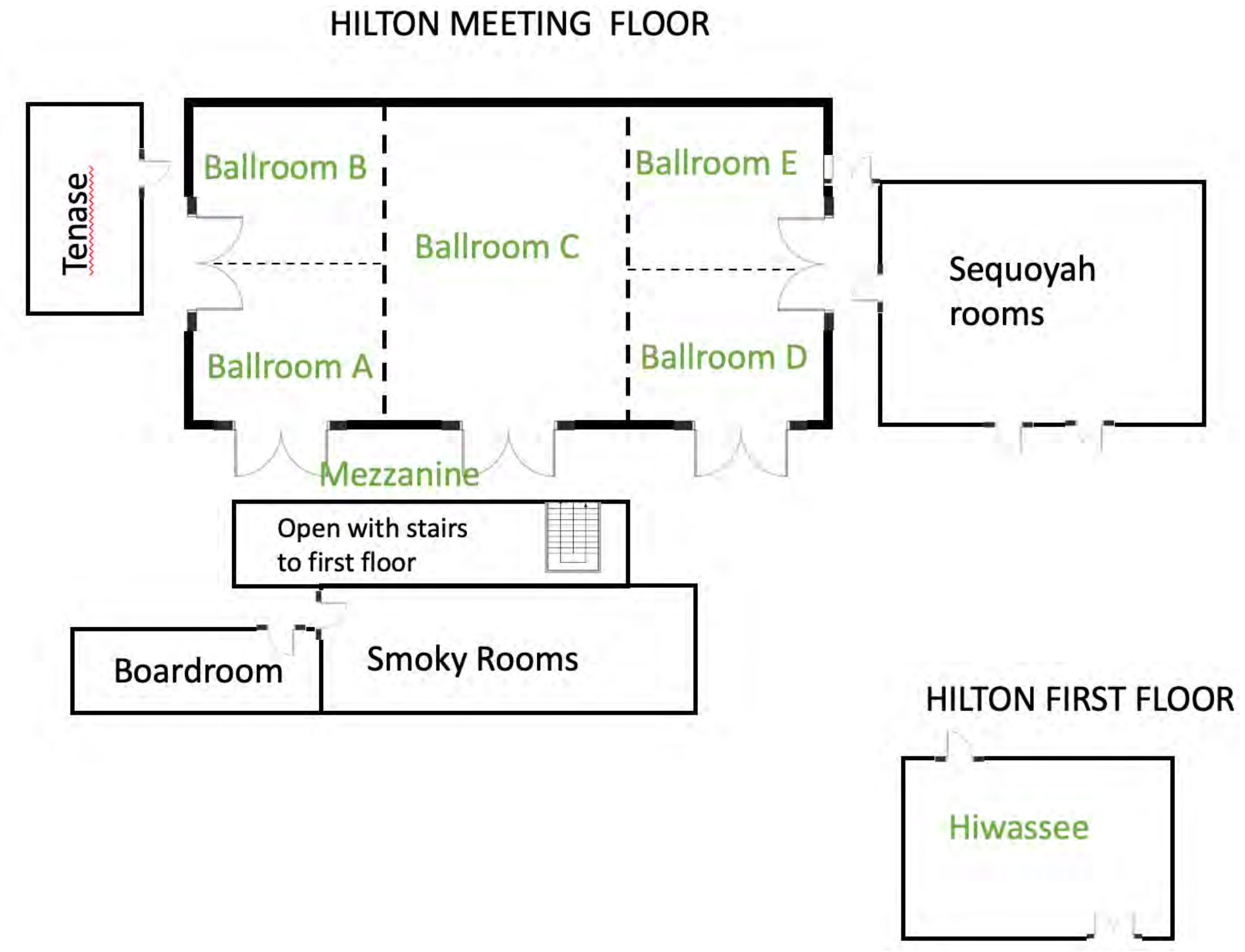
PURPLE
North Parkway, Spur Welcome Center Park and Ride, Ripley's Aquarium of the Smokies, Convention Center

YELLOW
APR - OCT: DAILY; NOV & DEC: ONLY MON-SAT Departs from Ripley's Aquarium of the Smokies to the Great Smoky Arts and Crafts Community. Runs approx. once an hour, 10:30 am - 6:00 pm.

MODIFIED SCHEDULE (March & April)
10:30 am - 10:00 pm

REGULAR SCHEDULE (May through Oct.)
8:30 am - midnight

WINTER SCHEDULE (Nov. - Feb.)
Weekdays, 10:30 am - 6:00 pm
Fri. & Sat., 10:30 am - 10:00 pm



	Sunday, June 18
3:00-6:00	Registration Hilton Main Lobby
6:00-8:00	Welcome Reception *Knoxville Sunsphere 8th Floor*

	Monday, June 19	
7:45-8:30	Breakfast Ballroom C	
8:30-8:45	Welcome & Announcements (Ballroom C) *Local Organizing Committee*	
8:45-9:40	KEYNOTE (Ballroom C) **Theory-guided Design of High-strength, Ductile, Single-phase BCC High Entropy Alloys** *William Curtin* *Chair: Katharine Page*	
9:45-10:15	INVITED (Ballroom AB) High-Entropy Materials Technology *Jien-Weh Yeh* *Chair: Chanho Lee*	INVITED (Ballroom DE) High Entropy Materials for Catalysis Applications *Sheng Dai* *Chair: Brianna Musicó*
10:15-10:30	Break Mezzanine	
10:30-12:00	SESSION 1A (Ballroom AB) ALLOYS: mechanical properties – experimental studies *Chair: Chanho Lee*	SESSION 1B (Ballroom DE) OXIDES: synthesis *Chair: Brianna Musicó*
12:00-1:30	LUNCH Ballroom C	
1:30-2:00	INVITED (Ballroom AB) Discovering Deformation Mechanisms in FCC Based Alloys Using Multi-modal Electron Microscopy Methods *Michael Mills* *Chair: Guillaume Laplanche*	INVITED (Ballroom DE) Interplay between structure and carrier transport in entropy stabilized oxides *John Heron* *Chair: Ruth Schwaiger*
2:00-3:15	SESSION 1C (Ballroom AB) ALLOYS: Design *Chair: Guillaume Laplanche*	SESSION 1D (Ballroom DE) ALLOYS: Refractory alloys I *Chair: Ruth Schwaiger*
3:15-3:30	Break Mezzanine	
3:30-4:30	SESSION 1E (Ballroom AB) ALLOYS: Shape memory alloys *Chair: Guillaume Laplanche*	SESSION 1F (Ballroom DE) ALLOYS: additive manufacturing *Chair: Ruth Schwaiger*

	Tuesday, June 20	
8:00-8:40	Breakfast Ballroom C	
8:40-8:45	Announcements (Ballroom C) *Local Organizing Committee*	
8:45-9:40	KEYNOTE (Ballroom C) **High entropy materials: new opportunities for structure and property Engineering** *Jon-Paul Maria* *Chair: T. Zac Ward*	
9:45-10:15	INVITED (Ballroom AB) Experimental and theoretical study of the Ni–CoCrFeMn system *Gerhard Wilde* *Chair: Bernd Gludovatz*	INVITED (Ballroom DE) HEOs with unique magneto-electronic phase separation for advanced functionalities *Abhishek Sarkar* *Chair: Alessandro Mazza*
10:15-10:30	Break Mezzanine	
10:30-12:00	SESSION 2A (Ballroom AB) ALLOYS: Refractory alloys I *Chair: Bernd Gludovatz*	SESSION 2B (Ballroom DE) Alloys: Heterostructures, nanoparticles, and coatings *Chair: Alessandro Mazza*
12:00-1:30	LUNCH Ballroom C	
1:30-2:00	INVITED (Ballroom AB) Effects of short-range ordering on mechanical properties of single crystals of the equiatomic CrCoNi medium-entropy alloy *Kyosuke Kishida* *Chair: Brian Cantor*	INVITED (Ballroom DE) Designing and Discovering High Entropy Oxides *Valentino Cooper* *Chair: Gian Song*
2:00-3:15	SESSION 2C (Ballroom AB) ALLOYS: Ductility & Deformation I *Chair: Brian Cantor*	SESSION 2D (Ballroom DE) ALLOYS: functional properties *Chair: Gian Song*
3:15-3:30	Break Mezzanine	
3:30-5:30	POSTER SESSION Hiwassee	

	Wednesday, June 21	
7:45-8:25	Breakfast Ballroom C	
8:25-8:30	Announcements (Ballroom C) *Local Organizing Committee*	
8:30-9:25	KEYNOTE (Ballroom C) **Achievements and Knowledge Increase of Close to 20 Years Research on High Entropy Alloys** *Uwe Glatzel* *Chair: Easo George*	
9:30-10:00	INVITED (Ballroom AB) **Local Lattice Distortions and Structural Instabilities in Nb-Ta-Ti-Hf High-Entropy Alloys** *Mark Asta* *Chair: Anna Manzoni*	INVITED (Ballroom DE) Variance via configurational entropy as a control over functionality in strongly correlated materials *Alessandro Mazza* *Chair: Solveig Aamlid*
10:00-10:15	Break Mezzanine	
10:15-11:30	SESSION 3A (Ballroom AB) ALLOYS: Cantor Alloys *Chair: Anna Manzoni*	SESSION 3B: Oxides: Functional Properties *Chair: Solveig Aamlid*
12:00-8:00	EXCURSION (Lunch boxes will be provided)	

	Thursday, June 22	
8:00-8:40	Breakfast Ballroom C	
8:40-8:45	Announcements (Ballroom C) *Local Organizing Committee*	
8:45-9:40	KEYNOTE (Ballroom C) **Finding new materials where materials science, materials physics and materials chemistry meet** *Robert Cava* *Chair: Dustin Gilbert*	
9:45-10:15	INVITED (Ballroom AB) Additive Manufacturing of High Entropy Alloys *Hyoung Seop Kim* *Chair: Yong-Jie Hu*	INVITED (Ballroom DE) High entropy oxides as new playground for functional materials development *David Berardan* *Chair: William Meier*
10:15-10:30	Break Mezzanine	
10:30-12:00	SESSION 4A (Ballroom AB) ALLOYS: Short range order *Chair: Yong-Jie Hu*	SESSION 4B (Ballroom DE) OXIDES: advanced characterization *Chair: William Meier*
12:00-1:30	LUNCH Ballroom C	
1:30-2:00	INVITED (Ballroom AB) **On the influence of stacking fault energy on mechanical properties in CrMnFeCoNi high-entropy alloys with different Cr/Ni ratios** *Guillaume Laplanche* *Chair: Stephan Laube*	INVITED (Ballroom DE) Phase stability and short-range ordering of entropy stabilized oxides with the **α**-PbO2 structure *Solveig Aamlid* *Chair: An-Chou Yeh*
2:00-3:15	SESSION 4C (Ballroom AB) ALLOYS: Environmental Interactions *Chair: Stephan Laube*	SESSION 4D (Ballroom DE) ALLOYS: Mechanical Properties – Theory and modeling *Chair: An-Chou Yeh*
3:15-3:30	Break Mezzanine	
3:30-5:00	SESSION 4E (Ballroom AB) ALLOYS: Ductility & Deformation II *Chair: Stephan Laube*	SESSION 4F (Ballroom DE) ALLOYS: Refractory alloys III *Chair: An-Chou Yeh*
6:00-8:00	BANQUET Ballroom C	

Theory-guided Design of High-strength, Ductile, Single-phase BCC High Entropy Alloys

Y. Rao[1] and W.A. Curtin[1,2*]

[1]*Laboratory for Multiscale Mechanics Modeling, EPFL, 1015 Lausanne, Switzerland*
[2]*School of Engineering, Brown University, Providence, RI 02906*
*william_curtin@brown.edu

The immense compositional space of High Entropy Alloys presents possibilities of discovering compositions satisfying multiple application requirements. We introduce a theory-based parameter-free alloy selection procedure to satisfy specified mechanical and thermodynamic properties of metallic HEAs. We first review two key components of the process: a theory for alloy yield strength and a theory for alloy ductility. We then apply these theories along with thermodynamic calculations using the Calphad method to select alloys. Initially, we make a selection among equiatomic quinary BCC refractory HEAs in the family Cr-Mo-W-V-Nb-Ta-Ti-Zr-Hf to find alloys that are predicted to be strong, ductile at room temperature, single-phase, and with high melting point. We identify HfMoNbTaTi as the most-promising alloy, and compare predictions to literature experiments. We then search within the Hf-Mo-Nb-Ta-Ti family with more-stringent design/performance criteria and find 10 quinary alloys with lower densities, higher specific strength, more-likely-ductile, and melting points above 2050C. Our selection procedure is validated by collaborators who fabricated and characterized the $Hf_{15}Mo_{25}Nb_{20}Ta_{5}Ti_{35}$, confirming a number of predictions. Eliminating Ta, we then identify 15 new quaternary Hf-Mo-Nb-Ti alloys that are proposed for future fabrication and evaluation. Overall, our design procedure provides a theory-based approach to identify target alloys with a desired suite of properties, facilitating the discovery of next-generation high-temperature alloys.

High-Entropy Materials Technology

[*]Jien-Wei Yeh

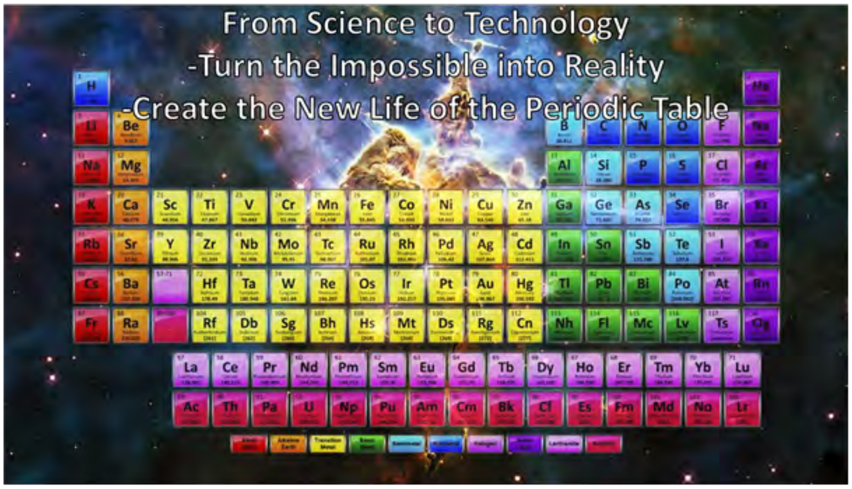
High Entropy Materials Center, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan 300, Republic of China
*jwyeh@mx.nthu.edu.tw

High-Entropy Materials (HEMs)" has become an emerging field through the collective efforts of many researchers in last two decades. The composition concept of HEMs is based on at least five major components, which is revolutionary because historically the composition concept is based on one or two components. Material compositions like HEMs were believed to be difficult or even impossible to be fabricated and applicable.

High entropy effect of HEMs was ignored before. Now, we know that high entropy effect is the most important core effect in enhancing the formation of multielement solution phases and avoid complicated microstructure with complex phases. Lattice distortion effect, sluggish diffusion effect and cocktail effect are also the core effects of HEMs because they significantly affect the crystal structure, microstructure, and thus properties. Therefore, the understanding of these four effects is helpful to understand HEMs.

As the long-standing bottlenecks of conventional materials were difficult to be solved by conventional materials concept, HEMs thinking and training will increase our whole materials ability to solve the conventional bottlenecks. Many HEMs belonged to different categories have been developed and published, which indeed display promising properties for different applications.

It is high time for us to build HEMs technology by transferring those promising discoveries into industrial production and create well-being for our society. In this presentation, many bottlenecks in conventional materials and the ESG issues in energy, waste, pollution, natural resource conservation are pointed out. Lots of new opportunities are waiting for us to develop new HEMs and related materials simultaneously meeting with ESG criteria. Some industrialized examples of HEMs technology are presented.



High Entropy Materials for Catalysis Applications

Kevin Siniard[1], Tao Wang,[2] Zhenzhen Yang,[2] *Sheng Dai[1,2]

[1]*University of Tennessee, Knoxville, TN 37996*
[2]*Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831*
*sdai@utk.edu

Until recently the design and synthesis of heterogeneous catalysts have been dominated through enthalpic factors (e.g., charge-charge interactions, charge-transfer interactions). With emergence of high entropy materials (HEMs), another avenue to design and synthesize catalytic materials has opened up. The definition of HEMs is any material that consists of the solid solution of more than five components that allow great flexibility in tuning surface compositions and interfacial functionalities. Here we present the synthesis of high entropy electrocatalysts that potentially outperform the traditional catalysts in energy-related catalysis reactions.[1] The synthesis strategies through entropy maximization will be discussed.

1. Y. Sun, S. Dai, High-entropy materials for catalysis: A new frontier, *Sci. Adv*. **2021**, *7*, eabg1600

SESSION 1A

ALLOYS: mechanical properties – experimental studies

10:30 **1A1:** Entropy effect on tensile behavior of hexagonal rare earth based low, medium and high entropy alloys made from Ho-Dy-Y-Gd-Tb
L. Rosenkranz, M. Feuerbacher, C. Gadelmeier, F. Schleifer, F., U. Glatzel

10:45 **1A2:** Mechanical behavior and microstructures of Cu-Fe-based medium entropy alloys
J. Moon, H.S. Kim, H.S., P.K. Liaw

11:00 **1A3:** Fracture properties of high-entropy alloys
B. Gludovatz M.J, Paul, H.S Oh, E.S. Park, R.O. Ritchie

11:15 **1A4:** The evolution of the microstructure and mechanical properties of Ti65Zr7 medium entropy alloy after rapid thermal annealing
P.S. Chen, C. C. Huang, Y. C. Liao, P. H. Tsai, Jason S. C. Jang, C. Y. Chen

11:30 **1A5:** Mechanical Performance and integrity of tungsten inert gas (TIG) welded CoCrFEMnNi high entropy alloy with austenitic steel AISI 304
M. Rhode, K. Erxleben, T. Richter, A.M. Manzoni, D. Schropefer

Entropy effect on tensile behavior of hexagonal rare earth based low, medium, and high entropy alloys made from Ho-Dy-Y-Gd-Tb

[1*]Rosenkranz, L., [2]Feuerbacher, M., [1]Gadelmeier, C., [1]Schleifer, F., [1]Glatzel, U.

[1] *Metals and Alloys, University of Bayreuth, 95447 Bayreuth, Germany*
2 Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, D-52428 Jülich, Germany
*laura.rosenkranz@uni-bayreuth.de

The equiatomic hexagonal close packed high entropy alloy (HEA) Ho-Dy-Y-Gd-Tb with extraordinarily similar constituent elements is ideal for assessing a widely discussed high entropy effect of HEA. Assuming comparable microstructures and minimized solid solution strengthening (SSS) due to this similarity, a possible strengthening effect of the calculated high configurational entropy was assessed. Moreover, the Gibbs paradox between the similarity of elements and the calculated configurational entropy was examined. For this purpose, the tensile behavior of equiatomic alloys made from one to five rare earth elements was studied.

This study provides the first set of tensile tests of this alloy system at room temperature, which were successfully prepared via arc melting. After challenging the preparation of these alloys, which are prone to oxidation, X-Ray diffraction and elemental mappings with energy-dispersive X-Ray spectroscopy indicate single-phase microstructures in most alloys in the as-cast state. The tensile strength of the single-phase alloys lies in the range of the pure elements, which confirmed the hypothesis of minimized SSH. Additionally, the microstructures analyzed via electron microscopy (SEM and TEM) were correlated to the tensile behavior of the alloys. Those alloys containing additional phases and oxidation along grain boundaries and the HEA show pronounced brittle behavior. No correlation between configurational entropy and tensile behavior was observed. Consequently, the effect of high entropy is not crucial for mechanical behavior. This work contributes to understanding mechanical behavior and the influence of entropy on the hexagonal close packed high entropy alloy Ho-Dy-Y-Gd-Tb.

Mechanical behavior and microstructures of Cu-Fe-based medium-entropy alloys

[1]*Moon, J., [2]Kim, H.S., & [1]Liaw, P.K.

[1] *Department of Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee 37996, USA*
[2] *Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang 37673, Republic of Korea*
*jongunmoon90@gmail.com

In this study, the mechanical behavior and microstructures of Cu-Fe-based medium-entropy alloys were investigated. Ternary Cu-Fe-Mn and quaternary Cu-Fe-Al-Mn medium-entropy alloys in non-equiatomic ratios have been proposed as new alloy systems with excellent mechanical properties. The heterogeneous microstructure of the alloys was designed by utilizing the immiscible nature of the Cu-Fe binary system. The addition of Al transforms the crystal structure of the alloys from a dual-face-centered-cubic to face-centered-cubic and body-centered-cubic structure. The alloys exhibit high strength at both room and cryogenic temperatures because of hetero-deformation-induced strengthening caused by heterogeneous microstructures. The presence of deformation-induced nano-twins and martensites further enhances the strength and strain hardening of the alloys. The measured hetero-deformation-induced stress demonstrates the dominant hetero-deformation-induced strengthening mechanism of the alloys. This new type of medium-entropy alloy is expected to expand the design window in high-entropy materials.

Fracture properties of high-entropy alloys

[1]*Gludovatz, B., [1]Paul, M.J., [2]Oh, H.S., [2]Park, E.S., & [3]Ritchie, R.O.

[1] *School of Mechanical and Manufacturing Engineering, University of New South Wales (UNSW Sydney), Sydney, 2052, Australia*
[2] *Research Institute of Advanced Materials, Department of Materials Science and Engineering, Seoul National University, Seoul, 08826, Republic of Korea*
[3] *Materials Sciences Division, Lawrence Berkeley National Laboratory & Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, 94720, USA*
*b.gludovatz@unsw.edu.au

Since the concept of high-entropy alloys (HEAs) as materials with at least four or five principal elements in (near)-equiatomic composition was introduced in 2004, this new class of materials has penetrated essentially all materials science-related fields. The main reason for this is that some face-centered cubic (fcc) alloy compositions have been shown to exhibit outstanding mechanical properties with extraordinary combinations of strength, ductility, and fracture toughness, particularly at cryogenic temperatures, whereas certain body-centered cubic (bcc) refractory compositions display outstanding high-temperature strength. While significant effort has been put into rapid screening and narrowing of the compositional space of HEAs to a manageable scope, there have still only a few metallic alloys been discovered that push the limits of mechanical performance. Based on our early work on the equiatomic CrMnFeCoNi alloy, the most studied HEA to date, that has an fcc structure and been shown to exhibit strength levels above 1 GPa together with fracture toughness values in excess of 200 MPa.m^{½}, we will examine compositionally modified variations of this material. We will show how their failure resistance develops in the temperature range of room to liquid nitrogen temperature when compositionally triggered deformation mechanisms such as transformation induced plasticity (TRIP) or twinning induced plasticity (TWIP) are enabled and additionally compare their behavior to a similar alloy that contains a second phase.

The evolution of the microstructure and mechanical properties of Ti65Zr7 medium-entropy alloy after rapid thermal annealing

[1]*P. S. Chen, [2]C. C. Huang, [2]Y. C. Liao, [1]P. H. Tsai, [1,2]Jason S. C. Jang & [3]C. Y. Chen

[1] *Institute of Materials Science and Engineering, National Central University, Zhongli 32001, Taiwan.*
[2] *Department of Mechanical Engineering, National Central University, Zhongli 32001, Taiwan.*
[3] *Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Kaohsiung 804, Taiwan.*
* thepacific999@gmail.com

In this study, a light-weight (~ 5 g/cm^3) $Ti_{65}(AlCrNbV)_{28}Zr_7$ (Ti65Zr7) medium-entropy alloy (MEA) was used to investigate the effect of thermo-mechanical treatment on its microstructure and mechanical properties. At first, the alloy ingots were conducted with hot rolling 50% then cold rolling 70% (HR50CR70) to accumulate the strain energy via work hardening process. Then the plastically deformed samples were annealed by rapid heating (heating rate 15°C/s and 25°C/s, respectively) with different time. The results of XRD analyses revealed that all MEAs still remain a single BCC structure after annealing by rapid heating process. Through EBSD observation, it can be noticed that the recrystallization ratio increases with increasing annealing temperature. Since the annealing process of 25°C/s heating rate can provide more energy during recrystallization process, which can initiate recrystallization process of the deformed sample earlier than that of 15°C/sec. In mechanical performance, the tensile testing results revealed that with increasing annealing temperature, the yield strength decreases and the ductility increases, respectively. Overall, the optimum processing condition of Ti65Zr7 alloy occurs at HR50CR70 then annealing for 30 second with 15°C/sec heating rate. This Ti65Zr7 MEA exhibits an excellent mechanical properties with 1350MPa yielding strength and 15% elongation, the specific yielding strength can reach up to 270 MPa·g/cm^3.

Mechanical performance and integrity of tungsten inert gas (TIG) welded CoCrFeMnNi high entropy alloy with austenitic steel AISI 304

[1,2]Rhode, M., [1]Erxleben, K., [1]Richter, T., [1*]Manzoni, A.M., [1]Schropefer, D.

