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Theoretical Study on Electrical Conductivity of Water Adsorbed Graphene

By the development of microprocessing technology of silicon, which is the most famous semiconductor material, the performance improvement of electronic devices have progressed, and the progress of information society has taken place. However, in recent years, the performance improvement of devices by microprocessing of silicon is reaching its limit. As one of the proposals to overcome the limit, graphene is attracting attention as the substitute material for silicon.

The graphene consists of single-layer carbon atoms arranged in a hexagonal lattice and it is expected to be used as the channel material of the transistor because it has very high mobility that is 200,000 cm^2/Vs in the case of free-standing graphene [1]. However, graphene is said to be susceptible to the surrounding environment because all carbon atoms in graphene are exposed to the environment. Especially, the influence of water molecules around graphene can be serious for the operation of the electrical properties of the graphene device under an electric field perpendicular to the graphene.

The graphene is one of the famous hydrophobic materials, and therefore it had long been believed that water molecules don't adsorb on the graphene surface. However, both the previous computational and the experimental studies revealed that there are single or double water layers on the surface of the graphene in a water vapor atmosphere [2,3,4,5]. The microscopic structure of the surface water layer parallel to the graphene had been clarified by our research. According to this study, the two-dimensional (2D) hydrogen-bond network is formed in the water layers on the graphene surface [5]. Following these previous studies, we investigated the influence of such a 2D network on the electrical properties of the graphene and how the gate voltage range of the graphene field effect transistor operates without being influenced by surface water.

In this work, we constructed the microscopic structure of water layers around graphene on a hexagonal boron nitride (h-BN) substrate using classical MD simulations. For the obtained structures, we calculated the electric dipole of water molecules when the electric field applied in the direction perpendicular to the graphene. By using these results, we estimated the electrical conductivity of the graphene using the Boltzmann equation. We explain the correlation between electric dipole of water layers and the electrical conductivity of graphene at the poster session.

References

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Figures

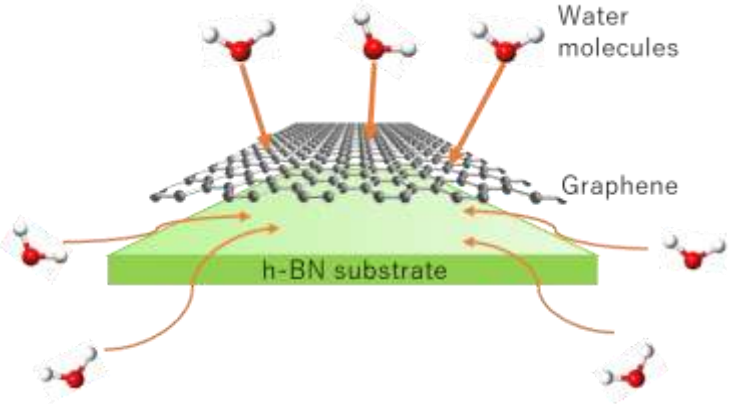

Figure 1: The illustration of the simulation model. Water layers around graphene on a h-BN substrate.