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Temperature and Substrate Orientation Effects on the Thermal Stability of Graphene Sheet Attached on the Si Surface

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Abstract : The graphene binding with silicon substrate has apparently Schottky barriers property, which can be used in the application of solar cell and light source. Because graphene has only one atom layer, the atomistic structure of graphene binding with the silicon surface plays an important role to affect the properties of graphene. In this work, temperature effect on the morphology of graphene sheet attached on different crystal planes of silicon substrates are investigated by Molecular dynamics (MD) (LAMMPS, developed by Sandia National Laboratories). The results show that the covered graphene sheet would cause the structural deformation of the surface Si atoms of stubtrate. To achieve a stable state in the binding process, the surface Si atoms would adjust their position and fit the honeycomb structure of graphene after the graphene attaches to the Si surface. The height contour of graphene on different plane of silicon surfaces presents different pattern, leading the local residual stress at the interface. Due to the high density of dangling bond on the Si (111)7x7 surface, the surface of Si(111)7x7 is not matching with the graphene so well in contrast with Si(100)2x1and Si(111)2x1. Si(111)7x7 is found that only partial silicon adatoms are rearranged on surface after the attachment when the temperature is lower than 200K, As the temperature gradually increases, the deformation of surface structure becomes significant, as well as the residue stress. With increasing temperature till the 815K, the graphene sheet begins to destroy and mixes with the silicon atoms. For the Si(100)2x1 and Si(111)2x1, the silicon surface structure keep its structural arrangement with a higher temperature. With increasing temperature, the residual stress gradually decrease till a critical temperatures. When the temperature is higher than the critical temperature, the residual stress gradually increases and the structural deformation is found on the surface of the Si substrates.

Keywords : molecular dynamics, graphene, silicon, Schottky barriers, interface
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