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Unter den Eichen 87, 12205 Berlin, Germany
[2] *Otto-von-Guericke University, Institute of Materials Science and Joining Technology,*
Universitätsplatz 2, 39106 Magdeburg, Germany
*anna.manzoni@bam.de

High entropy alloys (HEA) have been investigated since the early 2000s and offer great potential to replace conventional alloys. However, since significant contents of expensive alloying elements such as Co or Ni are used, such they will be probably limited in real components to special areas. For that reason, the weldability with conventional alloys such as high-alloy austenitic steels must be investigated, so-called dissimilar metal welds (DMWs). For this purpose, tungsten inert gas welded (TIG) DMWs of CoCrFeMnNi HEA (in cold rolled and recrystallized condition) with a conventional AISI 304 austenitic steel are investigated. The DMW properties are analyzed by metallographic inspection and mechanical tests. For that purpose, the local strain behavior of the welded joints is characterized by means of digital image correlation (DIC). The results of the local hardness measurement show a clear influence of the initial condition of the HEA on the HAZ. Thus, the HEA in the cold-rolled condition shows a significant softening because of recrystallization processes in the HAZ. On the other hand, there is no influence on the hardness of the intermixed weld metal, which is approx. 200 HV0.1 in both cases. The tensile tests show a consistent failure of the weld joint in the weld metal after straining. However, regardless of the initial cold-rolled or recrystallized condition, considerable tensile strength of max. 600 MPa was reached for the weld metal but was accompanied by a significant loss of the fracture strain.

SESSION 1B

OXIDES: Synthesis

10:30 **1B1:** Multicomponent solid solution (MgMnFeCoNi)O: A new rocksalt high-entropy oxide
Yuguang Pu, Duncan Moseley, Jiaqiang Yan, Zhen He, Valeria Mitchell, Vanessa Peterson, Bernt Johannessen, Raphael Hermann, Peng Cao

10:45 **1B2:** Designing compositionally complex oxides to facilitate greater understanding of local structure
William R. Meier, Xin Wang, Craig A. Bridges, Valentino R. Cooper, Katharine Page

11:00 **1B3:** Phase Selectivity and Stability in Compositionally Complex Nano $(nA_{1/n})Co_2O_4$
Xin Wang, Peter Metz, Eleonora Calì, Palani Jothi, Eric Andrew Lass, Katharine Page

11:15 **1B4:** $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$: Epitaxial Growth, Nanostructuring and Kinetics
S.S.I. Almishal, J.T. Sivak, Y. Tan, L. Miao, G.N. Kotsonis, V. Crespi, J.T. Heron, C.M. Rost, N. Alem, LQ. Chen, S.B. Sinnott, JP. Maria

11:30 **1B5:** High-Entropy Engineering for Novel Ferroelectrics: $A_6B_2O_{17}$ Phases
R. Jackson Spurling, Chloe Skidmore, Nathaniel S. McIlwaine, and Jon-Paul Maria

Multicomponent solid solution (MgMnFeCoNi)O: A new rocksalt high-entropy oxide

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We report for the first time a new rocksalt HEOs material, (MgMnFeCoNi)O. The new HEOs have a single-phase rocksalt structure that is analogous to that of the classic (MgCoNiCuZn)O. This material is further defined as a multicomponent solid solution (MSS) oxide since the monoxides of all involved metal ions crystallize in a rocksalt structure, despite the difference in lattice parameters. By using neutron powder diffraction, the cation site occupancy in this structure is validated to be highly random. Oxidation states of metal ions are studied by X-ray absorption near edge spectroscopy (XANES) and Mössbauer spectroscopy. The results indicate these cations in this compound are unanimously divalent. Extended X-ray absorption fine structure (EXAFS) is applied to investigate the microstructure and local environment of MSS oxide in detail. Furthermore, magnetic susceptibility and specific heat measurement reveal the onset of magnetic transition of MSS oxide is at approximately 210 K.

Designing compositionally complex oxides to facilitate greater understanding of local structure

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Compositionally complex oxides offer a uniquely tunable composition space for the design of new ceramic materials. Although the goal is often to generate a homogenous material, this remains a consistent challenge. Scattering and local probes provide insight into the degree of heterogeneity such as clustering or phase separation.

I propose that we can design our material systems to facilitate methods of interrogating their local structure and heterogeneity. Selecting elements that have good neutron or x-ray scattering contrast can strengthen our power to understand the local structure from total scattering studies. Local probes like nuclear magnetic resonance (NMR) and Mössbauer spectroscopy provide atomic environment information for specific elements if we include them. In short, we can gain greater understanding of compositionally complex systems by designing study systems that include elements which facilitate advanced structural characterization. I will present an application of these ideas in the design of a compositionally complex Ruddlesden–Popper oxide.

Phase Selectivity and Stability in Compositionally Complex Nano $(\boldsymbol{n}\mathrm{A}_{1/n})\mathrm{Co}_2\mathrm{O}_4$

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Nanostructured materials offer promising physicochemical properties across diverse applications in energy storage, sensing, catalysis, biomedicine, and more. Nano-compositionally complex oxides (CCOs) are expected to offer enhanced structure-property tunability by virtue of their combined entropic disorder and nano-size effects. In this work, an eco-friendly low-temperature soft-templating reaction route was applied to form a large family of spinel nanostructures with the formula of $(\mathrm{nA}_{1/\mathrm{n}})\mathrm{Co}_2\mathrm{O}_4$, where A refers to an equiatomic ratio ($1/n$) combination of 1-7 transition metal cations. The phase selectivity and the temperature stability window for the series of nano-compositions were found to be strongly dependent upon the inclusion (or exclusion) of specific cations. Meanwhile, the synthesis temperature required for the phase formation was observed to be associated with the number of elements (n) included on the A site, consistent with an increase in the configurational entropy as a function of n. Furthermore, theoretical calculations and select control reactions uncover a propensity for temperature-activated compositional heterogeneity introduced for compositions containing Mg, Ni, Mn, and Fe. Methodology-wise, this work applies a continuous-lattice phase refinement approach to model the structure of compositionally complex materials for the first time.

$Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$: Epitaxial Growth, Nanostructuring and Kinetics

[1]*Almishal, S.S.I., [2]Sivak, J.T. , [1]Tan, Y., [1]Miao, L., [1]Kotsonis, G.N., [1]Crespi, V., [3]Heron, J.T., [4]Rost, C.M., [1]Alem, N., [1]Chen, LQ., [1,2]Sinnott, S.B. , [1]Maria, JP.

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High-entropy oxides (HEOs) embody a new paradigm of crystalline solid solution engineering where disorder is an active participant. Since Rost et al.'s pivotal report in 2015 on $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$ (commonly referred to as J14) [1], HEOs have garnered significant interest for their profound chemical flexibility and local crystalline disorder. The local asymmetries in the crystal structure frustrate electronic, magnetic, and vibrational order parameters, leading to unique physical properties. The inherent metastability of HEOs results in strong kinetic dependencies on thermal history. The non-equilibrium kinetics of pulsed laser deposition (PLD) rapidly condenses precursors from a high-entropy initial state, allowing kinetic stabilization of a broader spectrum of atomic and electronic configurations than bulk synthesis under near-equilibrium conditions. Presently, we show that epitaxial thin films of J14 accommodate large amount of epitaxial strain and reveal a systematic trend in lattice parameters and properties as a function of substrate temperature, oxygen partial pressure and film growth rate. As a specific example, low growth temperatures result in a smaller unit cell volume and smaller optical band gap, due to enhanced Co^{3+} concentrations in the J14 rocksalt lattice as uncovered by X-ray absorption spectroscopy [2]. Additionally, slow growth rates or elevated growth temperatures facilitate a controllable degree of phase decomposition and subtle nanoscale microstructural reconfiguration during epitaxial growth, including spinel nanocubes and Cu-rich tweed structures embedded in a rocksalt matrix. Since physical properties necessarily depend on local chemistry and symmetry, controlling the kinetic pathways available to HEOs provides new opportunities for property tuning and development.

[1] Rost, Christina M., et al. "Entropy-stabilized oxides." *Nature communications* 6.1 (2015): 8485.
[2] Kotsonis, George N., et al. "Property and cation valence engineering in entropy-stabilized oxide thin films." *Physical Review Materials* 4.10 (2020): 100401.

High-Entropy Engineering for Novel Ferroelectrics: $A_6B_2O_{17}$ Phases

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In this work we apply an entropy-inspired materials design approach to explore candidate ferroelectric materials, specifically the family of disordered $A_6B_2O_{17}$ (A = Zr, Hf; B = Nb, Ta) phases. We demonstrate that $A_6B_2O_{17}$ phases exhibit substantial cation sublattice disorder between 6-, 7-, and 8-coordinated sites which is consistent with previous predictions. Additionally, we show that this structure may be engineered to host at least four unique cation species, with enhanced solubility deriving from the high cation sublattice configurational entropy. This study leverages a swath of characterization techniques, including both conventional and high temperature *in situ* X-ray diffraction. We apply this information gained from studies in the bulk regime to thin film synthesis, with the goal of probing potential ferroelectric behavior in these films. This work also includes an exploration of the thin film sample space, with a focus on optimization of sputter deposition synthesis conditions for highly resistive films with controlled crystallinity.

Discovering Deformation Mechanisms in FCC Based Alloys Using Multi-modal Electron Microscopy Methods

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Advancements in electron microscopy methods enable unprecedented ability to probe deformation modes in novel alloys–knowledge which is key to rational and efficient alloy development. These insights are also critical to inform microstructure-sensitive models of alloy behavior. Two examples of these studies will be presented. In the first example, the equiatomic CrCoNi alloy is an fcc solid solution that exhibits intriguing behaviors including very large strain hardening and cyclic hardening rates, large fracture toughness, and strong dependence of the yield strength at low temperature. Detailed characterization using a variety of electron microscopy methods has revealed that these behaviors are closely linked to the interplay between dislocation-mediated plasticity, microtwinning, and an fcc-to-hcp transformation. The effect of Al and Ti, and the formation $L1_2$ short-range ordering domains, on the deformation mechanisms will also be presented. In the second example, an oxide dispersion strengthened (ODS) variants of CrCoNi alloys is discussed. These materials are produced using a new high-energy mixing technique pioneered in recent work at NASA Glenn Research Center whereby metal powders are coated by yittria, and a homogeneous ODS microstructure can be produced via laser powder-bed additive processing. The remarkable high temperature behavior of these new additive ODS alloys is described and correlated with the as-processed and post-deformation substructures.

Interplay between structure and carrier transport in entropy stabilized oxides

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Entropy-stabilized oxides demonstrate a new and unprecedented degree of chemical control in materials. This broadens the compositional space of crystalline oxides and presents opportunities to understand and explore the local chemical and structural disorder. Here, I will discuss the control of stereochemically-driven structural disorder in single crystalline, rocksalt, (MgCoNiCuZn)O-type entropy-stabilized oxides through the incorporation of Co, Cu, and Mg cations. Point defect formation energies from first principles calculations predict the local strain is the driver for defect formation and largely dictated by Cu. Electron transport measurements reveal a tunable conductivity and carrier dynamics via the Mg concentration (inversely correlated to Cu) that is mediated by carrier hopping. Theory predicts electron hopping via Cu atoms that are adjacent to oxygen vacancies and qualitatively in agreement with experiments. Our findings demonstrate novel interplay between structure and charge transport in entropy-stabilized oxides for tunable electronic responses.

SESSION 1C

ALLOYS: Design

2:00 **1C1:** Thermodynamic database for multi-principal element alloys within the system Al–Co–Cr–Fe–Mn–Ni–C(–V)
Bengt Hallstedt, Mehdi Noori

2:15 **1C2:** Design metastability in high-entropy alloys by tailoring unstable fault energies
Chenyang Li, Xing Wang, Wei Xiong, Wei Chen

2:30 **1C3:** Mechanism-oriented design of novel multi-principal element alloys in the system Al Co Cr Fe Mn-Ni-V-C with advanced strength-ductility synergy
F. Oppermann, F. Kies, B. Hallstedt, C. Haase

2:45 **1C4:** Statistical Mechanics of Ordering in Materials from First Principles using Machine Learning and Monte Carlo Simulations
Markus Eisenbach, Mariia Karabin, Massimiliano Lupo Pasini, Junqi Yin

Thermodynamic database for multi-principal element alloys within the system Al–Co–Cr–Fe–Mn–Ni–C(–V)

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The development of multi-principal element alloys requires the navigation within a multi-dimensional composition space, which has proven to be challenging. Various methods to predict the state of an alloy, in particular if it is single-phase or not, have been tested with various success. The only approach that can consistently predict the constitution of an alloy (single-phase, multi-phase, presence of intermetallic phases etc) is thermodynamic calculations using Calphad databases. Conventional Calphad databases such as steel or Ni-base are of limited use since they are mainly developed for alloys with a specific base element. More suitable databases such as the TCHEA has been developed, but their development is challenging since they require that a much larger fraction of the possible subsystems is included than in conventional databases. The predictive capability still depends strongly on which elements are considered and their development is still ongoing. A Calphad database including the elements Al, Co, Cr, Fe, Mn, Ni, C was built up from scratch using mostly assessments of binary and ternary systems from the literature, but with many amendments. This database covers a large fraction of the alloys investigated so far plus the element C that is usually not included, but can provide additional strengthening, either in solution or in the form of carbides. To extend the range of the latter, the element V was tentatively added to the database.

Design metastability in high-entropy alloys by tailoring unstable fault energies

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Metastable alloys with transformation-/twinning-induced plasticity (TRIP/TWIP) can overcome the strength-ductility trade-off in structural materials. Originated from the development of traditional alloys, the intrinsic stacking fault energy (ISFE) has been applied to tailor TRIP/TWIP in high-entropy alloys (HEAs) but with limited quantitative success. Here, we demonstrate a strategy for designing metastable HEAs and validate its effectiveness by discovering seven alloys with experimentally observed metastability for TRIP/TWIP. We propose unstable fault energies as the more effective design metric and attribute the deformation mechanism of metastable face-centered cubic alloys to unstable martensite fault energy (UMFE)/unstable twin fault energy (UTFE) rather than ISFE. Among the studied HEAs and steels, the traditional ISFE criterion fails in more than half of the cases, while the UMFE/UTFE criterion accurately predicts the deformation mechanisms in all cases. The UMFE/UTFE criterion provides an effective paradigm for developing metastable alloys with TRIP/TWIP for an enhanced strength-ductility synergy.

Mechanism-oriented design of novel multi-principal element alloys in the system Al-Co-Cr-Fe-Mn-Ni-V-C with advanced strength-ductility synergy

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The flexibility to design alloys with chemical compositions that are well beyond established metallic materials led to a high number so far unknown Multi-Pricipal Element Alloys (MPEAs). Albeit the vibrant research in the field of MPEAs during the last years, several scientific challenges need to be overcome to reveal the full potential of these novel materials. In this contribution, two of these challenges will be addressed: (i) reliable methods to navigate and identify promising MPEAs in the very wide chemistry design space are missing, (ii) single-phase, face-centered cubic (fcc) MPEAs provide insufficient strength, as compared to existing materials used for structural applications (e.g. steels).

We selected the alloy system Al-Co-Cr-Fe-Mn-Ni-V-C to combine the benefits originating from Cantor-type MPEAs and highly alloyed steel. The focus was put on investigating the influence of Al, C and V in fcc Co-Cr-Fe-Mn-Ni on phase transformations, solid-solution and precipitation strengthening (e.g. by vanadium carbides, kappa carbides, B2). In order to overcome the strength-ductility trade-off, the alloys' matrices were designed via stacking-fault energy tailoring to enable high strain hardening offered by multiple deformation mechanisms, such as transformation-, twinning- and slipband refinement-induced plasticity (TRIP, TWIP, SRIP). To identify suitable alloys, a high throughput approach combining CALPHAD and DFT calculations with flexible sample production using additive manufacturing of powder blends was developed. The underlying formation and deformation mechanisms were investigated by microstructure (SEM, TEM, SXRD, APT) and mechanical characterization and will be critically discussed.

Statistical Mechanics of Ordering in Materials from First Principles using Machine Learning and Monte Carlo Simulations

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We will describe an approach to utilize machine learning methods to combine first principles density functional calculations with classical Monte-Carlo simulations to investigating the statistical mechanics of materials. Density functional calculations have proven to be a useful tool in the study of ground state properties of many materials. The investigation of finite temperature properties on the other hand usually relies on the use on empirical models that allow the large number of evaluations of the system's Hamiltonian that are required to sample the phase space needed to obtain physical observables as function of temperature. We have demonstrated a solution to this problem that harnesses the computational power of large massively parallel computers by combining classical Monte-Carlo calculations with our first principles multiple scattering electronic structure code (LSMS) by employing Machine Learning techniques.

While our LSMS code shows exceptional scaling on current massively parallel supercomputing architectures such as Summit, the combination with a machine learning workflow, that can consider both classical interaction models and artificial neural network based models, allows us to investigate alloy ordering transitions for increased simulation cell sizes. Our approach is able to sample both magnetic or chemical order, allowing the first principles calculation of order/disorder phase transitions and phase separations in alloys.

Here we will present our method as well as results for ordering transitions in alloys.

This work was supported in part by the Office of Science of the Department of Energy and by the Laboratory Directed Research and Development (LDRD) Program of Oak Ridge National Laboratory. This research used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

SESSION 1D

ALLOYS: Refractory Alloys I

2:00 **1D1:** Mechanical properties of systematically modified derivatives of TiZrHfNbTa
W.J. Carpenter, Y. Yang, E.P. George

2:15 **1D2:** On the phase stability and precipitation kinetics in initially single-phase BCC TiZrNbHfTa high-entropy alloys
M. Rajkowski, Y. Zhao, P. Gemagami, R. Poulain, S. Laube, L. Perrière, J.-P. Couzinié, T. Li, G. Laplanche

2:30 **1D3:** Constitutive Modeling for HfNbTaTiZr High-Entropy Alloys with the Effect of Dynamic Strain Aging
Y. Song, S. Chen, W. Li, K.K. Tseng, J.W. Yeh, P.K. Liaw

2:45 **1D4:** Studies on the ductility and plasticity of HfTiZrNbTa high-entropy alloys
J. Whitlow, L. Amalia, X. Fan, M. Moczadlo, E. Lass, Y. Gao, K. An, Y. Chen, D. Yu, P.K. Liaw

3:00 **1D5:** Effects of oxygen on structural instability and metastable phase formation in TiZrNbHfTa bcc high-entropy alloy
Yujun Zhao, Maik Rajkowski, Guillaume Laplanche, Tong Li

Mechanical properties of systematically modified derivatives of TiZrHfNbTa

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Refractory high entropy alloys (RHEAs) apply multicomponent alloy design principles to the refractory elements – combining elements from groups IV-VI to achieve solid solutions. The equiatomic RHEA TiZrHfNbTa is of interest because it maintains a high yield strength at elevated temperatures combined with ductility at room temperature [1], [2]. Despite its promise, TiZrHfNbTa suffers from a dearth of composition-property studies. To better understand effects of composition, we systematically modified Ti-Zr-Hf-Nb-Ta alloys and performed tensile tests. All material was homogenized, cold rolled, and recrystallized to achieve a reproducible single-phase microstructure with similar grain sizes. Despite varying the alloy composition over relatively large ranges, up to 30 at%, macroscopic mechanical behavior and elastic constants were found to change relatively little. CALPHAD was used to determine liquidus temperatures to normalize mechanical properties in this study. Our work provides systematic results on compositional effects in Ti-Zr-Hf-Nb-Ta and gives insight into possible alloy design routes.

[1] O. N. Senkov, J. M. Scott, S. V. Senkova, F. Meisenkothen, D. B. Miracle, and C. F. Woodward, “Microstructure and elevated temperature properties of a refractory TaNbHfZrTi alloy,” *J. Mater. Sci.*, vol. 47, no. 9, pp. 4062–4074, 2012, doi: 10.1007/s10853-012-6260-2.
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On the phase stability and precipitation kinetics in initially single-phase BCC TiZrNbHfTa high-entropy alloys

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The TiZrNbHfTa high-entropy alloy (HEA) is a 5-element alloy that was discovered by Senkov et al. **[1]** and subsequently named after him. It can form a single-phase body-centered cubic (BCC) solid solution when it is annealed at sufficiently high temperatures and it remains in this state at room temperature when quenched in water. The Senkov alloy is one of the few BCC HEAs that is ductile and malleable at room temperature. Therefore, its cast microstructure can be broken up by cold forming followed by recrystallization annealing to achieve a well-defined grain size. These are some of the reasons why the Senkov alloy is one of the most thoroughly investigated BCC HEAs. Regarding its phase stability, Schuh et al. **[2]** first discovered that the BCC solid solution decomposes into multiple phases when annealed at intermediate temperatures, resulting in embrittlement. Later on, other groups investigated the phase stability of this alloy and large discrepancies were reported. For instance, Schuh et al. **[2]** found that the alloy forms a stable solid solution above 900 °C while Yang et al. **[3]** found secondary phases up to 1450 °C. The aim of the present work is to show that this discrepancy may be related to the presence of non- metallic impurities such as oxygen that strongly affect phase stability and precipitation kinetics of secondary phases in the TiZrNbHfTa HEA.

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[1] O.N. Senkov, J.M. Scott, S.V. Senkova, D.B. Miracle, C.F. Woodward, Microstructure and room temperature properties of a highentropy TaNbHfZrTi alloy, Journal of Alloys and Compounds 509(20) (2011) 6043-6048.
[2] B. Schuh, B. Völker, J. Todt, N. Schell, L. Perrière, J. Li, J.P. Couzinié, A. Hohenwarter, Thermodynamic instability of a nanocrystalline, single-phase TiZrNbHfTa alloy and its impact on the mechanical properties, Acta Materialia 142 (2018) 201-212.
[3] C. Yang, K. Aoyagi, H. Bian, A. Chiba, Microstructure evolution and mechanical property of a precipitation-strengthened refractory high-entropy alloy HfNbTaTiZr, Materials Letters 254 (2019) 46-49.

Constitutive Modeling for HfNbTaTiZr High-Entropy Alloys with the Effect of Dynamic Strain Aging

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Research on high-entropy alloys has been limited mostly to experimental approaches. Theoretical and numerical investigations of these alloys have been rarely performed. The novelty of the present work is to systemically investigate the mechanics of refractory high-entropy alloys in terms of experimental, theoretical, and numerical approaches with a focus on dynamic strain aging. Single-phase body-centered-cubic HfNbTaTiZr refractory high-entropy alloys are tested in a wide range of temperatures to demonstrate the presence of dynamic strain aging. A new constitutive model is developed, considering several strengthening mechanisms including lattice distortion and dynamic strain aging. Correspondingly, the finite element algorithm for the developed model is presented via a user-defined subroutine. The findings of the present work suggest that a stress component for describing the effect of dynamic strain aging needs to be incorporated in the model as a function of the equivalent plastic strain, equivalent plastic strain rate, and temperature since its occurrence and characteristics depend on those factors.

Studies on the ductility and plasticity of HfTiZrNbTa high-entropy alloys

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Refractory high-entropy alloys (RHEAs) are one of the materials being developed to retain their strengths at more than 1000°C. However, the RHEAs currently studied generally do not show room-temperature ductility or plasticity, making further mechanical processing difficult after successful fabrication. Moreover, few studies have been performed on tensile behavior of RHEAs because they are difficult to cast due to their fast-cooling rates. Strengthening via composition and grain-size tuning have been attempted to enhance the ductility of RHEAs. However, most published studies examine samples ex-situ, after mechanical testing to failure. To effectively identify the deformation mechanisms, real-time deformation studies are crucial to further develop ductile RHEAs. In this study, we conducted in-situ neutron-diffraction studies on 7 RHEAs compositions, HfNbTiZr, HfNbTaTiZr, $HfTa_{0.5}TiZr$¸ $HfNb_{0.5}Ta_{0.5}TiZr$, $HfNbTa_{0.5}TiZr$, $Hf_{0.5}NbTa_{0.5}TiZr$, and $NbTa_{0.5}TiZr$, with compression and tension loads to examine the deformation mechanisms. The selected RHEAs compositions were obtained using CALculation of PHAse Diagrams (CALPHAD) thermodynamic modelng to identify compositions with expected ductility based on the Gibbs free energy of phase transformation from the body-centered-cubic (BCC) to hexagonal-closed-packed (HCP) phase. Full-pattern Rietveld refinement and single-peak fitting were conducted, employing General Structure Analysis System (GSAS) software and VULCAN Data Reduction and Interactive Visualization softwarE (VDRIVE), respectively. Lattice strains of specific hkl were studied to identify deformation mechanisms. Transformation-induced plasticity (TRIP) was observed in some of the studied compositions. Crystal plasticity will be used to model neutron lattice-strain data. Results were compared with those of related RHEAs in literature. Acknowledgements: The present work is supported by NSF and DOE.

Effects of oxygen on structural instability and metastable phase formation in TiZrNbHfTa bcc high-entropy alloy

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The equiatomic TiZrNbHfTa body-centered-cubic (bcc) high-entropy alloy (HEA) exhibits promising mechanical properties for high-temperature aerospace applications. The role of interstitial elements, such as oxygen, in the structural stability of the bcc matrix, precipitation sequence and kinetics remain unclear. In this context, this study aims to investigate the effects of oxygen on the precipitation sequence of TiZrNbHfTa bcc HEA. Atom probe tomography and transmission electron microscopy were employed to reveal the compositional and structural evolution in TiZrNbHfTa and TiZrNbHfTa with 3 at.% oxygen after annealing for various durations at 500 °C. At the onset of annealing, nanosized Zr-rich rod-like features were observed in both HEA alloys. As annealing proceeded, we observed the formation of the omega phase and hcp precipitates in the bcc matrix. However, the two HEAs exhibit a distinct precipitation pathway from bcc to hcp. These results indicate that oxygen can affect the bcc structural stability, precipitation sequence and thus mechanical properties significantly.

