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

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Academic Disciplines:
Materials Science and Engineering, Chemistry

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

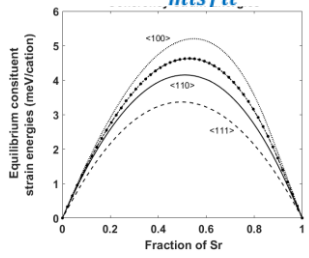
→ **Structure**
- 2nd-Phase Nanostructures

→ **Properties**
- $\mu_{el}^{prec} \rightarrow \sigma$
- $\kappa_{lattice}$

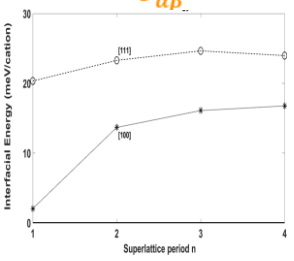
→ **Thermoelectrics figure of merit: ZT**

First Principles Inputs

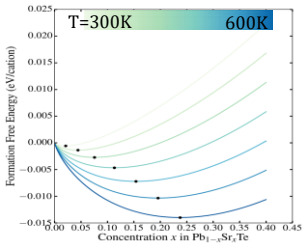
ΔG_{misfit}



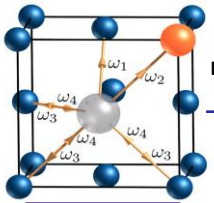
$\sigma_{\alpha\beta}$



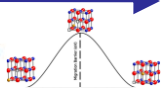
ΔG



Five Frequency Model



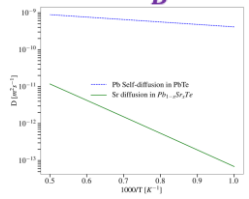
Nudged-Elastic Band (NEB) Method



DFT

Diffusion Type	Diffusion Barrier (eV)
E_0	1.13
E_1	0.68
E_2	1.04
E_3	1.15
E_4	1.14

D_B



Classical Nucleation Theory

Steady state nucleation rate

$$J_{SS} = \beta(g^*) n_1 \exp\left(\frac{-W^*}{kT}\right)$$

- Work of Formation

$$W = V_\beta \Delta G_{misfit} + A_{\alpha\beta}\sigma_{\alpha\beta} + V_\beta \Delta G_v$$

- β parameter for dilute solution

$$\beta(g^*) \approx \frac{s_1 (g^*)^{2/3} D_B c_o}{a^4}$$

Diffusion Coefficient D_B

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