Integration of first principles calculations into nucleation theory for design of multi-phase thermoelectric materials

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RESEARCH OBJECTIVE
The objective of this PSED project is to use first-principles inputs, including interfacial energies, strain energies, accurate thermodynamic quantities, and kinetic information in classical nucleation theory (CNT) to systematically study and predict secondary phase nucleation. A theory of first principles nucleation will help guide material synthesis experiments and help us better understand nanostructure formation and stability in order to design nanostructured materials with improved thermoelectric performance.

Processing
- Initial Alloy Composition
- Thermal Treatments

Structure
- 2nd-Phase Nanostructures

Properties
- \( \mu_{el}^{\text{prec}} \rightarrow \sigma \)
- \( \kappa_{lattice} \)

Thermoelectrics figure of merit: ZT

First Principles Inputs

Classical Nucleation Theory
Steady state nucleation rate
\[
J_{ss} = \beta(g^*)n_1 \exp\left(-\frac{W^*}{kT}\right)
\]
- Work of Formation
\[
W = V_{\beta} \Delta G_{\text{misfit}} + A_{\alpha \beta} \sigma_{\alpha \beta} + V_{\beta} \Delta G_{\text{v}}
\]
- \( \beta \) parameter for dilute solution
\[
\beta(g^*) \approx \frac{s_1 (g^*)^{2/3} DB C_0}{a^4}
\]
Diffusion Coefficient \( DB \)

Five Frequency Model
Nudged-Elastic Band (NEB) Method