Molecular dynamics simulation of glass formation and crystallization in binary Pd-Ni and Cu-Ni alloys.

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Abstract

Molecular dynamics (MD) using Quantum Sutton-Chen potentials were used to obtain an atomistic description of melting, glass formation and crystallization processes for amorphous Cu, Ni and Pd to study the PdNi and CuNi alloys. The thermodynamic and mechanical properties were calculated in the 0-2000K temperature range from the MD trajectories.The formation of amorphous Cu, Ni and Pd and their alloys by rapid quenching was investigated from MD at constant pressure and temperature (TPN ensemble). The structural properties were analyzed by means of pair distribution functions and volume *vs* temperature, at cooling rates ranging from 40 K/ps to 0.4K/ps. The relation between the cooling rate and glass transition temperature, or crystallization, was described. The radial distribution function agrees well with experimental results for amorphous phases. Upon cooling rates in the range of 5K/ps to 0.4K/ps, Cu, Ni, Pd and CuNi alloys were formed a crystalline structure while PdNi alloys formed a glass. The radius ratios of crystal former (CuNi) has 1.02 while glass former (PdNi) has ratios 1.134. Therefore, the role of mismatch in atomic size favoured to glass formation.

Keywords: Molecular dynamics, Quantum Sutton-Chen potentials,Cu-Ni alloys, Rapid quenching, cooling rates.