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First-Principles Simulations for the Initial Stage of Graphene Growth Induced by Si Sublimation from Stepped SiC Surface[1]
YOUKY ONO, RIST, MARCEED, TAKAHIRO YAMASAKI, NIMS, MARCEED, TAKAHISA OHNO, NIMS, IIS Univ. of Tokyo, MARCEED — An epitaxial graphene sheet can be obtained by heat sublimation of Si atoms from the stepped SiC surface. Although this method is expected as one of the most encouraging procedure to make clean sheets, its atomic scale growth mechanism is yet not understood in detail. In this study, the initial stage of the graphene growth processes on a stepped SiC(0001) surface are analyzed by first-principles molecular dynamics (FPMD) simulations. A first-principles calculation code "PHASE" [1] which is appropriate for efficient large scale parallel calculations is used. Our FPMD simulations proceed as follows. Before the start, some of the Si atoms on the top layer are intentionally removed from the initial SiC substrate to emulate the Si heat sublimation. MD is executed for 1 psec. under the condition of high temperature and then relaxed. Next, additional Si atoms are removed from the 2nd top layer, and then the same MD is repeated again. We tracked the behaver of the redundant C atoms during the series of these procedures. Where, when and how do those C atoms start to re-create the new C-C networks will be discussed in detail by comparing the results from several different patterns of the SiC substrates.

[1] http://www.ciss.iis.u-tokyo.ac.jp/english/project/device/.

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