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Effect of the cooling rate on the solidification of Ag-X%Au alloy: Molecular dynamics simulation

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Abstract
This research aims to study the solidification processes of Ag-X%Au alloy by molecular dynamics simulation technique at the NPT ensemble. The quantum Sutton-Chen many-body interatomic potential is used to calculate the energy and forces experienced by the particles. The coupled differential equations of motion of the particles are solved using Velocity Verlet algorithm. The solidification temperature, the cohesive energy and the solidification latent heat of Au, Ag pure metals as well as Ag-X%Au alloys with various concentrations of Au are determined. Furthermore, the solidification process of alloy is studied at different cooling rates. The molecular dynamics simulation results show glass structure is achieved at fast cooling rates while crystallization occurs at slow cooling rates. Also, this cooling rate is different for various concentrations of Au.

Keywords: Ag-Au alloy, molecular dynamics simulation, solidification, thermal properties

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