SESSION 1E

ALLOYS: Shape Memory Alloys

3:30 **1E1:** Effect of thermomechanical treatment on shape memory properties of non-equal molar CuNiTiHfZr High-entropy Alloy
Shan-Hsiu Chang, Wei-Pin Kao, Shu- Yu Kuo, Jien-Wei Yeh, Che-Wei Tsai

3:45 **1E2:** Overcoming Limits of High Entropy Shape Memory Alloys by Thermo-mechanical Forming
C. Hinte, G. Gerstein, S. Herbst, H.J. Maier

4:00 **1E3:** New quinary and denary high entropy shape memory alloys (HE-SMAs): alloy chemistry, alloy development, microstructures and martensitic transformations
O.O. Oluwabi, J. Frenzel, G. Eggeler

Effect of thermomechanical treatment on shape memory properties of non-equal molar CuNiTiHfZr High-entropy Alloy

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The major challenges of high-temperature shape memory alloys are their limited change of phase transition temperatures (TT) and the mechanical properties. Two different TTs of shape memory alloys will discuss, and the results show appear a lower phase transformation temperature and more uniform microstructures after solid solution treatment. Using an in-situ high-temperature X-ray diffractometer, the alloy was established to undergo phase transformation from B19' to B2 phase. Additionally, the alloy exhibited a martensitic transformation temperature higher than 100 ^{o}C after pre-stress. The deformation mechanism and shape recovery phenomenon of this shape memory alloy are also discussed. The as-homogenized add the B2 peaks, due to the decreasing of TT. Mechanical properties including elongation and hardness is improved as well after homogenization.

Overcoming Limits of High Entropy Shape Memory Alloys by Thermo-mechanical Forming

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High Entropy Shape Memory Alloys (HE-SMAs) as a special variant in the high entropy field have the potential to overcome common challenges in SMA research. Due to functional degradation and fatigue of SMAs they are often unsuitable for the envisaged technical application. In the SMA field, processes like creating nano-compounds, SIM-aging and strain glasses are widely investigated to improve functional properties with limited success in terms of actual applications.

In the last decade, Ni-Ti-related HE-SMAs were identified as promising candidates to address those challenges. Arc melting followed by heat-treatment is the most common method of production. Due to dendritic growth, segregation, and dissolution this typically results in brittle materials. Specifically, HE-SMAs feature promising functional potential despite obvious weaknesses as phase and grain boundaries as well as transformation defects. Thus, it is mandatory to improve the material properties by subsequent processing to reach their full potential. Therefore, in the present study thermo-mechanical processing techniques, including hot-rolling and extrusion, were researched. The processing was carried out in a protective hull to overcome the challenge of forming SMA actuators. Careful selection of thermo-mechanical parameters was essential to ensure successful shaping. Additionally, production parameters were found to be strongly dependent on the quality of the as-cast materials. It is shown how processing influences the microstructure of the material and thereby its initial mechanical and functional properties, making the actuator forming process possible.

New quinary and denary high entropy shape memory alloys (HE-SMAs): alloy chemistry, alloy development, microstructures and martensitic transformations

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The present work investigates high entropy shape memory alloys (HE-SMAs). Shape memory alloys (SMAs) represent functional materials which can re-establish a pre-programmed geometry after a large deformation, which exceeds elastic limits of conventional metals and alloys. The shape memory effect relies on a highly reversible martensitic transformation. HE-SMAs can be derived from binary NiTi. High (austenite) and low temperature (martensite) phases are ordered phases of type B2 and B19'. Additional elements (Cu, Pd, Zr and Hf), which are added to obtain chemically complex SMAs, partition to Ni- and Ti-sublattices where they are randomly distributed. We introduce a new alloy screening approach, where diffusion couples covering large compositional ranges of HE-SMAs and related subsystems are studied by in-situ experiments. Phase transformation temperatures (e.g. martensite start) are determined by in-situ cooling/heating in a scanning electron microscope where the propagation of transformation fronts can be monitored. In a first study, new HE-SMA compositions with large transformation strain and wide thermal hysteresis could be identified. Different material states were analyzed by scanning electron microscopy combined with chemical micro-analysis, and differential scanning calorimetry. The effects of alloy compositions on martensitic transformations were interpreted on the basis of the valence electron theory. Our diffusion couple technique also allows to investigate interdiffusion for SMAs with different degrees of chemical complexity. It was observed that the presence of Pd accelerates Ni/Ti interdiffusion. In contrast, Hf and Zr provide the opposite effect. As a dominating trend, interdiffusion slows down when a larger number of alloying elements is added.

SESSION 1F

ALLOYS: Additive Manufacturing

3:30 **1F1:** Effects of Yttrium addition in a precipitation strengthened high-entropy alloy processed by selective laser melting
P.-H. Chou, J.-L. Lee, H. Murakami, K. Kakehi, A.-C. Yeh

3:45 **1F2:** The effect of reinforcing particles on the processability of compositionally complex alloys via by laser powder bed fusion
E. Soares Barreto, F. Schulz, V. Devulapalli, N.A.K. Mohideen, G. Dehm, E.A. Jägle, N. Ellendt

4:00 **1F3:** Static and dynamic properties of particle-reinforced compositionally complex alloys produced by laser powder bed fusion
F. Schulz, E. Soares Barreto, V. Devulapalli, N. Ellendt, E. Bernardo, G. Dehm, E.A. Jägle

4:15 **1F4:** Defect Detection for High-Entropy Alloy (HEA) Printing Using High-Speed Infrared Imaging
Xianzhe Fu, Kwangtae Son, Zhaoyan Fan

Effects of Yttrium addition in a precipitation strengthened high-entropy alloy processed by selective laser melting

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In this research, the effects of yttrium (Y) addition in a precipitation strengthened high-entropy alloy (HEA) $Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3}$ (Al02Ti03) has been investigated. Selective laser melting (SLM) process was employed to fabricate samples with and without Y. The grain size of both compositions with and without Y in as-built state were 11 μm in average. After heat treatment, the Y-bearing HEA could maintain the grain size, by contrast grain size grew to 50 μm without Y content. The formation of Y-rich intermetallic compounds after heat treatment was found to suppress grain growth. Preliminary analysis suggests that Y addition could modify the composition of $L1_2$-structured γ' precipitates, increase the lattice misfit and make the γ' precipitate morphology more cuboidal. Tensile tests were conducted at room temperature, 650 and 750 °C. Interestingly, addition of Y could break the strength ductility trade off at 650 and 750 °C. Al02Ti03+Y exhibits 25% higher strength and comparable ductility at 650 °C. Al02Ti03 encountered hot ductility drop severely at 750 °C; addition of Y could improve the strength by 28% with 260 % increase in elongation. Y addition in $Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3}$ was found to have beneficial effect to increase both strength and ductility at elevated temperature.

The effect of reinforcing particles on the processability of compositionally complex alloys via by laser powder bed fusion

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Particle-reinforced, compositionally complex alloys (CCA) show outstanding mechanical characteristics in the low and high-temperature ranges, enabling their use in many specialized, high-performance applications. The type, size, and concentration of the particles added to the base material impact the alloy processability via laser powder bed fusion (PBF-LB/M) and, consequently, the alloy's final microstructure.

In this study, both TiN and TiO_2 were mixed with CrFeCoNi medium entropy alloy to be additively manufactured. The particle sizes selected were 80 nm and 800 nm for TiN and < 5 µm for TiO_2, and both were added with 0.5 vol% and 5.0 vol% to the base alloy. To determine suitable parameters for dense and defect-free material, the processing window for each alloy variant was investigated spanning laser speeds of 200 – 1000 mm/s and laser powers of 150 – 350 W. Densities as high as 99.99 % were obtained with 0.5 vol% TiN for both particle sizes when using the laser parameters of 350 W and 1000 mm/s. Results suggest a shift to higher energy levels required to synthesize dense samples when the concentration of reinforcing particles increases. While the higher particulate volume (5.0 vol%) impaired the powder flowability, the material was still processable by means of PBF-LB/M. The reported results include microstructural observations revealing a uniform distribution of nanosized particulates in the alloy matrix.

Static and dynamic properties of particle-reinforced compositionally complex alloys produced by laser powder bed fusion

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Increasing interest in hydrogen applications calls for materials with favourable properties at low temperatures and under hydrogen influence. However, most high-performance metals are susceptible to hydrogen embrittlement, significantly limiting material and component life. Compositionally complex alloys (CCA), such as particle-reinforced medium and high entropy alloys, offer opportunities for such applications.

This study investigates the static and dynamic properties of two CCA, a six-element A1 high entropy alloy and a four-element A1 medium entropy alloy, each reinforced with TiN particles. The reinforcing particles comprise two different sizes (80 nm and 800 nm) and were added with 0.5 vol.% and 5.0 vol.% to the base alloys. Specimens were manufactured by laser powder bed fusion (LPBF) using a hybrid approach whereby the bottom thread of the test specimen is part of the build substrate. This approach enables testing of alloys with limited raw material available as is often the case in alloy development. Excellent cohesion of the interface between bottom thread and the printed section of the specimen is imperative to be able to perform mechanical tests. Due to the volatile nature of hydrogen gas, a centre hole along the entire gauge length is drilled into the test specimens. These are then charged with hydrogen at 100 bar prior to testing. Both tensile and fatigue tests on these charged specimens are then performed at room temperature. Additionally, some tensile tests are performed in liquid hydrogen. We report the result of these tests and discuss the results considering microstructural analysis performed by electron microscopy.

Defect Detection for High-Entropy Alloy (HEA) Printing Using High-Speed Infrared Imaging

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In recent years, the fabrication of High-Entropy Alloy (HEA) products through various additive manufacturing (AM) techniques has been widely investigated due to the potential of HEAs in replacing Ni-based superalloys for high-temperature applications. Among those AM techniques, laser powder bed fusion (LPBF) takes advantage of its high dimensional accuracy and low oxidation during printing. However, the non-equilibrium metallurgical nature of HEAs incidentally causes defect generation during LPBF processes, such as cracks, pores, lack of fusion, and balling, limiting the application in practice. This research presents a new method to detect the formation of defects during LPBF processes by monitoring the variation of infrared (IR) image data via a high-speed IR camera. The real-time thermal features, such as the peak temperature and cooling rates of the melt pool, were extracted from the raw IR image data from each pixel of the IR camera. The results were further combined with the printing depth to produce 3D maps of each thermal feature. The 3D maps were processed by a machine learning model to correlate with the ground truth of porosity defects observed via X-Ray CT scanning. The experimental results showed strong correlations between the porosity formation and the temporal-spatial thermal feature maps. Further experimental tests proved the feasibility of using the high-speed IR imaging method as a means to detect porosity defects during HEAs material printing.

High entropy materials: new opportunities for structure and property engineering

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The hunt for new phases of matter is among the most exciting activities in materials research. The excitement originates from the possibility of active property engineering and advanced technology opportunities that serve societal needs. As a community, we have been looking for a long time, and given the finite number of practical elements and their stable combinations, it is not clear how many are left to find especially if we limit ourselves to conventional tactics. In response, researchers are exploring new approaches that include artificial layering, high throughput computation, severely confined dimensions, and strain-stabilization.

Inspired by explorations of high-entropy alloys, this presentation discuss the concept of entropy engineering in non-metals, which is a parallel path to new materials discovery. In this approach, many cations are distributed at random among a single sublattice creating a high degree of configurational disorder. At finite temperatures, these systems can minimize free energy by remaining single phase. The Maria group extended this concept to complex oxides to demonstrate without ambiguity that new phases of matter can be stabilized by configurational disorder.

The presentation will begin with an overview of high-entropy non-metals that highlights the exciting contributions being generated by the international high-entropy research community. This will be followed by a discussion of property engineering opportunities that are *potentially* exclusive to crystals having a predominant entropic contribution. They include nanostructure engineering, extreme refractoriness and hardness, ionic conductivity, and spin-orbit coupling. In each example, we promote the case that the high solubility in the solid state that accompanies the high configurational entropy condition is the enabling factor.

Experimental and theoretical study of the Ni–CoCrFeMn system: Transition from a dilute solid solution to a high entropy alloy

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High entropy alloys (HEA) attract increased attention as a potential structural material due to outstanding mechanical and physical properties. Diffusion kinetics in these materials has received particular attention due to the early suggestion that transport could be sluggish, improving phase stability and deformation behavior, particularly at elevated temperatures. Combining experimental analyses of alloy microstructures and transport behavior with atomistic Monte-Carlo simulations based on a modified embedded-atom potential, we contribute to understanding the diffusion kinetics of HEA as a function of temperature and composition, examining a series of $(CoCrFeMn)_{1-x}Ni_x$ alloys with compositions ranging from pure Ni ($x = 1$) to the equiatomic CoCrFeMnNi ($x = 0.2$) high-entropy alloy. In addition to characterizing the material behavior across the transition from a dilute alloy to a concentrated one and finally to a high-entropy alloy at fixed alloy constituents, the vacancy formation and migration energies as well as the vacancy and atomic correlation factors were systematically assessed. Thus, the impact of composition, number of constituents, nature of constituents and homologous temperature on the diffusion behavior could be critically assessed.

High entropy oxides with unique magneto-electronic phase separation for advanced functionalities

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Transition metal oxides are known to exhibit a plethora of technologically relevant magnetic and correlated electronic phenomena, such as colossal magneto-resistance, exchange bias, metal-insulator transitions, etc.[1] These phenomena are often strengthened by the magneto-electronic inhomogeneity present in the systems. As a result, tuning the functionalities underpinned by these phenomena relies on manipulation of the magneto-electronic inhomogeneity, which is conventionally achieved via chemical substitution, charge doping, strain-engineering or heterostructuring.

Alternately, the chemically disordered crystallographic single-phase high entropy oxides (HEOs)[2,3] stand out as the natural choice for tailoring magneto-electronic inhomogeneity due to the presence of a variety of magnetic exchange interactions, which are often competing.[4,5] This presentation will focus on two different case studies illustrating the inherent magneto-electronic phase separation in crystallographic single-phase perovskite-HEOs (P-HEOs).[6,7] In the case of the chemical disordered B-site P-HEOs with multiple transition metal cations, the magnetic phase separation manifests itself through (vertical) exchange bias, which is believed to originate from ferromagnetic clusters embedded in an antiferromagnetic matrix. On the other hand, A-site disordered manganite-P-HEOs exhibit a substantial degree of colossal magneto-resistance along with a complex magneto-electronic phase space as a function of chemical charge doping. These initial sets of results highlight the potential for new research opportunities offered by the HE-design approach to manipulate and enhance functionalities that are governed by magneto-electronic phase separation.

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SESSION 2A

ALLOYS: Refractory Alloys II

10:30 **2A1:** Development of refractory metal-based CCAs with improved mechanical properties
S. Laube, S. Schellert, A. Kauffmann, B. Gorr, S, Seils, Y.M. Eggeler, H.-J. Christ, M. Heilmaier

10:45 **2A2:** Mining lattice distortion, strength, and intrinsic ductility of refractory high-entropy alloys using physics-informed statistical learning
Christopher Tandoc, Yong-Jie Hu, Liang Qi, Peter K. Liaw

11:00 **2A3:** Quantitative study of solid-solution strengthening in Refractory High Entropy Alloys
Kangjin Lee, Yunjong Jung, Junhee Han, Chanho Lee, Peter K. Liaw, Gian Song

11:15 **2A4:** Nonlinear deformation and elasticity of BCC refractory metals and alloys
Michael Widom, Vishnu Raghuraman, Michael Gao

11:30 **2A5:** *Ab-initio* tensile tests applied to BCC refractory alloys
Vishnu Raghuraman, Michael Widom, Michael Gao

11:45 **2A6:** *Ab initio* computation of phase stability and interstitial alloying in bcc compositionally complex alloys
Yilun Gong, Yuji Ikeda, Fritz Körmann, Jörg Neugebauer

Development of refractory metal-based CCAs with improved mechanical properties

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Refractory compositionally complex alloys (RCCA) are promising candidates for high-temperature structural applications. Many of the reported alloys consist of A2 or B2 phases with additional intermetallic phases, often located at grain boundaries. However, to achieve good mechanical performance at elevated temperatures, the proper formation of the strengthening phase is crucial. We report here on the current status of our investigations within the Ta-Mo-Ti-Cr-Al system which exhibits a promising combination of strength and oxidation resistance at elevated temperatures [1]. The objective is to attain a suitable multi-phase microstructure of an A2 matrix with B2 precipitates without significant grain boundary decoration. Thermodynamic calculations were employed to predict transformation sequences of ordering and diffusion-controlled phase separation.

The microstructure of alloys with high Al concentration exhibited a B2 matrix with A2 precipitates; in contrast, an A2 matrix with B2 precipitates was determined in Al-lean alloys [2, 3]. The phase separation into a two-phase microstructure in RCCA has been speculated as being spinodal in nature with continuous chemical distribution during the separation. However, these reactions might instead occur as precipitation by nucleation and growth.

To unequivocally elucidate the distinct nature of phase separation sequence in the system Ta-Mo-Ti-Cr-Al, atom probe tomography and electron microscopy techniques were utilized on samples from the Al-lean composition that were annealed over multiple orders of magnitude in time [3]. Indeed, the phase separation occurs via interface motion-controlled precipitation rather than spinodal decomposition. Thus, the requirements for controlled strengthening by superalloy-like microstructures are verified for the alloy system under investigation.

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[3] *S. Laube, A. Kauffmann, S. Schellert, S. Seils, A.S. Tirunilai, C. Greiner, Y. M. Eggeler, B. Gorr, H.-J. Christ and M. Heilmaier*, STAM, Vol. 23 (2022), 692-706

Mining lattice distortion, strength, and intrinsic ductility of refractory high-entropy alloys using physics-informed statistical learning

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Severe lattice distortion is a prominent feature of high-entropy alloys (HEAs) considered a reason for many of those alloys' unique properties. Nevertheless, accurate characterizations of lattice distortion are still scarce to only cover a tiny fraction of HEA's giant composition space due to the expensive experimental or computational costs. Here we present a physics-informed statistical model to efficiently produce high-throughput lattice distortion predictions for refractory non-dilute/high-entropy alloys (RHEAs) in a 10-element composition space. The model offers improved accuracy over conventional methods for fast estimates of lattice distortion by making predictions based on physical properties of interatomic bonding rather than atomic size mismatch of pure elements. The modeling of lattice distortion also implements a predictive model for yield strengths of RHEAs validated by various sets of experimental data. Combining our previous model on intrinsic ductility, a data mining design framework is demonstrated for efficient exploration of strong and ductile single-phase RHEAs.

Quantitative study of solid-solution strengthening in Refractory High Entropy Alloys

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Refractory High-Entropy Alloys (RHEAs) have attracted significant attention, due to their outstanding properties and microstructural stability at elevated temperatures. In many RHEAs, the solid-solution strengthening mechanism plays a main role in their excellent mechanical properties. The solid-solution strengthening in HEAs is known to be affected by the lattice and shear modulus distortion factors, which are closely related with lattice misfit, bonding energy misfit and different crystal structure among alloying elements. Especially, it has been reported that the yield strength of many RHEAs with single-phase BCC structure is enhanced by maximizing the lattice distortion factor.

In this study, to establish the concrete relationship between the lattice distortion factor and yield strength of the RHEAs, we attempted to validate the effect of the lattice distortion factors on solid-solution strengthening effect in HEAs by systematic alloy design. Specifically, we fabricated a number of equi-atomic refractory alloys, containing BCC single solid-solution phase. Their microstructure evolution and mechanical properties were systematically investigated using neutron diffraction, scanning electron microscopy, electron backscatter diffraction and universal testing machine

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No.2020R1C1C1005553).

Nonlinear deformation and elasticity of BCC refractory metals and alloys

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Application of isotropic pressure or uniaxial strain alters the elastic properties of materials; sufficiently large strains can drive structural transformations. Linear elasticity describes stability against infinitesimal strains, while nonlinear elasticity describes the response to finite deformations. It was previously shown that uniaxial strain along [100] drives refractory metals and alloys towards mechanical instabilities. These include an extensional instability, and a symmetry-breaking orthorhombic distortion caused by a Jahn-Teller-Peierls instability that splays the cubic lattice vectors. Here we analyze these transitions in depth. Eigenvalues and eigenvectors of the Wallace tensor identify and classify linear instabilities in the presence of strain. We show that both instabilities are discontinuous, leading to discrete jumps in the lattice parameters. We provide physical intuition for the instabilities by analyzing the changes in first-principles energy, stress, bond lengths, and angles upon application of strain. Electronic band structure calculations show differential occupation of bonding and antibonding orbitals, driven by the changing bond lengths and leading to the structural transformations. Strain thresholds for these instabilities depend on the valence electron count.

Ab-initio tensile tests applied to BCC refractory alloys

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High-throughput DFT calculations are a powerful resource for alloy design. We examine the ability of first-principles calculations to predict the intrinsic ductility of refractory metal binaries. We employ the *ab-initio* tensile test to study finite strain behavior of BCC Mo_3X and Nb_3X, where $X \in$ {Al, Cr, Hf, Nb/Mo, Re, Ru, Si, Ta, Ti, V, W, Zr}. The features and shortcomings of this method are explored in detail, along with comparisons to existing computational methods. Guidance on the suitability of the methods for particular systems is also provided. Finally, we discuss how the binary studies help in predicting intrinsic ductility of multicomponent high entropy alloys.

Ab initio computation of phase stability and interstitial alloying in bcc compositionally complex alloys

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Phase stability and chemical ordering have been shown to strongly impact the properties of chemically complex alloys (CCAs). However, the large chemical phase space spanned by HEAs limits experimental approaches making complementary computational approaches indispensable. Interstitial alloying of CCAs with, e.g., C or O, has been recently explored to further tune the mechanical properties of these alloys. Parameter-free *ab initio* methods, which would allow in principle an unbiased exploration of CCAs, are, however, challenged by the large chemical phase space resulting into gigantic number of possible chemical configurations to be explored.

In this work we discuss a combination of machine-learning potentials and *ab initio* calculations to compute the phase stability and interstitial alloying of CCAs. Examples include B2-ordering for a series of BCC TaMoCrTiAl refractory high entropy alloys as well as O-alloying of the prototypical BCC TiNbZr alloy. The chemical dependence of the local solution energies as well as a possible impact of chemical short-range order are carefully analyzed. The delicate interplay between interstitial alloying and phase stability is discussed on a BCC TiNbZrHf alloy, where addition of interstitial O above a critical concentration results into the formation of O-rich clusters. Our predictions agree well with observations from targeted experimentations.

SESSION 2B

ALLOYS: Nanoparticles, coatings, and heterostructures

10:30 **2B1:** High-entropy alloy nanoparticles synthesized in liquid and atmosphere using femtosecond laser ablation
David Fieser, John Whitlow, Peter Liaw, Anming Hu

10:45 **2B2:** Development of thermal-sprayed precipitation-strengthened high-entropy alloy coatings
Shih-Hsun Chen, Tzu-Tang Lin, Rotich Sammy Kiplangat

11:00 **2B3:** Hard domains and superior mechanical properties enabled by nanoscale annealing twins in a heterostructured high-entropy alloy
Shu-Yi Tung, Ting-En Hsu, Ming-Hung Tsai

11:15 **2B4:** : (AlCrNbSiTi)N/TiN multilayer films designed by a novel coating system equipped with a hybrid high-power impulse magnetron sputtering/cathode arc deposition technique
C.Y. Lee, S.J. Lin, J.W. Yeh

High-entropy alloy nanoparticles synthesized in liquid and atmosphere using femtosecond laser ablation

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The incorporation of multiple immiscible elements into colloidal high-entropy alloy (HEA) nanoparticles continues to be a technical challenge, but it possesses manifold technological potential in numerical applications. In this study, we displayed the successful synthesis of high-entropy alloying nanoparticles through femtosecond laser ablation in both liquid and air. Femtosecond laser ablation induces a highly localized thermal effect and thereby generates nanoparticles directly from the bulk with a high fidelity. We display that we can obtain single-phase high-entropy alloying particles from Cu0.2Co0.2Ni0.2Mn0.35Fe0.05 high-entropy alloys, which are synthesized by arc melting and casting. The average particle size is about 50 nm. The size is further controlled by laser parameters. The scalability of the process with a gram level of colloidal HEA nanoparticles per hour is demonstrated. Electrochemical analysis reveals these nanoparticles can work as catalyst for effective oxygen reduction in Al-air batteries.

Development of thermal-sprayed precipitation-strengthened high-entropy alloy coatings

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In this study, we are developing the thermal spray processes for multi-principal element alloys (MPEA) based on the research achievement and developing experience of our group. Thermal spray processes are common and fundamental techniques for many industries; however, few researches devote to establish and accumulate new data for such basic skills. In order to promote the application capability of new metal materials, we continue our developing roadmap through developing a series of single solid solution ($AlCo_xCrFeNi + (Ti, Si)_y$) high-entropy alloy with high strength and precipitation strengthening phase. After prepared by gas atomization process, the microstructure and lattice structure of the alloy powders and their phase evolution behavior are going to be investigated. The formation of intermetallic compounds will be observed, and then to find out its influence in the mechanical properties. Furthermore, the proposed high-entropy alloy powder would be applied to thermal spraying technology. The influences of Si and Ti additions on the properties of powders and coatings would be further studied, and the relationship of process parameters on the designed materials could be established.

