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Numerical Modeling of Wave Propagation in Polycrystals: A Pure Stress Formulation Approach

**Marzieh Bahremana; Ming Huangb; Melody Pngb; Bo Lanb; Christopher Kubea**\*

a 212 Earth and Engineering Sciences Bldg. University Park, PA 16802, USA.  
b City and Guilds Bldg. Imperial College London, UK.   
\*Corresponding Author

**Abstract**

Investigating wave propagation in polycrystals is crucial for various engineering applications, ranging from materials science to structural integrity assessments. In this talk, we present a novel approach to numerically model wave propagation in polycrystals by employing a pure stress formulation. The stress equation is derived from momentum balance followed by transformation and simplifications. Symmetry considerations yield a set of coupled partial differential equations or equations of motion for the six stress components. Finite difference discretization of spatial and temporal domains enables numerical solution techniques. This stress-based formulation offers a potentially more efficient and natural way of modeling wave propagation in polycrystals compared to displacement-based approaches. Polycrystals are often assumed to exhibit uniform mass density and non-uniform stiffness, attributed to the statistical distribution of crystal orientations within the grains. Conventional displacement formulations require approximations of spatial derivatives on stiffness, potentially leading to inaccuracies and extra computational burden. However, these formulations lack spatial derivatives on mass density. Conversely, our proposed stress formulation incorporates spatial derivatives on density while omitting them on stiffness. Since density is uniform for polycrystals, our approach simplifies the computational process by eliminating the need to approximate spatial derivatives on quantities other than stresses, thus reducing computational overhead. By prioritizing the stress formulation and leveraging its inherent computational advantages, we can achieve more efficient simulations of wave propagation in polycrystals, thereby advancing our understanding of wave scattering behavior and facilitating the design of high-performance engineering materials. We employ this stress-based formulation to analyze the mechanical behavior of polycrystals generated through Dream3D software. The presentation will highlight the modeling background, computational implementation, and lastly results and discussion.