Molecular Dynamics Studies on Amorphous Formation of Si and Pd-Si alloy by Rapid Quenching

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Abstract:

This research aims at studying the structural properties of amorphous material, especially inorganic glass former, using classical molecular dynamic and first principles density functional theory (DFT). The amorphous supercell models of silicon (Si) and its binary alloy (PdSi) were built and investigated using molecular dynamics simulation (Classical and Ab-initio). The formation of amorphous silicon and palladium-silicon (PdSi) alloy by rapid quenching of the melt has studied using the EAM and PBE (GGA) potentials to model the interaction between silicon-silicon, and palladium-silicon atoms. By quenching the structure melts at a different rate to form amorphous Si and Pd-Si alloy. The rapid solidification of Si and Pd-Si alloy is studied to obtain the structural properties of glass formation using molecular dynamics technique at constant pressure and temperature (TPN). The structural properties are analyzed by means of pair distribution function and volume as a function of temperature at cooling rates ranging from 10 K/ps to 0.1 K/ps to see whether the Si and Pd-Si alloy pass through glass formation or it crystallizes. The relation between the cooling rate and glass transition temperature is revealed. The amorphous property of radial distribution function agrees well with experimental results.