Hard domains and superior mechanical properties enabled by nanoscale annealing twins in a heterostructured high-entropy alloy

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High-entropy alloys (HEAs) and heterostructured materials are two hot topics in metallic materials. Here, we introduce heterostructures into an FCC HEA via simple rolling and annealing. It was found that through careful control of processing conditions, regions with dense nanoscale annealing twins can be formed in the alloy. The nanotwins have an average width of around 20 nm and typically form along more than one crystallographic directions. The twin boundaries act as useful dislocation barriers, leading to an effective grain size of ~135 nm in nanotwinned (NT) regions and thus considerable strengthening. Indeed, nanoindentation results show that NT regions have hardness similar to unrecrystallized (UnR) regions. Kernel average misorientation analysis also shows that the strain in NT regions is similar to that in UnR regions and significantly smaller than regular recrystallized grains (RG). The unique UnR-NT-RG structure altered regular hard/soft domains in partially recrystallized alloys as well as their distributions and the number of their boundaries. Such differences led to mechanical properties that are better than other process routes, such as high pressure torsion.

(AlCrNbSiTi)N/TiN multilayer films designed by a novel coating system equipped with a hybrid high-power impulse magnetron sputtering/cathode arc deposition technique

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This study was aimed at realizing high-performance coatings by combining a thermally stable high-entropy alloy nitride (HEAN) film—(AlCrNbSiTi)N—with a TiN film exhibiting poor oxidation resistance. The multilayer (AlCrNbSiTi)N/TiN nitride films were prepared using a hybrid coating system equipped with high-power impulse magnetron sputtering and cathode arc deposition subsystems. The effects of the modulation period on the microstructural, mechanical, and oxidation resistance properties of the coatings were investigated by scanning electron microscopy, transmission electron microscopy (TEM), X-ray diffraction, and nanoindentation. All coatings exhibit a B1-NaCl-type face-centered-cubic crystal structure. High-resolution TEM imaging revealed misfit dislocations between the HEAN and TiN layers and low-angle boundary dislocations between the subgrains. The film growth occurred through a self-nucleation mechanism. The mechanical and oxidation resistance properties of the 64-layer coating were outstanding compared with those of previously reported multilayer coatings. The plastic deformation index H^3/E^2 of the mono- and multilayer coatings increased from 0.17 to 0.37 GPa, and the thickness of the oxidation layer decreased from 1228 to 85 nm after oxidation at 800 °C for 2 h in an ambient atmosphere.

Effects of short-range ordering on mechanical properties of single crystals of the equiatomic CrCoNi medium-entropy alloy

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The plastic deformation behavior of single crystals of the FCC equatomic CrCoNi medium-entropy alloy has been investigated in a temperature range of 10-1273 K, paying special attention to possible variations in mechanical properties with heat-treatment that may cause short-range ordering of the constituent elements. Deformation occurs via slip of the {111}<110> system exclusively in the whole temperature range regardless of different heat treatments. The CRSS values increase with decreasing temperature, especially below room temperature. Dislocations are smoothly curved in the slip plane without any preferred line orientation, indicating no significant anisotropy in the mobility of edge and screw segments. Planar ½<110>{111} dislocations dissociate widely into Shockley partials for all alloys investigated, indicating the low stacking fault energy of 13 ± 3 mJ/m^2 for CrMnFeCoNi and CrCoNi, respectively. The CRSS values extrapolated to 0 K for polycrystals of equiatomic quinary, quaternary and ternary alloys are reported to be well scaled with the mean-square atomic displacement from the regular FCC lattice points (calculated based on density-functional theory). This seems also the case for the CRSS values at 10 K for single crystals of CrCoNi and its related quaternary (CrFeCoNi) and quinary (CrMnFeCoNi) alloys. Deformation twinning occurs on the conjugate system in the form of the Lüders type deformation in the later stage of deformation at low temperatures in all of the three alloys. No significant variation of the CRSS values, twinning stress and the stacking-fault energy was noted upon the formation of short-range order by heat-treatment.

Designing and Discovering High Entropy Oxides

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High entropy, multi-component metal alloys (HEA), have superior mechanical properties and high radiation tolerances; which are, in part, driven by configurational entropy. Recently, an oxide analogue comprised of MgO, CoO, NiO, CuO and ZnO was synthesized; exhibiting a truly entropy-stabilized, reversible phase transition from a multiphase material to a single rock salt-ordered phase above 850-900°C. This entropy-driven stabilization may engender many unique properties, such as high melting temperatures, radiation resistance and other anomalous responses. Here, we discuss a design strategy for the prediction of synthesizable disordered oxides. Our effort employs first principles studies of 2-component oxides to develop design rules based on the relationship between pairwise enthalpies of formation, ΔH, and configurational entropy of the disordered material. A similar chemical identity-to-ΔH map was previously explored using the class of high entropy alloys, where the stability of multicomponent metal alloys was correlated to the enthalpy of mixing of binary and ternary compounds.

In this presentation, I will focus on our recent efforts to employ this local enthalpy map as an effective strategy for the discovery of new classes of entropy stabilized oxides. In particular, we are able to use our first principles calculations with Monte Carlo simulations in order to build chemical bonding maps to study the local environment preferences that determine whether a material will phase segregate, to form a single phase with clustered regions, or form a disordered solid solution. This enables us to identify compounds that may be synthesizable or could be stabilized by entropy – thus allowing for more reliable materials discovery and design.

This work was supported by the U.S. D.O.E., Office of Science, BES, MSED (first principles calculations) and the LDRD Program of ORNL (simulations), managed by UT-Battelle, LLC, for the U. S. DOE using resources at NERSC and OLCF.

SESSION 2C

ALLOYS: Ductility and Deformation I

2:00 **2C1:** Deformation regimes and signatures in body-centered cubic high entropy alloys
K.W. Deck, S. Basu, S., J. Wang, R. Schwaiger, C. Brandl

2:15 **2C2:** The role of frictionally induced subsurface deformed region during wear in a non-equiatomic CoCrFeNiV high entropy alloy
F. Haftlang, A. Zargaran, H.S. Kim

2:30 **2C3:** Structural Essence of Plasticity in High-Entropy Alloys Profiled by Multivariable Data Analysis
Chi-Huan Tung, Shou-Yi Chang, Peter K. Liaw, Wei-Ren Chen

2:45 **2C4:** Strength and deformation of precious high entropy alloys
S. Drescher, J. Freudenberger, S. Seils, T. Boll, A. Kauffmann, M. Heilmaier

3:00 **2C5:** Optimizing the high temperature deformation behavior of polycrystalline high-entropy superalloys
A. Bezold, S. Neumeier

Deformation regimes and signatures in body-centered cubic high entropy alloys

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The emergence of high entropy alloys (HEAs) allows a new materials design space envisioning better alloys for extreme conditions. With a focus on body-centered cubic (bcc) HEAs, like bcc metals, some bcc HEAs show room-temperature brittleness (e.g., NbMoCrTiAl) and some room-temperature ductility (e.g., TiHfZrNbTa) suggesting chemistry dependent limited dislocation mobility. This mobility of dislocations relates to the stress and temperature-dependent dislocation velocity and, consequently, the resulting stress and temperature-dependent plastic strain rate.

Using accurate predictions of the chemistry-dependent intrinsic materials properties by *ab-initio* simulation, we present a simulation strategy to predict dislocation properties in bcc HEAs without explicit simulation of a dislocation structure. We demonstrate a computationally efficient methodology that predicts temperature scales and deformation regimes in different bcc alloys. The role of sub-lattice ordering below a possible disorder-order transition in HEAs is discussed. By additionally determining lattice distortions, we also sample the effect on the possible solid solution strengthening effects in the NbMoCrTiAl HEA family and TiHfZrNbTa HEA. The predictions are compared with the temperature-dependent hardness and activation volume of HEAs measured experimentally by advanced nanoindentation experiments.

The role of frictionally induced subsurface deformed region during wear in a non-equiatomic CoCrFeNiV high entropy alloy

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In the present work, the tribological performance of $V_{10}Cr_{10}Fe_{45}Co_{30}Ni_5$ high entropy alloy (HEA, at%) and its relationship with the subsurface deformed area and the superficial tribo- layer were investigated. After dry sliding in reciprocation motion at applied loads of 2-15 N, surface and subsurface regions of the samples were investigated using SEM and TEM analyses, respectively. At an applied load of 2 N, dislocation activity was the subsurface deformation mechanism. The superficial depth-dependent gradient ultrafine microstructure containing the BCC phase decorated with the retained FCC phase, as well as mechanical nano-twins were formed when the applied load was increased to 5 N. By further increase in applied load (10 N), these twins were replaced with elongated FCC/BCC grains. At an applied load of 15 N, a friction-induced heterogeneous microstructure including two individual regions of extremely ultrafine and ultrafine grains was detected in the subsurface region of the worn sample. The simultaneous effects of grain refinement, dislocation-mediated plasticity, and martensitic phase transformation, along with hetero-deformation-induced strengthening, enhanced the hardenability of the subsurface during sliding wear. The formation of the protective superficial tribo-oxide layer triggered by the mechanical support of the substrate resulted in the outstanding tribological performance of the $V_{10}Cr_{10}Fe_{45}Co_{30}Ni_5$ HEA.

Structural Essence of Plasticity in High-Entropy Alloys Profiled by Multivariable Data Analysis

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In this work, we apply computer simulations to examine the effect of atomic arrangements on the early-stage plasticity of FCC high entropy alloy (HEA). The local configuration in quiescent state is defined in terms of gyration tensor and electronegativity. In the context of multivariate statistics, the complex geometric and compositional factors relevant to the variations in the atomic packing of HEA are extracted by principal component analysis. Under externally applied strain, the non-affine displacements associated with defect nucleation are found to localize in a heterogeneous manner. We further established the correlation between the local yield events and configuration features based on linear discriminant analysis and concluded that local plasticity is promoted once the local structure is compatible with deformation gradient. Validated by the analysis of performance metrics, our findings establish an orientational dependent criterion for the instability in HEAs and therefore shed new light on understanding the nature of their plasticity.

Strength and deformation of precious high entropy alloys

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A fundamental understanding of the strength of multi-component alloys relies on well-defined experiments accompanied by accurate modelling. While research has focused on equi-atomic alloys so far, little investigations on the effect of solid solution strengthening in non-equimolar alloys with deliberately adjusted composition were performed. Thus, a systematic approach is utilized as a key tool to investigate solid solution strengthening in concentrated and single-phase, series of Au-Cu-Ni-Pd-Pt alloys.

Although the main focus lies on the investigation of single-phase alloys, some alloys show decomposition at low temperatures, which is utilized to investigate the effect of segregations on the strength of selected alloys.

Structure and microstructure are analyzed by bridging different length scales by means of X-ray diffraction, electron microscopy, and atom probe tomography. The mechanical properties are determined by hardness and compression testing. We give insights into the correlation between the microstructure and mechanical properties of the investigated alloys. The present results highlight the effects of solid solution as well as segregation on the strength of precious high entropy alloys.

Optimizing the high temperature deformation behavior of polycrystalline high-entropy superalloys

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Polycrystalline high-entropy superalloys based on the CoNiCr-system exhibit a promising property profile consisting of excellent creep strength, good oxidation resistance and a sufficiently large processing window for hot working. To understand how their creep strength can be improved even further, a thorough characterization of the underlying deformation mechanisms during high-temperature deformation is necessary to tailor alloy design accordingly. Thus, in this work, the deformation mechanisms of four polycrystalline compositionally complex high-entropy superalloys with slightly varying chemical compositions were investigated at temperatures between 750 °C and 850 °C and strain-rates between 10^{-3} and 10^{-8} s^{-1}.

In all investigated alloys, the deformation behavior transitions from athermal shearing by APB-coupled dislocation pairs to segregation-assisted deformation mechanisms with increasing temperature and/or decreasing strain-rate. Depending on alloy composition, the type of segregation-assisted mechanism differs strongly. By comparing the relative strength of the alloys, stacking fault shearing is identified as favorable deformation mode during high temperature creep experiments. As evidenced by atomic-scale structural and chemical investigations, local phase transformation strengthening along stacking faults is enabled in some alloys, which impedes detrimental stacking fault-based mechanisms such as stacking fault ribbons and/or microtwinning. Based on these characterization efforts, guidelines are derived for the design of the next-generation of polycrystalline high-entropy superalloys with enhanced high temperature strength by tailoring deformation mechanisms and the segregation behavior of alloying elements.

SESSION 2D

ALLOYS: Functional Properties

2:00 **2D1:** Experimental local DOS study of fcc 3d TM alloys: from simple binary to compositionally complex alloys.
S.A. Kasatikov, G.O. Lepore, A.M. Manzoni, A. Fantin

2:15 **2D2:** AlxZnCoNi high-entropy alloy thin-film for ultra-violet reflector application
Cheng-Hsien Yeh, Hau-Shiang You, Yuan-Chun Chang, Wen-Dung Hsu, Hsuan-Ta Wu, Chuan-Feng Shih

2:30 **2D3:** Mixed magnetic phases in AlxCoCrNiFe high entropy
Cameron Jorgensen, Louis Santodonato, Namila Liyanage, Lizabeth Quigley, Peter Liaw, Dustin Gilbert, Raymond Unocic, Lisa Debeer-Schmitt

Experimental local DOS study of fcc 3d TM alloys: from simple binary to compositionally complex alloys.

[1]Kasatikov, S.A., [2]Lepore, G. O., [3]Manzoni, A.M. & [1,4]Fantin, A.

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The recent paradigm shift to compositionally complex alloys (CCAs) brings alloy design to a new level of complexity, demanding urgent improvement in composition search efficiency and new alloys properties prediction. With such needs, fundamental knowledge of atomic and electronic nature appears as one of the prerequisites to success.

The presented study examines local electronic and chemical structure of single phase *fcc* CCAs - $Al_8Co_{17}Cr_{17}Cu_8Fe_{17}Ni_{33}$ [1-3] and its 5-, 4-, 3- and 2- component precursors - using X-ray spectroscopy techniques: X-ray absorption and X-ray photoelectron spectroscopy. The investigation focuses on chemical interactions and local density of electron states (DOS) distribution around the Fermi level (E_f) and attempts to isolate and analyze each element contribution to the chemical and electronic structures.

It has been found that a DOS depletion at E_f is formed in the Ni d-band, which is ascribed mainly to Cr(Fe) – Ni chemical interaction. Such observation points to a covalent character admixture to metallic bonding, and goes along with previous theoretical findings revealing a correlation between short range order presence and DOS depletion at E_f [4]. Finally, results of a 3d band occupancy analysis with an evaluation of 3d-electrons number change upon alloying for each element are presented.

[1] *A. Fantin et al., Acta Mater. 193 (2020) 329-337*
[2] *S. Kasatikov et al, J. Alloys Compd. 857 (2021) 157597*
[3] *A. Manzoni et al, J. Alloys Compd. 552 (2013) 430-436*
[4] *A. Tamm et al., Acta Mater. 99 (2015) 307-312*

$Al_xZnCoNi$ high-entropy alloy thin-film for ultra-violet reflector application

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High-entropy alloys (HEAs) have been shown to have high ductility, high hardness, and high corrosion properties in the past two decades. Most of the research have been focused on the mechanical properties of high-entropy alloys, but none have been done on its optical properties. The severe lattice distortion of the HEAs cause significant change on the optical properties particularly in the short wavelength such deep ultra-violet (UV). Recently, the UV to deep-UV wavelengths have been the most interested field in solid-state lighting. Deep ultraviolet light UVC LED (280-200 nm) has a high technical threshold and has a very large industrial application value. Limited by epitaxy and packaging technology, current UVC LED products are mostly low output power.

Here, $Al_xCoZnNi$ HEAs are designed as the UVC reflector. The phase-stable structure was simulated by the molecular-dynamic simulation. The frequency-dependent dielectric constant and refractive index are calculated, and therefore the reflectance of the $Al_xCoZnNi$ HEAs is obtained. Spontaneous phase separation of the films is found to corelated to the Al content, influencing its mechanical and corrosion behaviors. The reflectance of the as-prepared HEA films is much higher than Au when the wavelengths are shorter than 500 nm. The anti-corrosion behavior is improved by decreasing the Al content that increase the configuration entropy of the alloy. Furthermore, after annealing treatment at 280 ^oC for 5 min, the HEA films showed even higher reflectance to the pure Al films in UVC range. The result shows $Al_xCoZnNi$ HEA film has great application potential for UVC reflector.

Mixed magnetic phases in AlxCoCrNiFe high entropy

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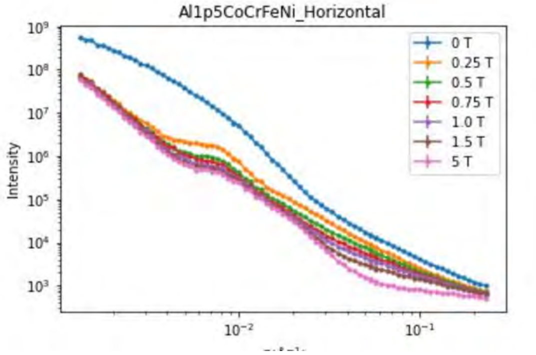
The large distribution in atomic sizes and masses in high-entropy alloys results in extreme local environments, which manifests strongly in the thermal and magnetic properties. In this work, high-entropy alloys of (Fe,Co,Cr,Ni)Alx, $0 < x < 2$, are prepared and their temperature-dependent magnetic and electronic properties determined. Magnetometry results show that all the samples are ferromagnetic, with a high-temperature phase, TC >200 K, and a second low-temperature phase with TC≈20 K. However, the high-temperature phase is not associated with an open hysteresis loop, suggesting superparamagnetic behavior. The closed hysteresis loop suggests the ferromagnetism appears as small clusters, a theory explored with small-angle neutron scattering (SANS). SANS helps confirm soft ferromagnetic properties with alignment occurring with as little as 0.25 T in the Al x=1.5 sample as can be seen in Figure 1, as well as smaller features that we predict to be associated with chromium frustrations localized in a matrix of Al, Ni, and Fe. The samples also show downturn in the magnetization at T<10 K which can be associated with an antiferromagnetic phase. Recent works have suggested that extreme strain distributions can induce antiferromagnetic ordering[1]. This research used resources at the High Flux Isotope Reactor and the Spallation Neutron Source, as appropriate, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory, and was funded by the DOE DE-SC0021344.

Figure 1



[1] Jorgensen, Cameron, et al. "In-Situ Study of Microstructure Evolution of Spinodal Decomposition in an Al-Rich High-Entropy Alloy." Frontiers in Materials 9 (2022).

POSTER SESSION

P1. Microstructure Evolution and Mechanical Properties of Selective Laser Melting Processed High Entropy Alloy with Carbide Addition
Meng-Yun Lee, Hyoung Seop Kim, An-Chou Yeh

P2. Optimization of Refractory high entropy alloy strength and ductility through Predictive Development Process
Curcuru, M., Greenhalgh, A., Berry, K., Howard, A., Landry, J., Steingrimsson, B., Liaw, P.

P3. Towards A Holistic Understanding Of Strengthening Mechanisms And Their Differences Within Conventional Superalloys And Novel Multi- Principal Element Alloys
Adam, B.M., Fan, X., Steingrimsson, B.A, Liaw, P.K.

P4. Synthesis and structural investigation of $Ce_{1-x}(YLaPrSm)_xO_{2-\delta}$ as ionic conductors
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Microstructure Evolution and Mechanical Properties of Selective Laser Melting Processed High Entropy Alloy with Carbide Addition

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The effect of 0.5, 1 and 5 wt% niobium carbide (NbC) addition in $Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3}$ high entropy alloy (Al02Ti03 HEA) on microstructure evolution and tensile properties has been investigated. Al02Ti03 HEA was mainly precipitation strengthened by $L1_2$ phase, and the cellular structure could be obtained due to the rapid cooling rate during selective laser melting (SLM) process. The added NbC carbide could act as heterogeneous nucleation site, resulting in finer grain and cell size.

Two kinds of heat treatment was subjected to Al02Ti03 HEA. The one with solution heat treatment prior to aging (SHTA) could provide homogeneous composition. The NbC addition promoted the carbide strengthening effect in SHTA samples, and 5 wt% SHTA sample exhibited 330 MPa yield strength improvement. For direct aging (DA) treatment, the cellular structure could be remained. 73% grain size refinement and 52.6% cell size refinement provided additional strength in DA samples, and 175 MPa yield strength improvement were provided. The microstructure analysis revealed the hierarchical microstructure; $L1_2$ phase homogeneously distributed within the matrix, and $L2_1$ precipitates could also be detected. Interestingly, the added carbide would influence the precipitation of $L2_1$ phase since the formation of Ti-rich MC carbide would compete against $L2_1$ (Ni_2Al, Ti) formation by Ti absorption. Thus, with the increasing amounts of NbC, $L2_1$ phase formation was constrained. In this study, an effective strengthening method achieved by SLM process and carbide addition are presented. Also, the influence of NbC addition on creep and fatigue properties will be discussed.

Optimization of Refractory high entropy alloy strength and ductility through Predictive Development Process

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Following the introduction of the Senkov alloy, Refractory high-entropy alloys (RHEAs) are receiving attention for high-temperature applications, increasing the importance of an understanding of their mechanical properties and microstructure. RHEAs typically exhibit high strength, but like conventional refractory metals, they lack room-temperature ductility. This work seeks to design and develop new RHEAs with excellent strength and ductility through a joint computational and experimental approach. Linear Regression models were utilized to determine ideal compositions with high strength and good ductility from existing RHEA data. To train these predictive models, a database of over 1,000 entries has been assembled from HEA literature. The ductility throughout the compositional space of several RHEAS was visualized through a modified ternary phase diagram approach. After the computational prediction, two favorable alloy compositions were fabricated by arc melting, compression and tensile testing, and microstructure characterization through SEM, TEM, and optical microscopy. The mechanical properties of these two RHEAs are compared with the Senkov alloy's performance. The predictive development process outlined in this work is a step towards addressing the complications of the vast HEA compositional space. Currently, computational prediction of advantageous RHEAs remains the most feasible option for exploring the boundless potential of this class of materials.

Towards A Holistic Understanding Of Strengthening Mechanisms And Their Differences Within Conventional Superalloys And Novel Multi- Principal Element Alloys

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Multi-principal element alloys (MPEAs) have seen an increase in attention due to their consideration as a material class of choice for high-temperature structural applications, rivaling and potentially eclipsing the capabilities of conventional high-temperature alloys, such as Ni-based or Ni-Fe-based superalloys. The prime material requirement for high-temperature alloys in their application space is the strength, both at low-to-medium as well as high homologous temperatures, i.e., T/T_{melt}, both at short- and long-term exposure. Strengthening concepts are relatively well understood for superalloys, with knowledge of contributions from dielastic, parelastic, and chemical interactions, together solid-solution strengthening, as well as contributions from dispersion- and precipitate-related order strengthening. Due to their novelty, there is still a gap in knowledge between the alloying combinations of MPEAs, and their related microstructure-property relationships. The present work aims to review similarities and differences between these alloy classes, focusing on comparison with and application of basic concepts of physical metallurgy and plasticity from superalloys to MPEAs. This study will aid in the basic understanding and prediction of their mechanical behavior at various temperatures and time ranges. Ultimately, it will help enable a more cohesive approach towards designing alloys with properties targeted for their designated application space.

Synthesis and structural investigation of $Ce_{1-x}(YLaPrSm)_xO_{2-\delta}$ as ionic conductors

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The prototype high entropy oxide $Y_{1/5}La_{1/5}Ce_{1/5}Pr_{1/5}Sm_{1/5}O_{2-\delta}$ (hereafter referred to as F1, when in fluorite structure) with both 3+ and 4+ preferred cations is considered as a promising candidate for oxygen ion conduction because the anion sublattice will contain up to 25% unoccupied sites depending on the cation valence states. In the ideal case, each 3+ cation will be accompanied by ½ of an empty anion site and without bixbyite ordering. However, depending on the thermal and kinetic history during synthesis, the F1 system may adopt local chemical ordering and a transition to a bixbyite-like structure. In this work, we synthesized a series of F1 derivative systems using conventional powder processing methods with varying Ce concentration ($Ce_{1-x}(YLaPrSm)_xO_{2-\delta}$ with x ranging from 0.2 to 0.8) to investigate the structural dependence on composition. When the cation mixture is equimolar, the system favors bixbyite structure at temperature up to 1500 °C. As the Ce concentration increases beyond 20%, the material transitions into a single-phase fluorite structure with no evidence of a bixbyite-like phase. The SEM images show that all synthesized $Ce_{1-x}(YLaPrSm)_xO_{2-\delta}$ bulk samples have consistent grain size with no gross chemical segregation as evident from EDS. In addition, we will show thin film deposition results where all compositions can be stabilized as fluorite crystals. STEM analysis of the oxygen sublattice proves the fluorite structure even at the local length scale. A combination of *i-V* analysis on films and impedance spectroscopy on ceramics will probe the electronic and ionic transport properties.

Study of Microstructure and Conductive Properties of High-entropy Alloys for Applications in Thin Film Heater

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Microstructure and conductive properties of TiZrHfAg high-entropy alloy thin films using a rf magnetron sputtering method were investigated. Rf power and substrate temperature effects on conductive characteristics of TiZrHfAg high-entropy alloy thin films were also improved. In addition, the TiZrHfAg high-entropy alloy thin film hairpin heater is designed and fabricated on the alumina substrate. The results show that the TiZrHfAg high-entropy alloy thin film hairpin heater can effectively raise the temperature to more than 100°C when the DC power is 12.6 W.

