

Polyamorphic transformations in liquid and amorphous silicon: A first-principles molecular-dynamics study

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Structural transformations between disordered phases, such as liquid-liquid and amorphous-amorphous transformations (polyamorphic transformations), have been a focus of interest for the past years. In water, amorphous-amorphous transformation was experimentally observed and transformation between two distinct liquid forms has also been examined [1]. Since a typical atomic configuration of silicon (Si) is the same as that of water (i.e., tetrahedral structure), similar polyamorphic transformations are expected in liquid and amorphous silicon. In this study, isothermal-isobaric first-principles molecular-dynamics simulations [2] were performed to investigate polyamorphism in amorphous and liquid silicon.

In our simulations, a new high-density amorphous (HDA) form of Si was discovered by pressurizing a normal amorphous Si [a low-density amorphous (LDA) form] up to ~ 12 GPa [3]. Detailed analyses show that the structure of HDA Si is found to be very close to that of HDA water. Reverse transformation to the LDA form was also observed by depressurization as in the LDA-HDA transformation of water. We will discuss this amorphous-amorphous transformation in connection with structural change in liquid Si under supercooling [4].

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[3] T. Morishita, *Phys. Rev. Lett.* **93**, 055503 (2004).

[4] T. Morishita, *Phys. Rev. Lett.* **97**, 165502 (2006).