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Carbon atom reactions in CVD graphene growth on copper surface: A first principles study[1] NOBUO TAJIMA, TOMOAKI KANEKO, JUN NARA, TAKAHISA OHNO, National Institute for Materials Science — Graphene has attracted considerable research interest due to potential application to future electronic devices. Chemical vapor deposition using copper surface with hydrocarbon source is one of the practical methods to produce graphene. The carbon atom nucleation and cluster growth processes in the CVD reactions have been studied extensively as key steps that control graphene growth behavior. The initial carbon atom bonding process is especially important, since carbon atom nucleation density dominates graphene quality. In the present study, carbon atom dimerizaiton on copper surfaces, the initial process of carbon atom nucleation in Cu-CVD graphene growth, have been studied with first principles MD simulations. The calculated results suggest that the copper surface almost melts at typical CVD temperature $\sim$ 1000 °C, and the surface roughening affects the carbon-metal interactions and the energetics of this reaction. Cu(111) and Cu(001) surfaces show different surface roughening behaviors, resulting in different energetics for the reactions on these surfaces. First principles simulation code PHASE (http://www.ciss.iis.u-tokyo.ac.jp/riss/english/project/device/) was used in these calculations.

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