

Abstract Submitted  
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**First-principles Study on Early Stage of Graphene Growth on SiC substrate by Si Sublimation.**<sup>1</sup> JUN NARA, TAKAHIRO YAMASAKI, TAKAHISA OHNO, National Institution for Materials Science — Graphene is known to have characteristic physical properties, such as high electron mobility and structural robustness, and then expected as future electronic device materials. Graphene growth on SiC substrate by Si sublimation is one of the promising graphene growth methods. However, the growth mechanism, especially, its early stage is not clear yet. In this study, we investigate the atomistic growth mechanism of the graphene growth by using first-principles molecular dynamics simulations. We used the PHASE/0 code [1] in this study. We found the remnant C atoms on SiC substrate after the Si sublimation preferably form one-dimensional (1D) structures than two-dimensional (2D) structures. Then, 2D structures are formed by the gathering of 1D structures. This is possible because 1D structures easily diffuse on the surface, differently from 2D structures, which are rather pinned on the surface. It seems that 2D structures have some difference depending on the distribution of surface Si dangling bonds. We will give the details of the result of FPMD simulations in the presentation. [1] <https://azuma.nims.go.jp>

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