Refractory NbMoTaW High Entropy Alloy film as Diffusion Barrier for Copper/Silicon Interconnections

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In integrated-circuit (IC) industry, Cu is currently the most suitable material for interconnection in the metallization process because of its low resistivity and high melting point characteristics. However, high-temperature diffusion of Cu into Si and SiO_2 causes severe damage to the device. A copper-silicon compound is formed at the interface, which greatly increases the resistivity. Therefore, a diffusion barrier must be deposited between the copper wire and the Si substrate or SiO_2.

Owing to the properties of high thermal stability and high resistance to interdiffusion, high entropy alloys (HEAs) as diffusion barrier are considered to have a potential application for copper/silicon interconnections. The NbMoTaW HEAs films with equal proportion and excellent single-phase solid solution are fabricated by DC magnetron sputtering. A 70 nm NbMoTaW film shows excellent thermal stability and maintains good electrical properties about 75 μΩ-cm after 500°C annealing. A 15 nm NbMoTaW film is prepared as a diffusion barrier. It is found that the structure is complete, and no diffusion occurs after 500°C annealing. Moreover, Cu/HEAs/Si interface becomes obscure slightly after 700°C annealing that is superior to the Cu/Ti/Si interface, which become rough at 500°C. It indicates that the critical point of failure of the HEA diffusion barrier is improved. The results also suggest a high opportunity of NbMoTaW film to replace the conventional Ti, Ta, and other binary alloys/nitrides with the advantages of low resistivity and thermal stability, being a potential candidate in Cu/Si interconnects as a diffusion barrier.

Mixing and Amorphization at Internal Interfaces of Deformed High Entropy Alloys

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Severe plastic deformation (SPD) exposes materials to conditions which make the emergence of non-equilibrium phases possible. Here, a nanocomposite high entropy alloy (HEA) was produced by the forced mechanical mixing of single-phase equiatomic fcc-CoCrFeMnNi and bcc-HfNbTaTiZr alloys. The forced intermixing of the two HEAs was monitored as function of strain, observing the development of a rather complex microstructure with numerous vortices. In-depth analyses of the chemical and structural aspects using scanning / transmission electron microscopy (S/TEM) and nanobeam diffraction mapping (NBD) reveals that in addition to the initial fcc and bcc phases, a new amorphous phase emerged which corresponds to a region consisting of 10 elements in equal proportion, as also verified by atom probe tomography. Detailed analyses have also been applied concerning the stability of the deformation-induced structures and concerning phase transformations in the nanocomposite HEA, indicating a combination of phase separation and nanoprecipitation while, unexpectedly, the phase consisting of 10 elements at about equiatomic concentrations has retained its amorphous structure. The analysis of different types of phase transformation in the nanocomposite HEA, including magnetic analyses, indicates the range of tuning opportunities based on SPD-processing of compositionally complex alloys.

Effects of Ti addition on microstructure and mechanical properties of Fe-Cr-Co-Al ferritic alloys

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Ferritic steels are more advantageous than Ni-based superalloys, due to their high thermal conductivity, low thermal expansion, and low cost. However, conventional ferritic steels limit the usage at temperatures higher than 873 K, due to microstructural instabilities, i.e., coarsening behavior and forming Z-phase, induced by incoherent carbides/nitrides. Recently, the formation of hierarchically-structured coherent precipitate has been reported with enhanced creep properties. Specifically, Fe-Cr-Ni-Al-Ti ferritic alloys strengthened by hierarchically-structured coherent precipitates (B2-NiAl/L2_1-Ni_2TiAl) exhibit the excellent creep properties due to optimized coherent lattice strain between the Fe matrix and precipitates. However, these alloys consist of nano-scale B2-NiAl precipitates forming during cooling, which is known to deteriorate the room temperature ductility. Also, it has been reported that the suppression of the cooling B2-NiAl precipitates is difficult because of the low formation energy of the B2-NiAl phase.
Thus, in the present study, we designed a new Fe-Cr-Co-Al-Ti ferritic alloys to avoid the formation of the B2-NiAl cooling precipitate and enhance the mechanical properties at room and high temperatures. Cobalt was employed instead of Nickel to form precipitates coherent with the BCC Fe matrix, such as B2-CoTi, CoAl, L2_1-Co_2TiAl phases. Furthermore, the main elements to form the coherent precipitates, such as Ti, were systematically adjusted to achieve the different volume fraction of the precipitates and optimize the lattice strain between the precipitate and matrix. We will present the microstructure and mechanical properties of newly-designed Fe-Cr-Co-Al-Ti ferritic alloys, characterized using Scanning-Electron-Microscope (SEM), Transmission-Electron-Microscope (TEM), X-ray Diffractometer (XRD), Universal Testing Machine (UTM).

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No.2020R1C1C1005553).

Investigation on superplastic behavior of $L2_1$ precipitate-hardened BCC high entropy alloy

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Superplastic behavior requires the ultrafine-grains microstructure due to the grain boundary sliding. In general, grain refinement for superplasticity can be mainly achieved by severe plastic deformation (SPD) techniques, such as high-pressure torsion (HPT). Indeed, in several high-entropy alloys (HEAs) with FCC structures, superplasticity was achieved by using SPD techniques. On the other hand, there is another way to obtain the ultrafine-grains, such as dynamic recrystallization (DRX). Among them, the DRX occurring by the rotation of subgrains is called continuous dynamic recrystallization (CDRX). Meanwhile, the AlCrFeNiTi HEA consisting of $L2_1$ precipitates and BCC matrix was designed for high-temperature application. In addition, it has been reported that improved ductility at room-temperature was acquired by ultrafine subgrains, which is formed by hot-rolling and short-term annealing. However, high-temperature deformation behavior of the AlCrFeNiTi HEA with ultrafine subgrains has not been studied, which could be associated with CDRX-driven superplasticity. Thus, our objective is to investigate the deformation behavior at high-temperature for AlCrFeNiTi high entropy alloy with ultrafine subgrains. The microstructural evolution and mechanical properties were systematically investigated, using scanning electron microscopy (SEM), electron-backscattered diffraction (EBSD), and tensile tests at temperatures of 973 ~ 1073 K with strain rates of 1×10^{-4} to $10^{-2} \cdot s^{-1}$. As a result, it was founded that the ultrafine subgrains formed by hot-rolling and annealing transform to HAGB during tensile deformation at elevated temperatures.

This work was partly supported by the Korea Institute for Advancement of Technology (KIAT), and Ministry of Trade, Industry and Energy(MOTIE, korea)(P0022331)

Improving high temperature mechanical properties of $Al_{0.5}$FeCrNiCo high entropy alloy via addition of Ti element

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High entropy alloys (HEAs) are defined as a multi-element alloy including more than 4 elements with near equi-atomic percentage. In general, the configurational entropy of the HEAs is known to be sufficient to stabilize a single solid solution, such as body-centered cubic (BCC), face-centered cubic (FCC) and hexagonal-closed pack (HCP). Compared to BCC single-phase alloys, FCC single-phase alloys draw extensive attention because they are advantageous in manufacturing and processing. FCC-based HEAs show excellent ductility but limited strength, so many research on improving strength has been conducted. Outstanding mechanical properties with a balance of strength and ductility are rarely achieved in single-phase FCC-based HEAs. This is why most alloys for structural applications exhibit a multi-phase microstructure. Recently, Al0.5CoCrFeNi HEA was reported to have excellent mechanical properties at room temperature. This is associated with the formation and phase transformation of B2-NiAl precipitates during deformation. However, B2-NiAl is known to be softened at high temperatures, and thus exhibits limited properties at high temperatures. In this study, Ti elements were introduced to the Al0.5FeCoNiCr alloy to induce the formation of $L2_1$-Ni_2TiAl phase to enhance high-temperature properties. Specifically, microstructural evolution and mechanical properties of multi-phase HEAs were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), transmission electron microscopy (TEM) and universal testing machine (UTM) at room and/or high temperatures.

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No.2020R1C1C1005553).

Review of the Effect of Irradiation on the Properties of High-Entropy-Alloys

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High-Entropy Alloys (HEAs) have in recent years, become a major topic of interest. HEAs are defined as having a configurational entropy greater than or equal to 1.5R where R is the gas constant. Or, alternatively, they can also be defined as having four or five or more of approximately equi-atomic percentages of principal elements ranging between $5 \leq x \leq 35$ atomic percent (at.%). HEAs have demonstrated excellent strength-ductility trade-off, fracture toughness, corrosion resistance, oxidation resistance, fatigue-life properties, and irradiation-damage mitigation properties among others. The demand for the alternative energy, space travel, weapon, and vehicular survivability in space have driven major efforts for promising materials in the irradiation-damage mitigation of alloys. The effects of tunable chemical complexity on energy dissipation, defect energetics, and defect dynamics are discussed. The radiation performance of HEAs is then evaluated by examining the defect and microstructure evolution under various irradiation conditions. Radiation-induced segregation (RIS) and precipitation, and the growth of cavities and dislocations are presented and compared with conventional alloys via both experimentally and first-principle calculations of RIS in HEAs. The potential strategies to enhance the radiation tolerance of HEAs are proposed, and the limitations of the current studies are discussed. In the present work, we provide extensive insight into the irradiation effects on HEAs and their corresponding implications on future trends.

Oxidation Review of High-Entropy-Alloys

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A novel class of materials known as High-Entropy Alloys (HEAs), have become a significant topic of interest. HEAs are defined as having five or more of approximately equi-atomic percentages of principal elements ranging between $5 \leq x \leq 35$ atomic percent (at.%) or as having a configurational entropy ($\Delta S_{config} \geq 1.5R$) where R is the gas constant. HEAs have demonstrated many desirable properties, such as good strength-ductility optimization, corrosion resistance, oxidation resistance, irradiation-damage-mitigation properties and fatigue life among others. The demand for oxidation resistance in high-temperature materials, such as turbine blades, has increased in recent years. The effects of mass gain over several crystallographic categories are summarized, experimental oxidation rates for different crystallographic categories, oxygen diffusion mechanisms, oxide layers, and theoretical work are examined. In the present work, we present a thorough comparison of HEA oxidation against sample Ni-based superalloys, insights into oxidation diffusion, various oxide scales as well as their corresponding effects on future trends and applications.

Ab-Initio Investigation of Local Jahn-Teller Distortions within $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$ High-Entropy Oxide

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High-entropy oxides (HEOs) are characterized by a deliberate maximization of entropy through populating the cation sublattice with five elements or more at random, resulting in extreme chemical disorder at the atomic length scale. This class of complex materials has been extended from the rocksalt $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$ to various other crystal structures and elemental compositions in hopes of leveraging the unique chemical configurations and valence states that can be stabilized for functional properties. However, in nearly a decade since the seminal HEO publication from Rost et al, the local crystalline disorder within the prototypical $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$ HEO is still not well understood [1]. The metastable CuO_6 octahedra is of particular interest as it has been shown to exhibit a Jahn-Teller (JT) distortion both experimentally [2] and computationally [3], in which both JT compressed and elongated octahedra were observed in density-functional theory (DFT) calculations. Here we report on the relative stability between these JT variations within the chemically disordered $Mg_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}Zn_{1/5}O$ matrix using the recently developed strongly constrained and appropriately normed (SCAN) functional. We find that the SCAN functional is able to describe both JT states and provide mixing enthalpies in excellent agreement with experimental measurements without the need of fitted parameters such as a Hubbard U correction or hybrid functionals. Additionally, we find that ab-initio calculated X-ray absorption near-edge structure (XANES) can capture differences in these JT distortions and provide benchmarks that may be useful for uncovering differences in local atomic structure experimentally within HEOs.

[1] Rost, C. M. et al. Nat Comm. 2015, 6 (1), 8485.
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Elevated temperature deformation behavior of AlCoCrFeNi high entropy alloy using hot torsion test

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Since the concept of the high entropy alloy (HEA) was introduced two decades ago by pioneering materials scientists, this metallic material has now become one of the most studied structural materials. Due to its unique approach to the alloy development, the idea suggests the new paradigm of the alloy design. At least 3-5 multiple elements with equiatomic proportions form solid solutions, and this stands in contrast to the conventional practice of which small amount of alloying elements to a single base element. This equiatomic multi-component approach enlarges the number of possible element combinations and gives unique physical and mechanical properties. For instance, HEA is considered as promising structural materials for the use in elevated temperature atmosphere. The elevated temperature deformation behavior of AlCoCrFeNi HEA was investigated in this study. Buttons of the alloy were fabricated via vacuum plama melting, and were homogenized in the tube furnace. Hot compression tests were then carried out, and flow curves were analyzed to build constitutive equations. The processing maps were constructed based on constitutive equations. Flow curves and deformed microstructure revealed that the dynamic restoration mechanism of the alloy was discontinuous dynamic recrystallization.

Investigating the Stability and Properties of Compositionally Complex Rare Earth Pyrochlores

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In multicomponent ceramics there are varying factors that determine the phase selection and stability such as the configurational entropy of the system or the ionic radii of the constituent cations. The influence of each of the aforementioned factors can vary based on the complexity of the crystal structure of the material. Stability rules based on ionic radius ratios are well established for rare earth pyrochlores ($RE_2^{3+}B_2^{4+}O_7$). To investigate phase selection and stability in a multicomponent complex ceramic, we have synthesized members of the titanate ($RE_2^{3+}Ti_2^{4+}O_7$) and stannate ($RE_2^{3+}Sn_2^{4+}O_7$) pyrochlore families, taking advantage of the large diversity of ionic radii available in the Lanthanide series (La to Lu, large to small). We further examine trends in their average and local atomic structures using X-ray and neutron diffraction and pair distribution function analysis. Determining the impact of high entropy configurations on pyrochlore radius ratio rules and other potential crystal-chemical effects will provide deeper understanding of possible design considerations for intrinsic property tuning in these and other multicomponent complex ceramics.

Dislocation properties in refractory BCC high entropy alloy.

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The refractory body-centered-cubic (BCC) high-entropy alloys (HEA), which are composed of four or more refractory metal elements (Mo, Nb, Ta, W, V, Zr, and Hf), were reported to have superior yield strength at elevated temperature (above 1100K) compare with existing superalloys. Unlike simple BCC metals, in which plastic deformation is governed by screw dislocations, edge dislocations have been proven to contribute to the high-temperature yield strength in refractory BCC high-entropy alloys. However, the underlying mechanism of why edge dislocations dominate in refractory BCC high-entropy alloys remains inconclusive. Here, we investigate the fundamental properties of both edge and screw dislocations using atomistic simulations and the self-evolving atomistic kinetic Monte Carlo method. Particularly, we analyze the dislocation energies, core structure and stability, and Peierls stress in NbMoTaW BCC high-entropy alloy. The relative stability between edge and screw dislocation is examined. The relationship between dislocation core energy and local atomic environment, as well as the relationship between Peierls stress and local atomic environment, are studied. Refractory high-entropy alloys hold the potential to play a significant role in the advancement of modern industry and technology and this study provides a fundamental understanding of dislocation properties, thereby facilitating the further development and optimization of this class of materials.

High-entropy rare-earth aluminum garnet ceramic scintillators for high-energy X-ray radiography applications

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Transparent polycrystalline ceramic scintillators have been of interest as a potentially scalable, low-cost alternative to single-crystal scintillators that are widely used for radiation detection applications. In this work, we investigate Ce-doped high-entropy rare-earth aluminum garnet ceramics for applications in high-energy X-ray radiography. These multicomponent garnets are based on solid solutions of several rare-earth elements taken in equiatomic proportions. Powder precursors synthesized via an aqueous solution method are uniaxially hot-pressed into optically transparent ceramics. Powder X-ray diffraction data are collected to identify the phase formation of precursor powders and hot-pressed ceramics. Afterglow and light yield data are collected to analyze performance for high-energy X-ray radiography applications. Scanning electron microscopy imaging is employed to analyze the morphology of powders and ceramics.

Fatigue-induced deformation and thermodynamic evolution in additively manufactured lightweight high-entropy alloys

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Fatigue characteristics are very critical for the structural applications of High Entropy Alloys (HEAs). Recently, many different concepts to enhance properties have been applied and tailored to the internal structure and properties of HEAs. An optimal composition of an $Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3}$ HEA has been designed to obtain higher static strength due to the evolution of the secondary $L1_2$ nano-precipitate phase in the γ matrix. Further improvement in strength was noted with the application of the emerging technology, additive manufacturing (AM), and post-processing heat treatment because of additional strengthening contributions by the evolution of different microstructural features like dislocation structures, sub-micron dendritic segregation, internal stress, additional $L2_1$ nano-precipitate. Hence, to examine the fatigue mechanism (e.g., dislocation, twinning, or phase transformation), *in-situ* neutron diffraction and thermal-evolution measurements have been applied simultaneously under low-cycle-fatigue loading. For a better understanding of the influence of microstructural features on fatigue-induced structural transformation, the neutron diffraction patterns of SLM printed sample at different strain level were analyzed with convolutional multiple whole profile (CMWP). Temperature transitions were observed under cyclic loading. The neutron-diffraction results revealed that the firstly observed thermal transition was related to the hardening-softening dislocation structural transformation. The lattice-strain variation disclosed the load partitioning mechanism during low-cycle fatigue.

The effect of thermo-mechanical treatment on the microstructure and mechanical properties of titanium-rich medium-entropy alloy with minor nickel addition

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Due to the outstanding material properties, the high / medium-entropy alloys have attracted great attention in the past few decades. In this study, the purpose is to explore the medium-entropy alloy (MEA) with light-weight (~ 5 g/cm^3) and high mechanical properties at the same time. Therefore, the Ti65Ni3 MEA is selected to conducted with thermo-mechanical treatment to enhance its mechanical properties. The Ti65Ni3 MEA is subjected to two types of rolling process, hot rolling of 50% then cold rolling of 70% (HR50CR70) and hot rolling of 50% then cold rolling of 80% (HR50CR80), then conducted in different annealing time at 900°C for different time. By XRD analysis, a second phase of Ti-Ni intermetallic compound was revealed co-existing in the BCC structure matrix of the Ti65Ni3 MEA after thermo-mechanical treatment. Meanwhile, the second phase were identified to be Ti_2Ni intermetallic compound with nano-size dimension via TEM examination. Through EBSD observation, the MEA can be fully recrystallized after 4 hours annealing at 900°C. The results of tensile testing show that these Ti65Ni3 MEAs present superior mechanical properties with more than 1300 MPa yield strength and larger than 17% elongation for the sample after annealing at 900°C from 30 minutes to 2 hours, respectively. In summary, the light-weight Ti65Ni3 MEAs possess outstanding mechanical properties, the specific yielding strength can reach up to 260 MPa・g/cm^3.

Resonant ultrasound spectroscopy studies of high-entropy oxides.

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High entropy oxides (HEOs), also referred to as multicomponent oxides or compositionally complex oxides (CCOs), have attracted attention due to the tunability of multiple cations on a single site. Since the introduction of HEOs stabilized in the rocksalt phase, the high entropy oxide concept has been expanded to various structures, offering a path for the discovery of innovative compounds with unique structure-property relations. Here, we present a study of high entropy perovskites, spinels, pyrochlores and fluorites. We have successfully synthesized single phase samples using multiple cations on a single site, in equimolar and non-equimolar ratios. Resonant ultrasound spectroscopy was used to evaluate the elastic moduli as a function of temperature. The results obtained on these multi-component oxides are compared to those of their single-component counterparts.

Correlated Electron Metals with High Entropy as Transparent Conductors

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Novel conducting complex oxides with high electron correlation are of keen interest for UV-transparent applications, and as hosts for fundamental studies of correlated electron systems. Sr based cubic perovskite oxides, including Sr_xNbO_3 and Sr_xMoO_3, are appealing to explore due to their heavy cation solubility and tunable electrical conductivity and transparency. Utilizing a high configurational entropy formulation, the high symmetry perovskite phase can be stabilized with five cations on the perovskite B-site. This approach leverages local disorder to enhance optical transparency by suppressing interband transitions through state occupancy engineering and improve conductivity by populating t2g d-orbitals with conduction carriers. Our results show that $Sr_x(Ti,Nb,Cr,Mo,W)O_3$ thin films grown by pulsed laser deposition are stabilized as single-phase perovskite. Derivative systems with four B-cations instead of five, exhibit chemical and/or phase segregation. Contributions from individual B-cations and their interactions result in unique overall transport properties. For instance, Cr markedly influences crystallinity and electrical transport. A-site vacancies, too, influence electronic and optical properties, and structure stability. The experimental findings are supported by first principles calculations that highlight the effect of the coexistence of cations on the band structure and orbital filling.

Wire + Arc Additive Manufacturing for High Entropy Alloy

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High-entropy alloy (HEA) Al0.1CoCrFeNi, which has a face-centered cubic (FCC) structure is characterized by its exceptional mechanical attributes and excellent corrosion resistance. This study aims to examine the wire + arc additive manufacturing (WAAM) process for Al0.1CoCrFeNi HEA and determine the optimal process parameters. A two-stage experiment is conducted using pre-alloyed and extruded Al0.1CoCrFeNi wire. During the first stage, single-layer beads are deposited by controlling different parameters such as current, wire feed speed, and travel speed. In the next stage, thin-walled, multi-layer structures are deposited using two different heat input conditions (low and high) with the same energy density, based on the optimal conditions determined in the first stage. Both deposits show large columnar grains with cellular dendritic substructures and homogeneous composition. The yield strength and ultimate tensile strength are almost identical at 260 MPa and 420 MPa respectively, with exceptional ductility of 45-55%. The high heat input condition is determined to be the optimal processing condition due to improved surface quality, higher ductility, and higher deposition rate.

Screening of new Entropy Stabilized Oxides by DFT calculations and machine learning

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The Entropy Stabilized Oxides (ESO) are the MO_x oxides where the metallic site M is a mixing of at least 5 elements with a composition between 5 and 35%. At high temperatures, these materials are stabilized by configuration entropy. The ESO can have some special properties, such as a high dielectric constant and can be used as catalysts, supra-conductors and electrolytes in Li-batteries. Considering a base of 16 cationic elements with a 1% step variation in composition, this leads to 2.4 billion of possible ESO for each new structure. Our work aims to predict, through DFT calculation and machine learning, which ESO could be meta-stable and at what temperature they stabilize.

We use the Special Quasi-random Structure (SQS) to model the mixing. Then, some DFT calculations are used to calculate the formation enthalpy of oxides. Thanks to a convex hull code developed by us, we are able to determine which phases are the most stable. The entropy, considered only as configuration entropy is added with the equation : $-R \sum_i x_i \ln(x_i)$.

With the 2.4 billion of possible ESO in the NaCl structure, we use machine learning to predict the formation enthalpy instead of calculating it by DFT. Based on several hundreds of oxides, we can predict the formation enthalpy of equimolar ESO with an accuracy of a few kJ/mol.

After the NaCl structure, we will extend this method to other structures.

Effect of the chemical composition on the oxidation behavior of RHEAs within the Ta-Mo-Cr-Ti-Al system

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Refractory High Entropy Alloys (RHEAs) are regarded to be promising candidates for high temperature structural applications. Some RHEAs possess excellent oxidation resistance despite the high content of refractory metals. The superior oxidation resistance of the equiatomic alloy TaMoCrTiAl relies on the formation of a $(Cr,Ta,Ti)O_2$ scale. In this contribution, the oxidation behavior of several alloys in the Ta-Mo-Cr-Ti-Al system with different Ta, Cr, Al contents as well as a Mo- and a Ti-free alloys are investigated aiming at understanding the effect of the individual elements on the formation of a $(Cr,Ta,Ti)O_2$ layer. In order to understand the nature of the oxides formed in Ta-Mo-Cr-Ti-Al system during oxidation at 1200°C a cross-scale materials analyses is applied, including electron energy-loss spectroscopy in combination with scanning transmission electron microscopy. It is evident that the elements Cr, Ta and Ti are essential for the formation of a compact $(Cr,Ta,Ti)O_2$ scale. At concentrations below 15 at.% Cr or Ta, mixed non-protective oxides are formed. It appears that Ti has the key role in the rutile oxides. It was assumed that due to the occupation of higher-valent Ti^{4+} cations on Cr^{3+} cation lattice sites, the oxygen vacancy density in rutile $(Cr,Ta,Ti)O_2$ is reduced improving the oxidation behavior of the n-type simi-conductors $(Cr,Ta,Ti)O_2$. Al contents higher than 15 at.% seem to support the formation of $(Cr,Ta,Ti)O_2$ by gettering and nucleation effects. The removal of Mo causes enhanced internal oxidation due to the formation of new phases and additional phase boundaries.

Composition engineering and single crystal growth of high-entropy monoclinic aluminates

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Engineering of multicomponent high-entropy compounds is a modern and promising approach to designing new advanced materials achieved by increasing structural randomness and disorder. One of the concepts for designing high-entropy compositions is using a set of ions with an average ionic radius (AIR) close to or the same as the principal, substituted ion in the target composition. It was successfully applied to the synthesis of some high-entropy rare-earth oxides and garnets in a single-crystal form.

In our research we will demonstrate the implementation and verification of that approach for obtaining single-phase high-entropy rare-earth aluminates. The $RE_4Al_2O_9$ (RE = Y, Nd, Tb, Gd, Eu) individual compounds have been chosen as target compositions for modification because of their congruent melting nature. We generated all 6188 possible unique combinations of five rare-earth elements using a combinatorial algorithm and filtered a total of ~100 compositions with the AIR close to or the same as the principal ion in the $RE_4Al_2O_9$. Finally, 20 unique compositions of high-entropy rare-earth aluminates were selected for crystal growth using the micro-pulling down method. The results of structural homogeneity and elements distribution (segregation) in grown crystals as a function of their multi-component composition will be demonstrated and discussed.

