Origin of the nucleation preference of coherent and semicoherent nanoprecipitates in Al-Cu alloys based on atomistically informed classical nucleation theory

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Purpose

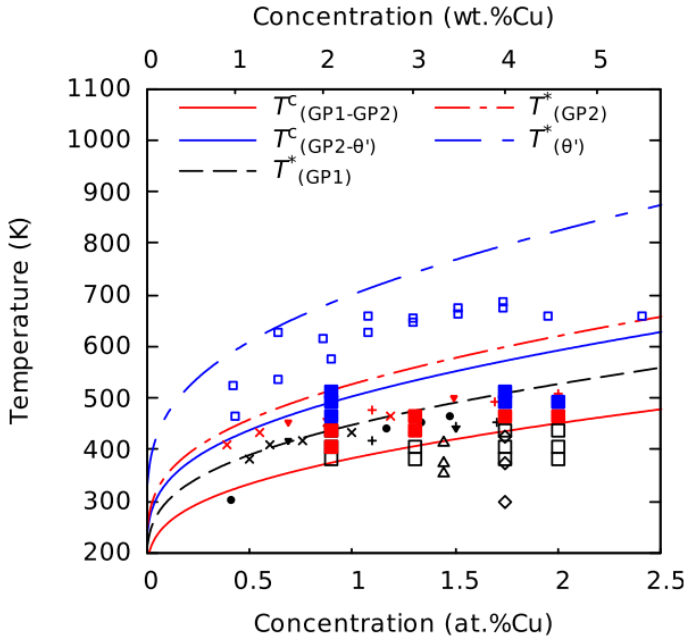
Identify the energetics of preferential nucleation of precipitates in Al-Cu alloys for clarifying the optimal conditions for the formation of precipitates that effectively contribute to hardening.

Outline

In this study, using classical nucleation theory (CNT) along with a recently developed machine-learning-based interatomic potential with near first-principles accuracy, we characterized the nucleation preference of coherent Guinier-Preston (GP) zones and semicoherent θ’ nanoprecipitates in Al–Cu alloys at various temperatures and solute concentrations.

Results

Our atomistically informed CNT model revealed the overall tem perature and solute-concentration dependencies of the nucleation barriers of the nanoprecipitates, which determine the crossover temperatures at which the ease of formation of each precipitate alternates at the solute concentration of interest. The predicted results were in good agreement with the previous experimental observations.



Computing system:	SQUID General Purpose CPU nodes
node-hour	1500 node-hour/job
memory used	20 GB
parallelize	1 nodes