Formation of metastable silicide during crystallization of Si-Al nanoparticles

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The mechanism of Al-Si alloy crystallization from an amorphous state is still unclear. Despite the absence of equilibrium compounds for this binary system, there are several experimental evidences conrming the formation of metastable silicide at annealing of amorphous Si mixed with Al. Classication of this metastable structure is a missing puzzle piece in the description of Al-Si alloy crystallization kinetics. Here, we considered the properties of aluminum silicide Al_2Si structure, which is a probable candidate for the role of the observed metastable compound. Our investigation was based on the atomistic simulations with the interatomic potential developed recently and DFT approach. All used methods revealed that there are several crystal structures of Al_2Si with close geometry and relatively low formation energies. The chemical ordering in such structures is similar to the one in Si-Al melt. We also showed that the combination of these structures allows to form a crystal with different degree of ordering.