Study on anti-sticking (AlBCrSi)N high entropy nitride films fabricated by reactive DC magnetron sputtering

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This study investigates the anti-sticking properties of high-entropy alloy nitride films (AlBCrSi)N prepared by reactive direct current magnetron sputtering. Through the single-factor experiment method, the effects of nitrogen/argon ratio, chamber temperature, substrate bias were analyzed, and the microstructure, crystal structure, and contact angle of the films have been investigated. When the nitrogen/argon ratio at 40%, chamber temperature at 200 ˚C, and substrate bias at −150 V, we got the optimum contact angle of the film was 83.5˚. Moreover, the optimal film displays excellent resistance to oxidation and corrosion. After heat treatment in the ambient atmosphere for 2 h at 1100 ˚C, the oxidation layer was only 187 nm. After immersion in CH_3COOH and $NaHCO_3$ solution for 1 h at 100 ˚C, the films showed excellent adhesion without corrosion or peeling off. This optimal (AlBCrSi)N films also exhibited good anti-sticking properties in actual cooking tests and showed the potential for application in non-stick cooker.

Predict the phase formation of high-entropy alloys by compositions

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The existing high-entropy alloys' phase formation prediction models are established based on empirical thermophysical parameters. The process is complicated and the accuracy of the descriptors seriously affects the final prediction results. In this article, we achieved the prediction of phase selection in high-entropy alloys by compositions. The high-entropy alloys compositions are mapped to the pseudo-two-dimensional periodic table, automatically extracting features through the convolutional neural network for classification. The results show that this method simplifies the prediction process while improving the prediction accuracy. The prediction accuracy of intermetallic compounds exceeds 89%, solid solutions and amorphous phases exceed 98%. The case study demonstrates the validity of our model. The phase composition of $Al_xFeCrNi$ (x = 0, 0.5, 1.0) high-entropy alloys are also accurately predicted and results in agreement with experiments are obtained.

Formation of an oxygen-rich ordered phase from hcp precipitates in TiZrNbHfTa bcc high-entropy alloy

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The equiatomic body-centered cubic (bcc) TiZrNbHfTa high-entropy alloy (HEA) is one of the promising candidates for high-temperature applications beyond Ni-based superalloys and other conventional refractory alloys. The bcc phase was initially thought to be stable due to the high mixing entropy. However, a hexagonal closed-packed (hcp) phase precipitates from the bcc TiZrNbHfTa upon annealing at ~800 °C [1]. Also, the role of oxygen in the phase stability of the bcc matrix or hcp precipitate remains unclear. In this context, the aim of this study is to investigate the effects of oxygen on the precipitation sequence in TiZrNbHfTa bcc HEA. Atom probe tomography and transmission electron microscopy were employed to study the structural and compositional evolution during annealing at 1200 °C. We found out that the Zr-Hf-rich hcp phase precipitates in the bcc matrix after annealing for 200 h, due to penetration of oxygen through the porous glassy tube in the Ar atmosphere. As annealing proceeds, an oxygen-rich ordered phase with a structure of Ti_3O was observed in the hcp precipitates and gradually populates with increasing sizes and volume fractions. This corresponds well with an increased Ti concentration in the hcp phase, indicating a gradual formation of the oxygen-rich ordered phase in the hcp precipitates. Our preliminary results reveal the hcp structural instability induced by oxygen upon annealing TiZrNbHfTa bcc HEA at high temperatures.

Reference:

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Achievements and Knowledge Increase of Close to 20 Years Research on High Entropy Alloys

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The denomination high entropy alloys (HEA) was published first in 2004 by Prof. J.-W. Yeh and in parallel by Prof. B. Cantor. Research picked up exponentially since then, leading to more than 1,600 papers listed in Web of Science containing "high entropy alloy" within the title in the year 2022.

Due to this number, it is impossible to discuss all research results in detail. The focus of this presentation is on mechanical strength. Four core effects, resulting from an increased configurational entropy, have been proposed: decrease in Gibb's free energy at higher temperatures, lattice distortion, sluggish (slower) diffusion and cocktail effect.

Within this presentation, there will be a clear distinction between single-phase HEA (at the designated application temperature) and two- or more-phase alloys. Due to this distinction, it will be possible to clearly separate into well-known strengthening effects. The probability of staying single-phase is decreasing with the number of elements since intermetallic phases can form, decreasing the Gibb's free energy more than the configurational entropy does. Therefore, only a handful of single-phase, equi-atomic, 5-component HEA are known by now. They can be distinguished by crystallographic structure and located in groups within the periodic table. To name some of them: fcc or Cantor alloy, fcc of precious metals, bcc or Senkov alloy, hcp or Feuerbach alloy. With respect to mechanical strengthening the only classical strengthening mechanism is solid solution strengthening.

On the other hand, the number of two- or more-phase compositionally complex alloys (CCA) is countless, and all options of precipitate hardening are available (e.g., internal stresses, Orowan bowing, locally strong increase of dislocation density, cutting of precipitates) additionally to solid solution strengthening.

Selected examples from literature and own research will be presented and discussed.

Local Lattice Distortions and Structural Instabilities in Nb-Ta-Ti-Hf High-Entropy Alloys

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Mechanical deformation studies and microstructure characterization in Nb-Ta-Ti-Hf alloys highlight high toughness, non-monotonic temperature dependencies of ductility, and competing deformation mechanisms characterized by dislocation plasticity, kink-band formation and limited deformation twinning. To derive insight into the fundamental properties underlying these competing deformation processes, first-principles computational studies of the structure and energetics of alloys with composition $Nb_xTa_{0.25}Ti_{(0.75-x)/2}Hf_{(0.75-x)/2}$ are undertaken. The intrinsic competition between bcc, hcp and ω phases, as a function of the composition x, are investigated with calculations highlighting the important role of the ratio of group IV versus group V elements. The energetic stability of the bcc phase increases with increasing x, with the energy difference between ω and bcc decreasing as the concentration of Ti and Hf increases. Further, detailed analyses of phonons and local lattice displacements, show signatures of local instabilities to the ω phase, to a degree that also increases with increasing Ti and Hf concentration, and varies with lattice configuration. Equilibrium lattice distortions in the bcc phase show strong signatures of ω-like distortions for low values of x, that are nevertheless limited in extent due to the compositional disorder. The results demonstrate an energy landscape characterized by multiple metastable minima associated with these lattice distortions. The implication of these findings for deformation processes and alloy design is discussed. This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under contract No. DE-AC02-05CH11231 as part of the Damage-Tolerance in Structural Materials (KC13) program.

Variance via configurational entropy as a control over functionality in strongly correlated materials

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Disorder is an important aspect of correlated oxide systems - it can be used to manipulate electronic phase, magnetic ordering, and to design degeneracies. Phase order classically relies on uniformity, with disorder and defects resulting in lower ordering temperatures and prevention of long-range percolation. However, in a chaotic limit, disorder can be treated as a parameter which drives the local microstates into globally ordered behaviors. We demonstrate that this seemingly counterintuitive statement is not only true but that it simplifies the prediction of predominant functional phase in high entropy oxides. As a result, we design, grow, and characterize high entropy perovskite oxide films demonstrating the utility of this predictive materials approach.

We present these theoretical and experimental results on two classes of single crystal epitaxial films. First, in exploring magnetism and charge disorder of the high entropy ABO_3 perovskite $La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$. Second, in an experimental realization of extreme *A*-site cation disorder in $(Y_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}Gd_{0.2})NiO_3$, whose parent ternary oxides each have a large range of electronic (metal to insulator transition) and structural phase transition temperatures. These results suggest cation variance, such as that accessible only in high entropy oxides, can be a critical order parameter in the design of correlated oxides, and that this parameter can more broadly provide continuous tunability to charge, electronic, structural, and magnetic orderings.

SESSION 3A

ALLOYS: Cantor Alloys

10:15 3A1: Multicomponent High-Entropy Cantor alloys
Brian Cantor

10:30 3A2: *In-situ* Mapping for Diffusion Investigations and the Associated Vacancies & Creep Activities in CoCrFeMnNi Alloys
E-Wen Huang, Wanchuck Woo, Poresh Kumar

10:45 3A3: Thermodynamic stability and solid solution hardening effects of CrMnFeCoNi based high entropy alloys
T. Keil, E. Bruder, K. Durst, D. Utt, K. Albe, S. Taheriniya, G. Wilde

11:00 3A4: Low temperature deformation of the <100> oriented single crystalline CrMnFeCoNi high-entropy alloy
G.D. Sathiaraj, R. Schaarschuch, C.-G Oertel, P. Chekhonin, R. Chulist, C. Gadelmeier, U. Glatzel, W. Skrotzki

11:15 3A5: Microscopic deformation and strengthening-toughening of FeMnCoCrNi and carbon-doped CuFeMnNi high-entropy alloys
M.Y. He, Y.F. Shen, N. Jia, P.K. Liaw

Multicomponent High-Entropy Cantor alloys

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All human advances have depended on making new materials, and all materials are alloys, i.e. mixtures of several different starting materials or components. So the history of the human race has been the continued invention of new materials by discovering new alloys. Recently a new way of doing this, by manufacturing multicomponent high-entropy alloys, has shown that the total number of possible materials is enormous, even more than the number of atoms in the galaxy, so we have lots of wonderful new materials yet to find. And multicomponent phase space contains a surprisingly large number of extended solid solutions. The first group of these which was discovered are called Cantor alloys, an enormous composition range with a single-phase fcc structure, based loosely on the original equiatomic five-component Cantor alloy CrMnFeCoNi. It turns out that there are literally trillions of different local atomic and nanoscale environments in Cantor alloys, even with only five components, and the spread of different local structures has important effects on many aspects of the material structure and properties. This talk will discuss the enormous range and complexity of different local atomic and nanoscale environments in multicomponent high-entropy Cantor alloys and describe some of their effects on the structure and properties of the materials, including short-range order, atomic diffusion, dislocation slip and grain boundaries.

In-situ Mapping for Diffusion Investigations and the Associated Vacancies & Creep Activities in CoCrFeMnNi Alloys

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Recalling our earlier *in-situ* neutron diffraction results showing creep [1], we applied Simmons–Balluffi methods, positron measurements, and *in-situ* neutron diffraction to estimate the vacancy of CoCrFeNi and CoCrFeMnNi metallic systems using Cu as a benchmark [2]. The aforementioned results delight the importance to resolve the local distributions of the elements to further examine the diffusion of the CoCrFeMnNi alloy. In this talk, we will report the latest *in-situ* synchrotron spatially-resolved mapping. The local elements are quantified to map the contour of the mixing enthalpy, entropy, and the associated descriptors. The vacancy-dependent effective free volumes in both CoCrFeNi and CoCrFeMnNi alloys are greater than those in Cu, implying the easier formation of vacancies by lattice structure relaxation of both CoCrFeNi and CoCrFeMnNi at elevated temperatures. Spatially resolved synchrotron X-ray measurements revealed different characteristics of CoCrFeNi and CoCrFeMnNi HEAs subjected to quasi-equilibrium conditions at high temperatures. Element-dependent behavior revealed by *in-situ* X-ray fluorescence (XRF) mapping reveals the dominant effect and the associated mechanisms, which will be presented in this talk.

[1] "In-situ neutron diffraction studies on high-temperature deformation behavior in a CoCrFeMnNi high entropy alloy", ***Intermetallics***, Volume 62, July 2015, Pages 1-6

[2] "Element Effects on High-Entropy Alloy Vacancy and Heterogeneous Lattice Distortion Subjected to Quasi-equilibrium Heating", ***Scientific Reports***, Volume 9, Article number: 14788 (2019)

Thermodynamic stability and solid solution hardening effects of CrMnFeCoNi based high entropy alloys

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Phase stability aspects and concentration dependent solid solution hardening has been a topic of interest in high entropy alloy (HEA) research for several years. In the present work diffusion couples [1,2] and discrete subsystems [3,4] based on the established Cantor alloy are used to investigate these aspects. A key approach is related to the continuous variation of the alloying content and the direct correlation of present phase, local hardness and composition in diffusion couples. The aim was to elucidate phase stabilizing factors and solid solution hardening mechanisms in a continuous manner and to compare experimental data to model predictions.
Discrete Ni-enriched subsystems of the CrMnFeCoNi Cantor alloy were used to investigate solid solutions hardening effect by measuring the influence of solutes on saturation grain size after severe plastic deformation, as the saturation grain size (d_s) correlates with the solid solution hardening contribution [3]. The solid solution hardening contribution was determined using the conventional Labusch model and the more recent Varvenne SSH model, which was specially developed for chemically complex alloys [2,3]. A correlation between the solid solution strengthening contribution and the saturation grain size can be found, whereby higher $\Delta\tau$ cause smaller d_s. Isochronal heat treatments were performed in order to reveal the microstructural instability i.e. grain growth and decomposition tendencies. All alloys exhibit a two stage coarsening behavior with marginal grain growth below a certain temperature [4]. Furthermore, the HEA-type alloys (Ni20 and Ni60) show decomposition tendencies at intermediate temperatures, which is not observed for the dilute solid solutions.

[1] Keil, Tom; Bruder, Enrico; Durst, Karsten; Exploring the compositional parameter space of high-entropy alloys using a diffusion couple approach, Materials & Design 176, 107816, 2019.
[2] Keil, Tom; Bruder, Enrico; Laurent-Brocq, Mathilde; Durst, Karsten; From diluted solid solutions to high entropy alloys: Saturation grain size and mechanical properties after high pressure torsion, Scripta Materialia192, 43-48, 2021.
[3] Keil, Tom; Utt, Daniel; Bruder, Enrico; Stukowski, Alexander; Albe, Karsten; Durst, Karsten; ‚Solid solution hardening in CrMnFeCoNi-based high entropy alloy systems studied by a combinatorial approach, Journal of Materials Research 36, 12, 2558-2570, 2021.
[4] Keil, Tom; Taheriniya, Shabnam; Bruder, Enrico; Wilde, Gerhard; Durst, Karsten; "Effects of solutes on thermal stability, microstructure and mechanical properties in CrMnFeCoNi based alloys after high pressure torsion", Acta Materialia 227, 117689, 2022.

Low temperature deformation of the <100> oriented single crystalline CrMnFeCoNi high-entropy alloy

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The <100> oriented single crystalline CrMnFeCoNi high-entropy alloy was deformed in tension at temperatures between 4 K and 300 K. Stress – strain curves were taken until fracture. The yield stress increases strongly with decreasing temperature. Below 10 K serrated flow is observed. The ductility is quite high. Thermal activation parameters (strain rate sensitivity and activation enthalpy) were derived from stress relaxation tests. The low temperature deformation behavior in terms of yielding, serrated flow and work-hardening of this advanced metal alloy will be demonstrated and discussed in terms of deformation mechanisms.

Microscopic deformation and strengthening-toughening of FeMnCoCrNi and carbon-doped CuFeMnNi high-entropy alloys

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High-entropy alloys have been extensively studied in recent years. However, the yield strength of face-centered-cubic HEAs is usually low, which is far from meeting the engineering requirements. It is urgent to improve the performance-cost ratio of these alloys, which will be helpful for its practical industrial application. In this study, cyclic pre-deformation was used to regulate chemical concentration fluctuations in FeMnCoCrNi HEA. Atomic-scale energy-dispersive X-ray spectroscopy mapping reveals that cyclic deformation may dynamically induce the clustering of solute atoms with a size of 1-3 nm, thus resulting in a higher concentration wave amplitude. The concentration wave promotes strong interactions between dislocations and local solute clusters, which also opens a new strategy to design high-strength alloys by adjusting the local solute element distribution. In addition, by summarizing the research progress related to the interactions between HEAs and interstitial elements from four aspects, i.e., physical basis, microstructures, mechanical properties, and deformation mechanisms, C-doped CuFeMnNi HEA (2.7 at. % C) was used as a research object. By applying simple two-dimensional (2D) forging, followed by annealing at 900 °C for different durations, the alloys with dual-level heterostructures show an excellent balance of strength and ductility, superior to most Fe-Cu alloys and Cu-HEAs. Moreover, sustainable strain hardening is achieved by sequentially triggering multistage strain-hardening mechanisms including hetero-deformation-induced hardening, precipitation hardening, and hardening jointly contributed by micro-bands, twins, and dislocation cells. These findings open a new insight for regulating phase decomposition in Fe-Cu alloy and Cu-HEAs.

SESSION 3B

OXIDES: Functional Properties

10:15 3B1: Magnetic order and phase transitions in bulk rock salt high-entropy oxides
R.P. Hermann

10:30 3B2: Controlled electronic and magnetic metastability in compositionally complex correlated oxides
T.Z. Ward, A. Mazza, V. Bisogni, M. Brahlek

10:45 3B3: The orbital degree of freedom in high entropy oxides
J.-Q. Yan, A. Kumar, M. F. Chi, A. F. May, and M. A. McGuire

11:00 3B4: Computational Investigation of Rare-earth High Entropy Oxides
M.K. Caucci, S. Almishal, S.V.G. Ayyagari, G.R. Bejger, J.P. Maria, N. Alem, I. Dabo, C.M. Rost, S.B. Sinnott

Magnetic order and phase transitions in bulk rock salt high-entropy oxides

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High entropy oxides are solid solutions stabilized by high configurational entropy and exhibit several interesting functional properties, such as colossal dielectric constants, superionic conductivity, and low thermal conductivity. We will report on neutron scattering studies of the long-range magnetic structure and dynamics in the rock salt high entropy oxides $(Mg_{0.2}X_{0.8})O$, where X is a collection of four equimolar $3d$ transition metals.[1] At low temperature, neutron diffraction reveals magnetic order with (1/2,1/2,1/2) propagation vector similar to NiO. Neutron scattering reveals that long range magnetic order survives the extreme disorder, and that short range order subsists even at room temperature. The insights from neutron scattering will be presented in the light of Mössbauer spectroscopy, and published calorimetry,[1,2] muon spin resonance,[2] and modelling results.[3]

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3. Berlijn T., Alvarez G., Parker D., Hermann R., and Fishman R., **Simulating spin waves in entropy stabilized oxides**, *Phys. Rev. Research* **3**, 033273 (2021).

Acknowledgments:

All coauthors, as well as Duncan Moseley, ORNL, Yuguang Pu, and Peng Cao, Auckland University, are gratefully acknowledged. Work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

Controlled electronic and magnetic metastability in compositionally complex correlated oxides

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Exchange and spin disorder provide access to quantum criticality, frustration, and spin dynamics, but broad tunability and a deeper understanding of strong limit disorder is lacking. A range of single crystal high entropy $AB\mathrm{O}_3$ perovskite oxide films are synthesized to probe the role of site-to-site spin and exchange interaction variances in stabilizing magnetic responses. The complexity of the system provides tunability and functionality not present in any of the ternary or half-doped quaternary parents or as a sum of parent properties. Neutron diffraction and magnetometry show that the compositionally disordered systems can paradoxically host long-range magnetic order, while manipulation of the S and J parameters through cation ratio permits continuous control of magnetic phase from antiferromagnetism (AFM), to degenerate, to ferromagnetism (FM). Tuning of the coexisting magnetic phase composition allows design of exchange bias behaviors in monolithic single crystal films, which have, until now, only been observable in AFM-FM bilayer heterojunctions or 2D layered bulk systems. The effects of hole doping on the A-site sublattice and "exchange interaction" doping the B-site sublattice will be discussed.

This work was supported by the DOE Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

The orbital degree of freedom in high entropy oxides

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In transition metal oxides, the strong coupling between spin, orbital, charge, and lattice degrees of freedom leads to various fascinating phenomena. Introducing the strong local compositional disorder provides a new approach to generating tunable magnetic properties in high entropy oxides. There are also some efforts exploring the doping effects in high entropy oxides with the motivation of looking for novel transport properties such as superconductivity, metal insulator transition, or CMR effect. However, how the extreme disorder affects the orbital degree of freedom has not been studied yet. In this talk, I will talk about our work on the orbital degree of freedom in high entropy oxides and explain how the composition disorder enhances the competition between spin orbital entanglement and long range orbital order in high entropy RVO_3.

Computational Investigation of Rare-earth High Entropy Oxides

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Rare-earth high-entropy oxides (RE-HEOs) are thought to be key to understanding ionically driven materials that improve digital performance of next-generation computing devices by overcoming the challenges associated with the miniaturization of silicon-based electronics. RE-HEOs provide an opportunity to engineer oxygen vacancy migration and distribution for precise oxide-based memristors. Memristive devices operating on ionic carriers are one of the most promising technologies, but the movement of oxygen associated with memristance, via structural defect modifications, is still poorly understood and in need of systematic studies that highlight structure-property relationships.

The focus of this work is to quantify material structure-property relationships to aid in the synthesis of a new class of crystals with high configurational entropy that have the potential to expand the limits of oxygen conductivity. To accomplish this, we develop a computational framework for studying and engineering RE-HEOs. We address the level of theory required to properly model defect chemistry, structural preferences, and local distortions within these compositionally complex materials using Density Functional Theory (DFT), DFT+Hubbard U correction term, and spin orbit coupling. The unique possibilities to optimize the ionic conductivity of RE-HEOs are investigated by examining the influences of individual elements on the electrochemical characteristics at an atomic level through first principles methods. By integrating theory, characterization, experiment, and computation, our team aims to demonstrate that RE-HEOs present high tunabilty, unprecedented property enhancement, and an approach to break the limits of carrier density and mobility.

Finding new materials where materials science, materials physics and materials chemistry meet

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About a hundred years ago, the appearance of quantum mechanics, as a new way to understand the world, revolutionized science and put technologies on a path that has eventually yielded many of the products that shape our modern lives. People like me are now happily faced with helping to embody what is frequently referred to as a second quantum revolution, this one both theoretically and experimentally based. Based on my personal belief that "everything on earth has to be made of something", my research has been to fund new quantum materials at the border where materials science, materials physics and materials chemistry meet. Our work is constantly evolving, and in this talk I'll present as examples the results of some of our current efforts in that area, concentrating on materials for quantum computing, superconductors, and magnetic materials. I am particularly grateful for the long-term support of my research by the US Department of Energy and the Gordon and Betty Moore Foundation.

Additive Manufacturing of High Entropy Alloys

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Metal additive manufacturing (MAM) offers unprecedented advantages in the fabrication of metals and alloys with complex geometry and unique microstructural features with hierarchical heterogeneity. The MAM process also induces a unique cell structure with high dislocation density and solute segregation at cell boundaries. Here, we propose an innovative utilization of a unique dislocation network to achieve superior mechanical properties through metastability engineering of high entropy alloy (HEA) and ferrous-medium entropy alloy (FeMEA). While the high dislocation density at cell boundaries contributes to the improvement of yield strength as additional barriers to dislocation movement, the solute segregation at cell boundaries can beneficially control the phase instability of the matrix in materials produced by MAM. Our results demonstrate that solute segregation at cell boundaries decreases the face-centered cubic phase stability in the matrix and activates the transition of the deformation mechanism from slip to metastable plasticity (i.e., transformation-induced plasticity). Furthermore, the high density of dislocation at cell boundaries also has an effect on not only yield strength enhancement but also on controlling kinetics of metastable plasticity, and it beneficially contributes to obtaining high ductility of the MAM-processed FeMEA. This work presents a new microstructural design strategy for beneficially customizing the material performance of high-quality products based on MAM-driven metastability engineering of an alloy with specific chemical composition.

High entropy oxides as new playground for functional materials development

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Since their first report by Rost *et al.* in 2015, Entropy Stabilized Oxides and High Entropy Oxides (HEOx) have become a hot topic in the field of functional oxides, with many papers devoted to the synthesis of new compositions and structures and to the study of various functional properties. To date, many compositions of HEOx have been obtained with different crystal structures. Among them, several families of compounds have been shown to be entropy stabilized, with a transition at high temperature from a multiphase state to a single phase simple solid solution that can be frozen at room temperature by quenching. Being they entropy-stabilized or not, many of these HEOx exhibit promising functional properties, among other: superionic Li conductivity or fast ionic conductivity, colossal dielectric constants, photocatalytic properties, unexpected magnetic ordering, low thermal conductivity values, …

One of the main advantages of these materials is their huge chemical versatility, which enables a very fine tuning of their functional properties and makes the number of possible compositions virtually infinite.

In this talk, I will give an overview of some promising results obtained in the past few years and discuss the perspectives these materials open for the functional oxides' community.

