

Abstract Submitted
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Non-crystalline state of silicon studied by multicanonical simulation combined with first-principles calculation YOSHIHIDE YOSHIMOTO, Institute for Solid State Physics, University of Tokyo, Japan — By combining multicanonical ensemble molecular dynamics and first-principles calculations, non-crystalline state of silicon is studied. This attempt contrast with quenching molecular dynamics simulations whose speed is usually by far quicker than that of experimental quenchings. To make the molecular dynamics simulation tractable, a model interatomic potential is used. The parameter, however, is determined by first-principles calculation so that the discrepancy between the first-principles interatomic potential and the model one is minimized on the typical configuration set of the multicanonical ensemble. Because multicanonical ensemble represents the whole thermodynamics of the system, the obtained model will conserve the thermodynamics to a maximum extent. (thermodynamic downfolding of an interatomic potential [1]) The transition between amorphous silicon and liquid silicon, and the density maximum of liquid silicon as a function of temperature will be discussed. (Silicon has similar structure to that of water) [1] Y. Yoshimoto, J. Chem. Phys., 125, 184103 (2006)

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