N1-P002

Growth Mechanism of Graphene structure on 3C-SiC(111) Surface: A Molecular Dynamics Simulation

황유빈, 이응관, 최희채, 정용재

한양대학교 신소재공학과

Since the concept of graphene was established, it has been intensively investigated by researchers. The unique characteristics of graphene have been reported, the graphene attracted a lot of attention for material overcomes the limitations of existing semiconductor materials. Because of these trends, economical fabrication technique is becoming more and more important topic. Especially, the epitaxial growth method by sublimating the silicon atoms on Silicon carbide (SiC) substrate have been reported on the mass production of high quality graphene sheets. Although SiC exists in a variety of polytypes, the 3C-SiC polytypes is the only polytype that grows directly on Si substrate. To practical use of graphene for electronic devices, the technique, forming the graphene on 3C-SiC(111)/Si structure, is much helpful technique. In this paper, we report on the growth of graphene on 3C-SiC(111) surface. To investigate the morphology of formed graphene on the 3C-SiC(111) surface, the radial distribution function (RDF) was calculated using molecular dynamics (MD) simulation. Through the comparison between the kinetic energies and the diffusion energy barrier of surface carbon atoms, we successfully determined that the graphitization strongly depends on temperature. This graphitization occurs above the annealing temperature of 1500K, and is also closely related to the behavior of carbon atoms on SiC surface. By analyzing the results, we found that the diffusion energy barrier is the key parameter of graphene growth on SiC surface.

Keywords: graphene, silicon carbide, molecular dynamics