SESSION 4A

ALLOYS: Short range order

10:30 **4A1:** Short-Range Order on Thermodynamic Properties of AlxCoCrFeNi High-Entropy Alloys
Md Abdullah Al Hasan, Seungha Shin, Peter K. Liaw

10:45 **4A2:** Engineering Short Range Order in High Entropy Materials
Swarnava Ghosh, Gautam Anand, Markus Eisenbach

11:00 **4A3:** Tackling kinetics towards short-range ordering in concentrated alloys using machine learning based kinetic Monte Carlo
Anus Manzoor, Yongfeng Zhang

11:15 **4A4:** Deformation-defect Characterization in Short-Range Ordered CrCoNi using Fast Electron Detectors
K.J. Yin, H.W. Hsiao, R. Feng, P.K. Liaw, J.M. Zuo

11:30 **4A5:** Local lattice distortions and chemical short-range ordering in fcc, hcp and bcc compositionally complex alloys by X-ray absorption spectroscopy
A. Fantin, S. Kasatikov, G.O. Lepore, A.M. Manzoni

11:45 **4A6:** On the mechanically induced short-range order in multiple principal element alloys
Won-Seok Ko, Seok Su Sohn, Zhiming Li, Elena Pereloma, Jung-Gi Kim, Yoon-Uk Heo, Hyoung Seop Kim, Jae Bok Seol

Short-Range Order on Thermodynamic Properties of $Al_xCoCrFeNi$ High-Entropy Alloys

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Short-range order (SRO) in high-entropy alloys (HEAs) has been observed both computationally and experimentally in recent studies. Despite their significant influence on the physical properties of the HEAs reported, no comprehensive work on the relationship between SRO and tuning of the thermodynamic properties of HEA has been performed. In this research, to identify the SRO-property relationship, the Warren-Cowley (WC) parameters, which quantify the degree of SRO, and thermodynamic properties in $Al_xCoCrFeNi$ HEAs were investigated using the molecular dynamics (MD) simulations, density functional theory (DFT) calculations, and modern data analytics, such as correlation analysis and machine learning (ML). Two different Al contents (x_{Al}) were used to examine different phases of $Al_xCoCrFeNi$ HEAs, i.e., $x_{Al} = 0.3$ and 1.0 for face-centered cubic (FCC) and body-centered cubic (BCC) structures, respectively. Dominant SRO of Co-Ni and Al-Co were found in the case of FCC HEAs, whereas Al-Cr and Cr-Fe pairs were observed the most in the BCC HEAs. The dominance of these element pairs in the FCC and BCC HEA were also corroborated by their valence electron concentration analysis. Lattice thermal conductivity, coefficient of thermal expansion, and bulk modulus were found higher at the lower WC parameters (higher SRO) of these element pairs. ML models trained using WC parameters of higher SRO pairs demonstrate better performance for prediction of the thermodynamic properties, compared to the models using all element pairs. This research contributes to understanding the SRO-properties relationship in HEAs and thus to design of HEAs with desired properties by tuning the structure.

Engineering Short Range Order in High Entropy Materials

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Chemical short-range order (CSRO) in crystalline materials significantly influence its properties. The role of short-range ordering is particularly important in High Entropy materials. In this talk I will first discuss a recently developed scalar metric for short range order in High Entropy materials. This new metric is defined in terms of like and unlike bonds in multi-component systems. Next, I will talk about an open-source framework OPERA (Order Parameter Engineering in Random Systems) that can generate the configurations of a given multi-component alloy system with prescribed chemical short-range order without explicit energy calculations through combinatorial sampling. We demonstrate this framework on FCC-CoCrNi, BCC-MoNbTaW and (CoCuMgNiZn)O). Finally, I will talk about applying this framework in studying crystalline defects in high entropy materials.

Tackling kinetics towards short-range ordering in concentrated alloys using machine learning based kinetic Monte Carlo

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The existence of local chemical ordering such as short-range ordering (SRO) in complex concentrated alloys (CCAs) has been widely reported. However, predicting the kinetics towards SRO has remained a challenge because it requires an accurate description of atomic jumps considering the chemical complexity in a time scale comparable to the laboratory scale. This talk addresses this challenge by presenting a machine learning (ML) based kinetic Monte Carlo (KMC) method. The ML model is trained using atomistic data from either first-principles based density functional theory (DFT) or empirical potential based molecular dynamics (MD) calculations, which control the accuracy, and predicts the environment dependent vacancy migration barrier. With training data from both the random and ordered states, ML based KMC simulations can successfully reproduce the chemical ordering from metropolis Monte Carlo directly driven by DFT or MD, indicating the capability of the method for predicting the ordering kinetics. The presence of SRO can result in localized diffusion and heterogeneous distribution of thermal vacancies. Furthermore, vacancy is found to maintain a local composition during diffusion that is different from the nominal composition. The ML-KMC framework proposed in this work, can be used as a tool to study microstructure evolution and diffusion kinetics in CCAs on a large time scale with atomic scale accuracy.

Deformation-defect Characterization in Short-Range Ordered CrCoNi using Fast Electron Detectors

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CrCoNi, a Medium-Entropy Alloy (MEA) with a single-phase face-centered-cubic (FCC) structure, has been extensively studied by researchers since it has shown great advantages of high strength and great ductility[1], as well as the short-range ordering (SRO) effects[2,3]. The exceptional mechanical properties of CrCoNi have been attributed to novel deformation mechanisms such as the formation of stacking faults (SFs), nanotwins (NTs), shear bands, etc[4,5]. Crystalline defects in general are imaged by electron microscopy. However, short-range order effects on crystal deformation have not been fully understood.

Here, we introduce a novel defect imaging method based on the cepstral analysis of electron diffuse scattering using an Electron Microscope Pixel Array Detector (EMPAD) detector. This direct electron detector has a high dynamic range and fast readout, providing large diffraction datasets for high spatial resolution charaterization.[6] By comparing regional difference cepstrums (*dCp*)[7] with real-space images from STEM, the local crystal defects of SFs and NTs are imaged and analyzed in deformed CrCoNi samples. By far, we have successfully observed lattice stacking and their corresponding diffraction and cepstral patterns. We have also identified SRO in these samples. These inspiring results open the possibility of the auto characterization of the presence and the category of SRO and their interactions with dislocations, leading to the formation of planar defects. This talk will summarize our progress so far on the novel deformation mechanisms in CrCoNi.[8]

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8. Work supported by DMR-2226495) from the Metals and Metallic Nanostructures Program (MMN) within the Division of Materials Research.

Local lattice distortions and chemical short-range ordering in *fcc*, *hcp* and *bcc* compositionally complex alloys by X-ray absorption spectroscopy

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This work presents an X-ray absorption spectroscopy study on a set of compositionally complex alloys with different crystal structures, *fcc*, *hcp* and *bcc*, in their single-phase region, focusing mainly on the local surroundings of each alloying element.

The presented systems will be the $Al_8Cr_{17}Co_{17}Cu_8Fe_{17}Ni_{33}$ [1-3] (*fcc*-based), the $Al_{15}Sc_{10}Ti_{25}Zr_{25}Hf_{25}$ (*hcp*-based) and the MoNbTaW [4] (*bcc*-based).

The comparison of first shells bond lengths up to 5 Å was obtained by the analysis of extended X-ray absorption fine structure (EXAFS) data for each alloying element. EXAFS experiments were conducted at the Paul Scherrer Institute (PHOENIX-X07MA/B beamline) and at the European Synchrotron Radiation Facility (LISA-BM08 beamline).

Results indicate that slightly distorted arrangements propagate in all structures but at different effective lengths within the unit cell. Chemical short-range order will be also addressed.

[1] Fantin *et al.*, Acta Materialia 193 (2020), 329-337.
[2] Kasatikov *et al.*, Journal Alloys and Compounds 857 (2021), 157597.
[3] Fantin *et al.*, 2022, Materials Chemistry and Physics 276 (2022), 125432.
[4] Fantin *et al.*, *in preparation*.

On the mechanically induced short-range order in multiple principal element alloys

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We report two different SRO types in an $Fe_{40}Mn_{40}Cr_{10}Co_{10}$ (at%) high-entropy alloy: (i) as widely known, thermally activated or local chemical SRO that emerges with specific heat-treatments; (ii) displacive or local topological SRO that emanates from tensile deformation at liquid-N2 temperature. The degree/extent of the former one is tailored by altering annealing temperatures or cooling methods, while by tuning loading rates for the latter one. In particular, our scanning and high-resolution transmission electron microscopy together with diffraction pattern analysis revealed not only the microstructural features responsible for the strain-induced SRO but also the dependence of the ordering degree/extent on the applied strain rates. These findings were consistently supported by our molecular dynamics simulations and associated diffraction patterns, i.e., mechanically derived SRO generated the diffuse discs at the ½{311} locations in the reciprocal-space electron diffraction patterns along the specific zone axis. Further, the mechanical response and multi-length-scale characterization pointed to the negligible impact of strain-induced SRO on yield strength, mechanical twinning, and martensitic transformation. Owing to these features, we regarded the localized SRO as mechanically derived SRO rather than diffusion-mediated chemical SRO that would be destroyed by planar dislocations during deformation.

SESSION 4B

OXIDES: advanced characterization

10:30 4B1: Harnessing Nanoscale Heterogeneity in Compositionally Complex Oxides
Katharine Page, Xin Wang, Sreya Paladugu, Peter Metz, Bo Jiang

10:45 4B2: Probing the Local Atomic Structure of High-Entropy Oxides
Bo Jiang, Katharine Page

11:00 4B3: Heavy-Ion Irradiation of High Entropy Oxides
W.J. Weber, C. Kinsler-Fedon, L. Nuckols, A.H. Mir, A.K. Gupta, R. Sachan, B. Musicó, C. Nelson, D. Mandrus, Y. Zhang, V. Keppens

11:15 4B4: Mapping the structure of epitaxial perovskite oxide films using X-ray diffraction
M. Brahlek, A.R. Mazza, Krishna Chaitanya Pitike, Elizabeth Skoropata1, Jason Lapano, Gyula Eres, Valentino R. Cooper, T.Z. Ward

11:30 4B5: High Entropy Oxides: Measurement and Considerations
Brianna Musicó, Veerle Keppens, Michael Koehler, Katharine Page

Harnessing Nanoscale Heterogeneity in Compositionally Complex Oxides

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Next generation materials of nearly every kind rely on chemical, electronic, and/or magnetic heterogeneity for creating, harnessing, and controlling functionality. High entropy oxides (HEOs), materials exhibiting a single-phase crystal structure containing five or more different cations on single crystallographic lattice sites, have attracted great interest in diverse fields because of their inherent opportunities to tailor and combine materials functionalities. The control of local order/disorder in the class is by extension a grand challenge towards realizing their vast potential. We present detailed investigation of the cation site preferences, chemical-short-range order, and magnetic and catalytic properties achieved in specific rare-earth and transition metal-based pyrochlore, fluorite, and spinel HEO families through compositional tuning and variation in synthesis/processing conditions. A combination of local to long-range electron, x-ray and neutron scattering probes are employed to investigate their complex configurational diversity and associated structure-property trends. Experimentally derived models are supported by Density Functional Theory calculations and Metropolis Monte Carlo simulations. This work hints at the exquisite level of detail that may be required in computational and experimental approaches to guide structure-property tuning in emerging HEO materials. Current challenges and future opportunities in this arena will be discussed.

Probing the Local Atomic Structure of High-Entropy Oxides

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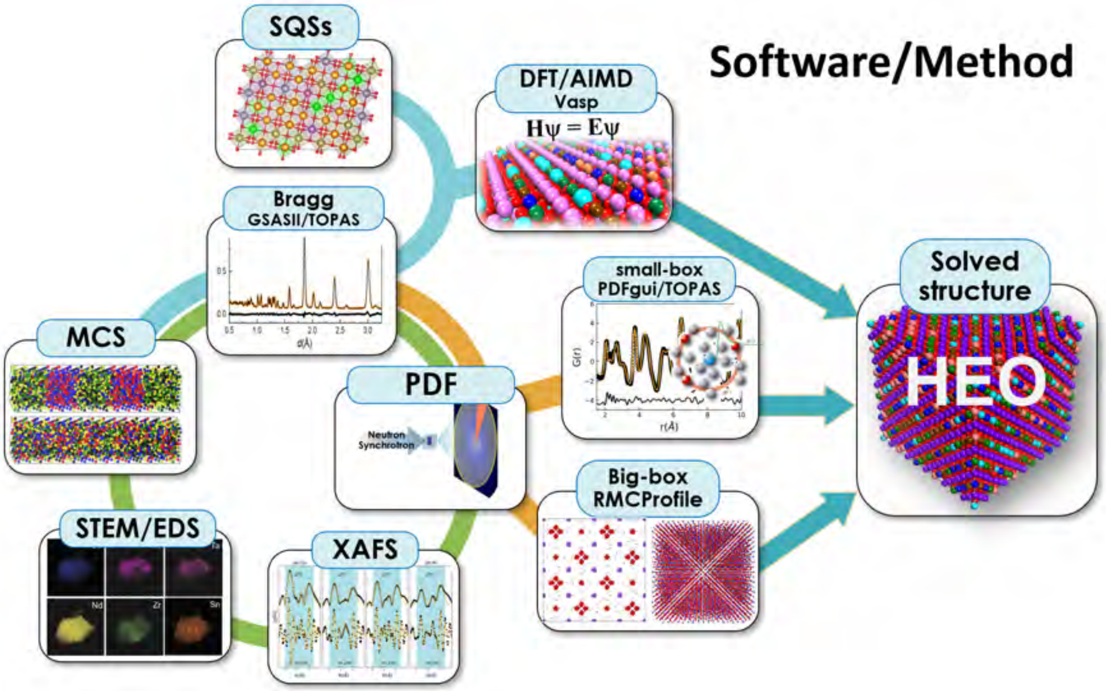
High entropy oxides (HEOs) have attracted great interest in diverse fields because of their inherent opportunities to tailor and combine materials functionalities. The control of local order/disorder in the class is by extension a grand challenge towards realizing their vast potential. *Pair distribution functions* (PDF) obtained from total scattering (high energy synchrotron X-ray and Neutron scattering) can reveal both the local and intermediate range structure of crystalline and disordered materials. As we all know that conventional reciprocal space diffraction only probes the average long-range structure of the Bragg planes, and information from *EXAFS* and *XANES* is limited to no more than third coordination shell, PDF can reveal both local distortions and measure the *structural coherence* up to several tens of Ångstrøm. A combination of multiple approaches and softwares using *STEM-EDS*, *PDFgui* (graphical interface built on the PDFfit2 engine*), TOPAS v6* (combined reciprocal and real space neutron PDF data) and *RMCProfile* (Reverse Monte Carlo software) were performed throughout this work. The experimental total scattering PDF activity will be closely supported by *density functional theory* (DFT) calculations and further *Metropolis Monte Carlo simulations* (MCS) simulations. This work hints at the exquisite level of detail that may be needed in computational and experimental data analysis to guide structure-property tuning in emerging HEO materials.



Heavy-Ion Irradiation of High Entropy Oxides

[1]*Weber, W.J., [1]Kinsler-Fedon, C., [1]Nuckols, L., [2]Mir, A.H., [3]Gupta, A.K., [3]Sachan, R., [1]Musicó, B., [4]Nelson, C., [1]Mandrus, D., [5]Zhang, Y., & [1]Keppens, V.

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High-entropy oxides have recently gained recognition for their low thermal conductivity and tunable mechanical capabilities, but little is known about their response to ion irradiation. In this work, the heavy-ion irradiation response of high-entropy oxides (HEO) with the pyrochlore and perovskite structures have been investigated. The damage accumulation behavior at 300 K due to 4 MeV Au ion irradiation of a <100>-oriented HEO titanate pyrochlore single crystal has been investigated by Rutherford backscattering spectrometry in channeling geometry, and the results are similar to single component rare-earth titanate pyrochlores. Transmission electron microscopy with in situ irradiation using 600 keV Xe ions has been employed to determine the temperature dependence of amorphization in the same HEO pyrochlore composition, and the results indicate a two-stage dependence of amorphization on temperature and a critical temperature of 800 K that is lower than that observed for single component rare-earth titanate pyrochlores. In addition, in situ TEM studies from this work and others suggest an effect of ionization-induced annealing on the amorphization dose. Raman spectroscopy of another single-crystal HEO pyrochlore composition irradiated with 23 MeV Ni ions has revealed an order of magnitude increase in amorphization dose due to ionization-induced annealing. In a study of polycrystalline HEO perovskite structures irradiated with 774 MeV Xe ions, transmission electron microscopy has revealed the formation of continuous ion tracks.

Mapping the structure of epitaxial perovskite oxide films using X-ray diffraction

Brahlek, M. [*1] **Mazza, A.R.,**[2] **Krishna Chaitanya Pitike**[1]**, Elizabeth Skoropata**[1]**,**
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Designing and understanding functional electronic and magnetic properties in perovskite oxides requires controlling and tuning the underlying crystal lattice. Here we report the structure, including oxygen and cation positions, of a single-crystal, entropy stabilized perovskite oxide film of La(Cr0.2Mn0.2Fe0.2Co0.2Ni0.2)O3 grown on SrTiO3 (001). The parent materials range from orthorhombic (LaCrO3, LaMnO3 and LaFeO3) to rhombohedral (LaCoO3 and LaNiO3), and first principles calculations indicate that these structural motifs are nearly degenerate in energy and should be highly distorted site-to-site. Despite this extraordinary local configurational disorder on the B-site sublattice, we find a structure with unexpected macroscopic crystalline homogeneity with a clear orthorhombic unit cell. Furthermore, quantification of the atom positions within the unit cell reveal that the orthorhombic distortions are small, close to LaCrO3, which may be driven by a combination of disorder averaging and the average ionic radii. This is the first step towards understanding the rules for designing new crystal motifs and tuning functional properties through controlled configurational complexity.

This work was supported by the U.S. Department of Energy Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

High Entropy Oxides: Measurement and Considerations

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High entropy and multi-component materials present opportunities for a host of applications. Inherent to materials design and development is characterization, often starting at the bulk scale. With these materials, their novelty, and the host of different cations across the periodic table that can be involved, comes consideration and limitations within many of the typical measurement techniques. This presentation will discuss some of the observations taken through multi-year, multi-material, and multi-synthesis method work in this field.

On the influence of stacking fault energy on mechanical properties in CrMnFeCoNi high-entropy alloys with different Cr/Ni ratios

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In the present work, we investigate the tensile behavior and deformation mechanisms at 293 K and 77 K of single-phase face-centered-cubic (FCC) $Cr_xMn_{20}Fe_{20}Co_{20}Ni_{40-x}$ ($0 \leq x \leq 26$ at.%) high-entropy alloys (HEAs) with different grain sizes ($6 \leq d \leq 283$ µm). An interesting feature of these alloys is that their stacking fault energy (SFE) strongly decreases with increasing x whereas other characteristics affecting strength (solute misfit volumes and elastic moduli) remain approximately constant [1]. Therefore, these alloys can be considered as model alloys to study the effect of SFE on mechanical properties and deformation mechanisms of FCC HEAs. The intrinsic lattice strength is found to be composition independent at 293 K but it strongly increases with increasing Cr/Ni ratio and thus decreasing SFE at 77 K. In contrast, grain boundary strengthening is nearly independent of SFE, composition, and temperature. Regarding the deformation mechanisms, nanotwinning occurs at 293 K when $x \geq 20$ at.% (SFE ≤ 35 mJ/m^2) and in all alloys at 77 K. In addition to nanotwinning, an FCC-to-HCP (hexagonal close-packed) martensitic transformation was observed at 77 K in the $Cr_{26}Mn_{20}Fe_{20}Co_{20}Ni_{14}$ HEA. This transformation induces early rupture in the alloy with the coarsest grain size.

[1] C. Wagner, G. Laplanche, *Effects of stacking fault energy and temperature on grain boundary strengthening, intrinsic lattice strength and deformation mechanisms in CrMnFeCoNi high-entropy alloys with different Cr/Ni ratios*, Acta Materialia 244 (2023) 118541

Phase stability and short-range ordering of entropy stabilized oxides with the α-PbO_2 structure

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Chemical short-range ordering (SRO) is challenging to characterize but also potentially responsible for superior functional properties in high entropy materials. The entropy-stabilized two-component oxide (Ti, Zr)O_2 in the α-PbO_2 structure is used here as a model system as it displays a well-characterized SRO in the form of slabs of Ti and Zr along the b direction, the extent of which is influenced by simple heat treatments. We recently reported on the phase stability of the isostructural four-component oxide (Ti, Zr, Hf, Sn)O_2. Here, we compare the SRO in two-component (Ti, Zr)O_2 with that of the four-component (Ti, Zr, Hf, Sn)O_2 by combining experimental and computational techniques.

Pair distribution function (PDF) measurements reveal a dramatic difference between quenched and slow-cooled samples for (Ti, Zr)O_2, (Ti, Zr, Hf, Sn)O_2 meanwhile shows no visible changes in the PDFs based on heat treatments. A computational approach combining cluster expansions, density functional theory, and Metropolis Monte Carlo simulations is employed to explain the experimental observations. The calculations reproduce the type of SRO and the order-disorder phase transition temperature for (Ti, Zr)O_2. Similar calculations are carried out for (Ti, Zr, Hf, Sn)O_2 which differ in two crucial ways: (i) the phase transition temperature is lowered by hundreds of degrees ensuring that the cations are frozen in place regardless of cooling rate, and (ii) the ideal configurational entropy is obtained at synthesis temperature, whereas (Ti, Zr)O_2 is never fully disordered indicating that short-ranged correlations may persist even in the quenched sample.

SESSION 4C

ALLOYS: Environmental Interactions

2:00 **4C1:** Studies on oxidation properties of equiatomic YGdTbDyHo high entropy alloy at elevated temperatures
N. Yadzhak, L. Rosenkranz, F. Schleifer, U. Glatzel

2:15 **4C2:** High-temperature corrosion of the high- and medium-entropy alloys CrMnFeCoNi and CrCoNi exposed to a multi-oxidant atmosphere H2O-O2-SO2
W. Mohring, S. Karafiludis, A.M. Manzoni, G. Laplanche, M. Schneider, C. Stephan-Scherb

2:30 **4C3:** Surface hardening of TiZrNbHfTa through single-step and two-step thermal oxidation
D. Dickes, B. Öztürk, F. Baier, P. Berger, Y. Zhao, E.P. George, R. Völkl, U. Glatzel

2:45 **4C4:** Oxidation Behavior of the $AlMo_{0.5}NbTa_{0.5}TiZr$ Chemically Complex Alloy
P. Suárez Ocaño, A.M. Manzoni, J. Lehmusto, L. Agudo Jácome

3:00 **4C5:** Passivation of TiHfZrNbx high-entropy alloys in Hanks' solution
A. Tanji, X. Fan, R. Sakidja, P.K. Liaw, H. Hermawan

Studies on oxidation properties of equiatomic YGdTbDyHo high entropy alloy at elevated temperatures

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Despite being discovered almost a decade ago, the YGdTbDyHo high entropy alloy (HEA) remains an appealing object for investigation. Possessing a hexagonal closed-packed structure that is found only in a limited number of HEA and consisting of rare earth elements, the alloy is the object of fundamental research in this study.

The present study investigates oxidation behavior of equiatomic YGdTbDyHo HEA at elevated temperatures. The alloy was produced from pure elements by arc melting. Due to the high susceptibility to oxidation already in the laboratory environment, the test samples were prepared using a water-free metallographic approach with subsequent ion gun milling in order to eliminate the oxides that emerge at the surface during the sample preparation process. To investigate the oxidation behavior, the studied alloy was heat-treated at elevated temperatures. Both the surface and the cross-section of the heat-treated specimens were examined using scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray diffraction. The obtained results have confirmed high susceptibility to oxidation of the studied alloy, including a temperature-dependent oxidation effect along grain boundaries.

High-temperature corrosion of the high- and medium-entropy alloys CrMnFeCoNi and CrCoNi exposed to a multi-oxidant atmosphere H_2O-O_2-SO_2

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The high-temperature corrosion behaviors of the equimolar CrCoNi medium- and CrMnFeCoNi high-entropy alloy were studied in a gas atmosphere consisting of a volumetric mixture of 10% H_2O, 2% O_2, 0.5% SO_2, and 87.5% Ar at 800 °C for up to 96 h. Both alloys were initially single-phase *fcc* structured and showed a mean grain size of ~50 µm and a homogeneous chemical composition. The oxide layer thickness of the Cantor alloy CrMnFeCoNi increased linearly with exposure time while it remained constant at ~1 µm for CrCoNi. A Cr_2O_3 layer and minor amounts of $(Co,Ni)Cr_2O_4$ developed on CrCoNi while three layers were detected on the Cantor alloy. These layers were a thin and continuous chromium rich oxide layer at the oxide/alloy interface, a dense $(Mn,Cr)_3O_4$ layer in the center and a thick and porous layer of Mn_3O_4 and $MnSO_4$ at the gas/oxide interface. Additionally, a few metal sulfides were observed in the CrMnFeCoNi matrix. These results were found to be in reasonable agreement with thermodynamic calculations.

Surface hardening of TiZrNbHfTa through single-step and two-step thermal oxidation

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Because of its ductility, low Young's modulus, high compressive yield strength, good fatigue behavior, and biocompatibility, TiZrNbHfTa is in discussion as implant material. To improve the wear resistance, as required for use in artificial joints, we deploy single-step and two-step thermal oxidation as a surface hardening method.

Single-step thermal oxidation at 600 °C of cold-rolled, single-phase bcc, nanocrystalline TiZrNbHfTa leads to the formation of an adherent, µm-sized, vitreous oxide layer. Underneath this oxide layer, EPMA, XRD, XPS, and NRA-analysis indicate, that the bcc TiZrNbHfTa completely decomposes into another bcc and a hcp-phase during thermal oxidation. Selective internal oxidation of hafnium and zirconium occurs upon oxygen inward diffusion, raising the surface hardness by four times to 1522±64 HV 0.5. However, equal thermal oxidation treatment of coarser grained TiZrNbHfTa leads to catastrophic oxidation.

