Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effect of Al_2O_3 deposition on electronic Transport in Graphene: DFT-NEGF study[1] TOMOAKI KANEKO, TAKAHISA OHNO, National Institute for Materials Science, MATERIALS RESEARCH CONSORTIUM FOR EFFICIENT ELECTRONIC DEVICES TEAM, UNIVERSITY OF TOKYO TEAM — In order to screen the charged impurities and to prevent the adsorption of contaminant on graphene, the deposition of high-k materials such as Al_2O_3 on graphene surface is important issue for graphene device application. Since the interfacial structure of graphene and high-k materials are not identified, theoretical study on the interfacial structure dependence on electronic transport is highly demanded. In this paper, we performed the electronic transport simulation in graphene under Al_2O_3 based on the density functional theories (DFT) and nonequilibrium Green's function method (NEGF). We investigated the effect of Al_2O_3 surface termination on the electronic transport properties. According to the calculation of stability of interfaces and electronic structures, the graphene's linear band structure is preserved in O_2 deficient condition. In O_2 rich condition, on the other hand, the graphene's unique electronic structure is disturbed. These properties are important for the electronic transport in graphene under Al_2O_3. Graphene shows relatively good transport properties in O_2 deficient condition, but transport is considerably suppressed in O_2 rich condition. Our results suggest O_2 deficient condition is desirable for the device application.

[1]A portion of this research was supported by the grant for "Strategic Programs for Innovative Research" Field No. 4: Industrial Innovations.

Tomoaki Kaneko
National Institute for Materials Science

Date submitted: 14 Nov 2014 Electronic form version 1.4