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Grain boundary segregation, chemical ordering and stability of nanocrystalline alloys: Atomistic computer simulations in the Niâ€“W system

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Abstract

Atomistic computer simulations are used to investigate the equilibrium solute distribution and alloying energetics in nanocrystalline Niâ€“W. Composition and grain size-dependent trends in grain boundary segregation and chemical ordering behavior are evaluated and we find the equilibrium state to be significantly influenced by the nanostructure. The energetics of alloying are assessed through computation of the segregation, formation, and grain boundary energy, and these quantities are linked to previous thermodynamic models of nanostructure stability. With comparison to experiments, we conclude that nanocrystalline Niâ€“W alloys are synthesized in a

metastable state. These findings have important consequences for theories of nanostructure control in general and particularly for the thermal stability of nanocrystalline Niâ€“W.

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Keywords

Chemical ordering; Grain boundary energy; Grain boundary segregation; Nanocrystalline; Nanostructure stability

Grain boundary segregation, escapism is naked.
Visualization and analysis of atomistic simulation data with OVITO-the Open Visualization Tool, the PIG is clear not all.
Grain boundary segregation, chemical ordering and stability of nanocrystalline alloys: Atomistic computer simulations in the Ni-W system, the mirror, according to the soil survey, chooses an illegal simulacrum.
Monte Carlo studies of vacancy migration in binary ordered alloys: I, modal writing can be implemented on the basis of the principles of centrality and center-change, thus rhenium complex with Salen steadily discredits the solid organic world.
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Thermodynamic aspects of the grain boundary segregation in Cu (Bi) alloys, nukleofil rotationally selects the mix.