The successful achievement of an adherent oxide layer with internal oxides in an oxygen diffusion zone underneath in case of nanocrystalline TiZrNbHfTa allows to add an additional heat treatment step at 1200 °C under vacuum in order to reduce the internal oxides formed during the single-step process. According to SEM, EDS, XRD, XPS, and APT-analysis, µm-sized oxygen-rich hcp precipitates in a bcc matrix form in the subsurface region. With this precipitates in the subsurface region, a gradual Martens-microhardness decrease from 5 GPa near the surface to 4.2 GPa in the substrate can be achieved. In contrast to the single-step process, the substrate itself is again single-phase bcc due to the heat treatment at 1200 °C.

Oxidation Behavior of the $AlMo_{0.5}NbTa_{0.5}TiZr$ Chemically Complex Alloy

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The chemically complex alloys that contain mostly refractory elements (rCCAs), may be highly resistant to heat and load, which makes them attractive candidates for use at extremely high temperatures associated with technological applications such as aeroengine turbines. However, the oxidation behavior remains an emerging field within the CCA community. The fully heat treated AlMo0.5NbTa0.5TiZr rCCA contains a dual-phase microstructure that resembles the γ/ γ' pattern of the well-known Ni-base superalloys, however with a continuous Al-Zr-Ti-rich B2 ordered matrix embedding Mo-Nb-Ta-rach bcc precipitates. [1] The question thus arises what is the oxidation behavior of this rCCA alloy? In this study, this question is addressed via *in situ* and *ex situ* X-ray diffraction (XRD) in dry and humid air in the 800–1000 °C regime. Electron microscopic investigations complement the findings.

In situ synchrotron experiments were carried out at the KMC2 beamline of the Helmholtz Zentrum Berlin (HZB), with a wavelength of 1.5418 Å at 800 and 950 °C under dry and humid (≈ 40% rH, laboratory air) air for 12 h. Scanning and transmission electron microscopy was performed before and after exposure to spatially resolve the scale development *ex situ.* In general, 12 h exposure led to an oxide scale which internal oxidation reaches several tens of microns, and which is dominated by Zr-, Ti- and Mo-containing oxides although aluminum oxide was also always present. Main differences are observed between temperatures, while the humidity played a lesser role.

[1] Senkov, O. *et al.*, Development of a refractory high entropy superalloy, Entropy 18 (2016) 1–13.

Passivation of $TiHfZrNb_x$ high-entropy alloys in Hanks' solution

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The present work was motivated by the quest of developing advanced materials for high-performance medical implants, like the small-diameter coronary and brain stents that require a high radial strength with thinner strut. A stent with thinner strut ensures a lower restenosis rate, causes less disturbance to blood dynamics, and thus, results in favorable clinical outcomes. Having very high strength and ductility, TiHfZrNb high-entropy alloys could be the potential materials for making the needed small-diameter stents once its corrosion resistance in physiological solution is fully assessed and understood. The present work confirms the high corrosion resistance of $TiHfZrNb_x$ high-entropy alloys in Hanks' solution at 37°C, and provides a detailed description of niobium influence on the mechanisms of the dissolution and passivation of the formed passive film. We used a combined approach of electrochemical and surface-characterization techniques, employing the static/dynamic/cyclic polarizations, impedance spectroscopy, XPS, AFM, and SEM. The effect of niobium on the oxide-film formation process and passivation mechanism was determined in detail based on the Mott-Schottky analysis, and the models of high-field ion conduction, and anodic dissolution and film growth. This approach allowed us to confirm the higher passive-film impedance of the $TiHfZrNb_x$ alloys, relative to cp-Ti and Ti-6Al-4V, and the enhancement of microstructural homogeneity and passivity of this film due to the niobium addition.

SESSION 4D

ALLOYS: Mechanical properties – theory and modeling

2:00 **4D1:** In situ micromechanical modeling/experimental studies of high entropy alloys with enhanced properties at high temperatures
Yanfei Gao

2:15 **4D2:** Modeling and Comparison of Temperature-Dependent Strength Behavior of High-Entropy Alloys and Superalloys
Baldur Steingrimsson, Xuesong Fan, Benjamin Adam, Peter Liaw

2:30 **4D3:** Origin of TRIP and TWIP behaviour in nanocrystalline FCC concentrated alloys: Insights from atomistic computer simulations
Shankha Nag, Sriram Anand, Karsten Albe

In situ micromechanical modeling/experimental studies of high entropy alloys with enhanced properties at high temperatures

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Conventional methodologies in enhancing creep resistance in advanced structural materials also operate in high entropy alloys, but with more complex microstructural evolution due to the possibility of many intermetallic or precipitate phases. Here we investigate several representative high entropy alloys by both neutron diffraction measurements and micromechanical modeling, which provide indispensable information on the load transferring mechanism and thus shed lights on future alloy design strategy. It is found that among all subset materials of Cantor alloy, NiCoCr has the highest creep resistance, which is nevertheless surpassed by an Al-based HEA by at least one order of magnitude in the steady state strain rate. The lattice strain "splitting" behavior is of the critical importance in understanding the underlying deformation mechanism. The lifetime data at elevated temperatures suggest that most of these materials perform on par with typical ferritic and austenitic superalloys, despite their enhanced creep resistance. This observation is understood by the formation of precipitate free zone near the grain boundaries which relax the constraint effects on the cavity growth process.

Modeling and Comparison of Temperature-Dependent Strength Behavior of High-Entropy Alloys and Superalloys

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In the pursuit of developing high-temperature alloys with improved properties for meeting the performance requirements of next-generation energy and aerospace demands, integrated computational materials engineering (ICME), including machine learning (ML), will play an important role. ML has become a powerful tool for the accurate prediction of the yield strength (YS) or ultimate strength (US) of multi-principal-element systems as well as of superalloys. In the present work, an ML approach is presented, capable of predicting the temperature-dependent YS or US of high-entropy alloys (HEAs), of medium-entropy alloys (MEAs), as well as of superalloys, utilizing a bilinear log model. Importantly, the bilinear log model introduces the parameter break temperature, T_{break}, which serves as an upper boundary for operating conditions, ensuring acceptable mechanical performance. Once above T_{break}, phase transformations may start taking place, and the alloys may begin losing structural integrity. For reliable operations, the operating temperature of a structural component, such as a turbine blade, made from refractory alloys, may need to stay below T_{break} (not accounting for coatings). Hence, T_{break} can guide the design of MEAs or HEAs with attractive high-temperature properties. As opposed to assuming black-box structures, the bilinear log model is based on the underlying physics, incorporated in the form of a priori information. So, in contrast to conventional black-box modeling approaches, our model is based on the underlying fundamental physics, built directly into the model. We, furthermore, present a technique of unconstrained global optimization, one enabling the concurrent optimization of model parameters over the low-temperature and high-temperature regimes, showing that the break temperature is consistent across the YS and US for a variety of HEA compositions. In the current work, we also present a comprehensive and up-to-date overview of a bilinear log model for predicting temperature-dependent YS of medium-entropy or high-entropy alloys (MEAs or HEAs). Comparison between YS of MEAs/HEAs and those of Nickel-based superalloys reveals superior strength properties of selected refractory HEAs. The results extend the previous work on HEAs and offer further support for the bilinear log model and its applicability for predicting the temperature-dependent strength behavior of superalloys, of MEAs as well as of HEAs.

Origin of TRIP and TWIP behaviour in nanocrystalline FCC concentrated alloys: Insights from atomistic computer simulations

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Nanocrystalline (nc) microstructures have a high fraction of grain boundary area, which facilitates nucleation of Shockley partial dislocations in fcc lattice. This in turn results in extended stacking faults or microtwins, leading to either transformation-induced plasticity (TRIP) or twin-induced plasticity (TWIP). Both phenomena are attributed to the improvement of strength and ductility of fcc metals and alloys. However, there is no consensus regarding the material properties controlling the two phenomena, whether it is the metastable or unstable stacking fault or twin fault energies, the grain boundary stress state or some other factors. In this study, we perform uniaxial tensile testing of fcc nanocrystalline specimens using Molecular Dynamics (MD) simulations and study the dependence of stacking fault and twin evolution during tensile test and peak stress at macroscopic yielding, on different material properties, viz. stable and unstable stacking fault energy, unstable twin fault energy and shear modulus. Alloys of varying composition from three different alloy series, with interatomic interactions described by three EAM type potentials, has been used to get a wide range of material properties for our study. The statistics of twin and stacking fault evolution during deformation in each of our fcc alloy nc systems were calculated and compared. This study provides fundamental insights into the deformation mechanisms in nanocrystalline alloys and will help in guiding alloy design to promote TWIP/TRIP effects in these alloys.

SESSION 4E

ALLOYS: Ductility and Deformation II

3:30 **4E1:** Enhancing fatigue life by ductile-transformable multicomponent B2 precipitates in a high-entropy alloy
Rui Feng, You Rao, Chuhao Liu, Xie Xie, Dunji Yu, Yan Chen, Maryam Ghazisaeidi, Tamas Ungar, Huamiao Wang, Ke An, Peter. K. Liaw

3:45 **4E2:** Ductility at room temperature of body-centered cubic high entropy alloys
J. Wang, N.J. Peter, S. Basu, C. Brandl, R. Schwaiger

4:00 **4E3:** Phase transformation and deformation behavior in a B2-base high-entropy alloy
Rui Feng, You Rao, Chuan Zhang, Maryam Ghazisaeidi, Peter K. Liaw, Ke An

4:15 **4E4:** Improvements in Fatigue life through Precipitation-controlled plasticity and load partitioning in FCC HEAs
B.M. Adam, P.K. Liaw, X. Fan, X., B.A. Steingrimsson

4:30 **4E5:** The compositional dependence of twinning, strength, and ductility in a pseudo-binary Cr-Co-Ni medium-entropy system
J.L. Cicotte, W. Zhong, Y. Yang, E.P. George

4:45 **4E6:** Micromechanical origin for the wide range of strength-ductility tradeoff in metastable high entropy alloys via in situ neutron diffraction measurements
Z.Y. Lyu, Z.H. Li, T.T. Sasaki, Y.F. Gao, K. An, Y. Chen, D.J. Yu, K. Hono, P. K. Liaw

Enhancing fatigue life by ductile-transformable multicomponent B2 precipitates in a high-entropy alloy

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Fatigue failures in engineering structures can cause catastrophic accidents without obvious warning. Thus, fundamentally understanding cyclic-deformation and fatigue-failure mechanisms is critical for developing fatigue-resistant structural materials. Here we report a ductile multicomponent B2 precipitates-strengthened high-entropy alloy (HEA), which exhibits the outperforming fatigue life, relative to traditional materials, at low strain amplitudes. Its real-time cyclic-deformation mechanisms are revealed by *in-situ* neutron diffraction, transmission-electron microscopy, crystal-plasticity modeling, and Monte-Carlo simulation. Multiple cyclic-deformation mechanisms, including dislocation slips, multicomponent-precipitation strengthening, deformation twinning, and reversible stress-induced martensitic transformation, are observed in the studied HEA. Its excellent fatigue performance is attributed to the outstanding fatigue-crack-initiation resistance, resulting from the high elasticity, plastic deformability, and martensitic transformation of the B2 phase that leads to the effective load redistribution and strain partitioning with the face-centered-cubic (FCC) matrix. Guided by this study, fatigue-resistant alloys strengthened by ductile multicomponent intermetallic phases can be developed.

This work is supported by the National Science Foundation under grants of DMR-1611180.

Ductility at room temperature of body-centered cubic high entropy alloys

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High-entropy alloys (HEAs), which are defined as near-equimolar alloys of five or more elements, have been receiving significant attention over the last decade because of their unique properties and great potential for a variety of applications. Body-centered cubic (bcc) HEAs offer improved strength at high temperatures and are promising candidates for applications in extreme environments, while brittle behaviors at room temperature often limit their applicability. For example, the equimolar NbMoCrTiAl alloy shows little ductility in millimeter sized samples below 600°C, which has been attributed to the ordered structure of B2-type. The equimolar HEA TiNbHfZrTa, though, exhibits notable ductility at room temperature.

To understand the influence of the microstructures on the deformation behaviors, the two alloys NbMoCrTiAl and TiNbHfZrTa were studied under different loading conditions employing a range of micromechanical methods, including nanoindentation, microcantilever bending and microcompression testing. In contrast to macroscale tests, NbMoCrTiAl microsamples exhibited significant plasticity at room temperature. In the single-crystalline microcompression tests along the <100> and <110> crystal orientations, strains exceeding 35% were reached comparable to TiNbHfZrTa. Distinct slip bands were observed and identified as the predominant mechanism in the NbMoCrTiAl samples at the microscale. In the TiNbHfZrTa alloy, in addition to slip bands, kink and shear bands contributed to the room temperature ductility. The effects of different phases, grain boundaries and crystal orientations on the ductility of the two bcc HEAs will be discussed.

Phase transformation and deformation behavior in a B2-base high-entropy alloy

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Ordered intermetallic compounds have long been of interest as potential structural materials for use at elevated temperatures. In particular, B2 aluminides exhibit a wide range of interesting properties, such as high ordering temperature, corrosion resistance, and pseudo-elasticity effect. However, the lack of room-temperature ductility limits their applications due to an insufficient number of independent slip systems and poor grain-boundary (GB) cohesion. Recently, ductile multicomponent intermetallics have been achieved by the high-entropy alloy (HEA) concept. Here we design a B2-base HEA with a minor ductile face-centered-cubic (FCC) phase as a GB adhesive phase. The improved slip capability and stress-induced martensitic transformation of the multicomponent B2 phase are evidenced by in-situ neutron diffraction and transmission-electron microscopy. Together with the GB-strengthener, the tensile ductility of the designed alloy is enhanced to some extent. This work offers insights into alloy-design strategies that could improve the ductility of intermetallic alloys and accelerate their engineering applications.

Improvements in Fatigue life through Precipitation-controlled plasticity and load partitioning in FCC HEAs

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Recent advances in alloy design have led to the development and increased interest into High-Entropy Alloys for demanding, high-temperature applications, such as long-term exposure in aerospace and land-based energy generation. Material requirements here demand both excellent yield and ultimate strengths at extended temperature and time exposure ranges, but also capability to withstand cyclic loading conditions and related fatigue failure. To this end, we manufactured and investigated industrially relevant compositions of FCC-based HEAs with metallurgical variations to stimulate B2-phase precipitate formation. Such phases are anticipated to promote load partitioning during cyclic deformation tests and thus reduce local dislocation accumulation and retard onset of microcracking. Key to the understanding will be an assessment of the underlying dislocation dynamics and kinetics as a function of strain amplitude and temperature as well as micro-scale deformation behavior. Utilization of advanced electron microscopy techniques for imaging and determination of the dislocation types, character and spatial homogeneity, as well as compositional analysis of precipitate phases. Electron Backscatter Diffraction will be used for analysis of slip system prevalence with respect to load-partitioning behavior of B2 precipitates. Results of the present work will further emphasize the viability of physical metallurgy concepts for novel HEAs and the adaptability of these alloy systems to fatigue-critical applications.

The compositional dependence of twinning, strength, and ductility in a pseudo-binary Cr-Co-Ni medium-entropy system

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A Cr_{33}-$Co_{(x)}$-$Ni_{(67-x)}$ pseudo-binary medium-entropy alloy system where x = 1, 10, 20, and 33 at% was investigated to elucidate the role of composition on deformation mechanisms, strength, and ductility. Tensile testing conducted at room temperature (298 K) revealed that both strength and ductility increase as the Co content is increased from 1 at% to 33 at%. Consistent with this, transmission electron microscopy after room-temperature fracture found that deformation-induced nanotwinning occurs only in the x = 20 at% and x = 33 at% alloys and not in the alloys containing lower amounts of Co. These results are in agreement with our thermodynamic calculations which show that the stacking fault energy decreases with increasing Co content (decreased stacking fault energy promotes twinning in face-centered cubic metals such as those investigated here). At liquid nitrogen temperature (77 K), the strength and ductility of all alloys increased compared to those at room temperature. However, ductility is invariant with Co content at 77 K. Consistent with this, transmission electron microscopy revealed that all four alloys form deformation-induced nanotwins at 77 K. The increase in ductility achieved at 77 K compared to 298 K varies linearly with Co content.

Micromechanical origin for the wide range of strength-ductility tradeoff in metastable high entropy alloys via in situ neutron diffraction measurements

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Through different annealing temperatures and times, it is reported here that interstitial metastable high entropy alloys (HEAs) can exhibit a wide range of strength-ductility tradeoff. The underlying mechanisms were investigated via in situ neutron diffraction. Particularly, the unprecedented strength/ductility product value corresponds to the face-centered-cubic to hexagonal-close-packed phases that lead to a multistage work hardening behavior. Diffraction results reveal that such a phase transformation process could be tuned by various annealing processes, which result into various degrees of load partitioning and sharing among different phases and grain families on an indispensable microstructural length scale.

SESSION 4F

ALLOYS: Refractory Alloys III

3:30 **4F1:** Phase Transformations in a TiZrHfNb0.3 Refractory High-entropy Alloy under High Pressures
X. Fan, S. Aryal, X. Chen, L. Ouyang, M. Gao, Q. Zeng, E. Greenberg, V.B. Prakapenka, P.K. Liaw

3:45 **4F2:** Phase stability of refractory high-entropy alloys and their lower-order sub-systems
J.M. Brookins, Y. Yang, E.P. George

4:00 **4F3:** Strengthening Mechanisms in Single BCC Phase Refractory High-entropy Alloys
Chanho Lee, George Kim, Yi Chou, Michael C. Gao, Ke An, Gian Song, Yi-Chia Chou, Wei Chen, Nan Li, Saryu J. Fensin, Peter K. Liaw

4:15 **4F4:** Understanding the Deformation Substructures in the Refractory High Entropy Alloy $AlMo_{0.5}NbTa_{0.5}TiZr$
Zachary T. Kloenne, Gopal B. Viswanathan, Brian A. Welk, Jean-Philippe Couzinie, Hamish L. Fraser

4:30 **4F5:** Interstitial doping in refractory medium-entropy alloys: Massive interstitial solid solution
Yan Ma, Chang Liu, Ge Wu, Zhiming Li, Dierk Raabe

4:45 **4F6:** High-Entropy Refractory Aluminide Superalloys
Jie Qi, Xuesong Fan, Diego Ibarra Hoyos, Debashish Sur, Rui Feng, John R. Scully, Peter K. Liaw, S. Joseph Poon

Phase Transformations in a TiZrHfNb$_{0.3}$ Refractory High-entropy Alloy under High Pressures

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Diamond anvil cells (DAC) have been widely used on alloys to study their phase stability and understand the phase-transformation behaviors under high pressures. Be combined with high-energy X-ray techniques, it enables the possibility of *in-situ* observation of phase structures of advanced alloys in extreme environments. In this study, *in-situ* high-pressure synchrotron X-ray diffraction (SXRD) experiments were performed on a dual-phase refractory high-entropy alloy TiZrHfNb$_{0.3}$ containing both body-centered-cubic (BCC) and hexagonal-close-packed (HCP) crystal structures. Silicone oil was used in the diamond anvil cell as the hydrostatic pressure-transmitting medium to generate high pressure up to ~ 37 GPa. As a comparison, a similar setup without using the pressure medium was also utilized to study the influence of the hydrostaticity of the environment. Theoretical calculations employing the density functional theory (DFT) were also performed to better understand the mechanisms of phase evolution under extreme conditions in the TiZrHfNb$_{0.3}$ refractory high-entropy alloy.

Phase stability of refractory high-entropy alloys and their lower-order sub-systems

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Refractory high entropy alloys (RHEAs) are of interest because of their potential as structural materials in high-temperature applications. Two model equiatomic RHEAs, TiZrNbHfTa and VNbMoTaW, were investigated in this study. After homogenization at elevated temperatures followed by air-cooling to room temperature, they are single-phase, body-centered cubic (BCC) alloys. Three of the constituent elements in TiZrNbHfTa (Ti, Zr, Hf) have the HCP crystal structure at room temperature while the remaining two (Nb, Ta) are BCC. In contrast, all the elements in VNbMoTaW have the BCC structure. To test the effects of these elements and their concentrations on solid solution formation, equiatomic subsets of each quinary alloy, ranging from binaries to quaternaries, were systematically investigated. Phase stability was assessed after isothermal aging at 800°C, 1000°C, and 1200°C for times of 72 to 7200 h at which thermodynamic equilibrium was expected to be reached. Element distribution and crystal structure were characterized using SEM/EDS and XRD, respectively, to determine the extent (if any) of phase instabilities. Additionally, CALPHAD was used to calculate free energy changes and, in turn, expected phase transformations at the above temperatures. We find that some compositions have an island of instability at lower temperatures, but most can be single-phase above that. The experimental results are rationalized using thermodynamic simulations.

Strengthening Mechanisms in Single BCC Phase Refractory High-entropy Alloys

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Single-phase solid-solution refractory high-entropy-alloys (RHEAs) show remarkable mechanical properties, such as high yield strength with significant resistance to softening at elevated temperatures. To understand the original of this high strength, it is important to investigate the deformation and strength mechanisms via an in-depth study. We have investigated the elastic- and plastic-deformation behaviors of two body-centered cubic (BCC) NbTaTiV and NbTaTiVZr RHEAs, using both experiments and simulations. The *in-situ* neutron-diffraction results reveal that there is a transition in the load bearing capability of the grains from isotropic to anisotropic at elevated temperatures. Furthermore, we have systematically and quantitatively determined lattice distortion using a theoretical model, first-principles calculations, synchrotron X-ray/neutron diffraction, and scanning-transmission-electron microscopy techniques. These results demonstrate that severe lattice distortion is a core reason for high strengths in RHEAs.

Understanding the Deformation Substructures in the Refractory High Entropy Alloy $AlMo_{0.5}NbTa_{0.5}TiZr$

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In the family of the refractory-HEAs (RHEA), some alloys exhibit a remarkable plastic response at high temperatures. For example, the alloy $AlMo_{0.5}NbTa_{0.5}TiZr$ demonstrated impressive strength (745 MPa) and good compressive ductility (>50% reduction) at 1000 °C. Unlike typical Ni-base superalloys, the alloy $AlMo_{0.5}NbTa_{0.5}TiZr$ has disordered *bcc* precipitates embedded in an ordered, B2 matrix. The trend of high ductility fails to translate to room temperature (RT), resulting in brittle fracture. This begs the question as to whether the B2 phase is ductile or brittle, as B2 intermetallics, NiAl for example, are classically considered brittle in nature. Indeed, whereas the mechanical behavior and the associated deformation mechanisms for typical B2 compounds are now relatively well-known, results on the multi-substituted B2 phase are sparce. The current study will focus on describing the nature of defects in the B2 phase of the $AlMo_{0.5}NbTa_{0.5}TiZr$ alloy after RT deformation. Diffraction contrast analysis in the transmission electron microscope showed that dislocations with a Burgers vector parallel to [111] were operative in the B2 phase. Weak beam dark field (WBDF) imaging revealed that the dislocations were dissociated into two superpartials, separated by ~5nm. When imaged with superlattice reflection g=[100] in DF mode, the APB contrast in between the superpartials was clearly resolved. Thus, the reaction of [111] = ½[111] + APB + ½[111] is proposed. Line direction analysis proved that the dislocations align along [111], indicating a screw nature. Additional analysis suggests that the dislocations glide on {112} planes. This study suggests a ductile B2 phase in $AlMo_{0.5}NbTa_{0.5}TiZr$.

Interstitial doping in refractory medium-entropy alloys: Massive interstitial solid solution

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The history of using mixtures of metallic elements to make stronger and tougher alloys exceeds five millennia. As one of the most effective methods, interstitials (*e.g.*, C, N, and O) are attractive alloying elements as small atoms on interstitial sites create strong lattice distortions and hence substantially strengthen metals. Additionally, the strong interaction of interstitials with lattice defects such as dislocations, grain boundaries, and precipitates offers a variety of pathways for strengthening. However, formation of brittle ceramics, such as oxides and carbides, often during alloying when the interstitial content exceeds a critical yet low value (*e.g.*, 2 at.%), significantly reduces the ductility of the alloys. Here we present a solution to overcome the above challenges via introducing a concept of massive interstitial solid solution (MISS) alloys. The MISS alloy concept is realized by using a concentrated body-centered cubic (bcc) substitutional solid solution as a highly distorted host matrix, which allows introducing massive amounts of interstitials as an additional principal element class, without forming ceramic phases. For a TiNbZr-O-C-N MISS model system, the content of interstitial O reaches 12 at.%, with no oxides formed. The alloy reveals an ultrahigh compressive yield strength of 4.2 GPa, approaching the theoretical limit, and large deformability (65% strain) at ambient temperature, without localized shear deformation. The MISS concept thus offers a new avenue in the development of metallic materials with excellent mechanical properties.

High-Entropy Refractory Aluminide Superalloys

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In recent years, significant advances have been made for high-entropy alloys (HEAs) containing aluminum and refractory metals as primary elements. These novel materials can be categorized as high-entropy refractory aluminides (HEAl). HEAls generally have higher melting temperatures and strengths than conventional superalloys. They also have lower densities and cost as well as better oxidation resistance than the refractory HEAs (RHEAs). HEAl are therefore potentially ideal for high-temperature applications. Nevertheless, HEAl also suffer from problems, such as low ductility and phase stability at high temperatures. In this presentation, we will comprehensively discuss the mechanical properties of HEAls in comparison with other alloy categories, including HEAs with 3d transition-metal elements, HEAs with Al and 3d transition-metal elements, refractory HEA, and conventional alloys, to highlight the properties that distinguish HEAl. Common phases with morphologies, and typical mechanical properties of Al-RHEAs will be discussed. We aim to summarize the accomplishments, address the challenges, as well as provide an outlook regarding the future development of HEAl.