

# Invar Effect in $\delta$ -Pu Alloys

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Several long-debated dynamical and elastic anomalies of  $\delta$ -Pu and its alloys (Pu-Al/Ga/In) [1,2] have been captured within an unprecedented unified theoretical framework. This achievement [3] is made possible by machine learning-accelerated *ab initio* simulations [4,5], which enable an accurate description of explicit temperature effects [6].

For pure  $\delta$ -Pu, the present simulations—within this unified framework—successfully reproduce the experimental observations of negative thermal expansion, equilibrium volume, and anomalous softening of elastic properties. Our analysis demonstrates that the distinctive behavior of  $\delta$ -Pu is almost entirely attributable to large anharmonic effects, which are linked to the extreme softening of the phonon spectrum [3].

This simulation approach has recently been extended to Pu-Al/Ga/In alloys. The results reveal significant anharmonic effects upon the addition of  $\delta$ -stabilizing elements and reproduce the well-known invar effect in  $\delta$ -Pu alloys, where thermal expansion transitions from negative to positive as a function of Al/Ga/In content. These results are a step forward toward a better understanding of alloying effects in plutonium.

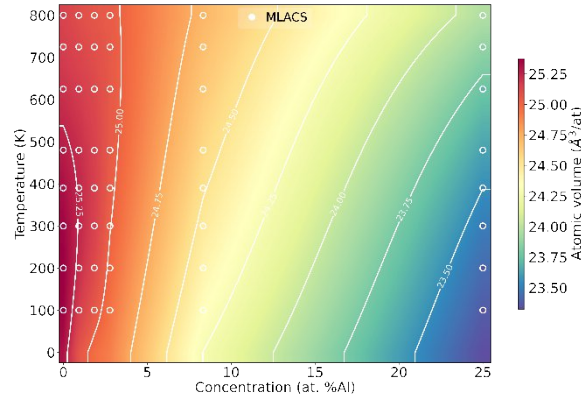


Figure 1: Atomic volume as a function of Al concentration and temperature.

## References:

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