

Chemisorption of hydrocarbons at the SiC surfaces – from *ab initio* to classical molecular dynamics

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Hydrocarbons of the type C_nH_m (like propane, methane, or benzene) are used as typical reactants for chemical vapor deposition (CVD) growth of epitaxial graphene on metals and silicon carbide. Understanding the kinetics of the CVD processes is important for further advancing of graphene layer growth. In the first stages of growth, the most important processes include chemisorption of hydrocarbons on the substrate's surface and further the surface catalyst dehydrogenation of hydrocarbons.

In this communication, we present results of classical molecular dynamics (MD) modeling of relevant chemical reactions leading to graphene growth on Si and C terminated surfaces of 4H-SiC. The classical MD allows for simulation of chemical reactions on larger time and length scales and as it turns out can provide reliable picture provided the potentials describing the interactions between atoms are carefully chosen. It turns out that a prerequisite for successful description of the chemical reactions are potentials that account for the coordination numbers of atoms [1], i.e., of the Brenner's type [2]. To perform our studies, we had to determine parameters of the potentials describing the interaction between following atoms Si-Si, Si-C, and Si-H. We used the existing analytic expressions for C-C, and C-H [1] and *ab initio* calculations in the framework of the density functional theory (as implemented in the VASP computer package) to determine potentials involving Si atoms. Having determined the potentials for systems involving Si, C, and H atoms we performed additional tests for systems of Si_nC_m small clusters [3] and found out the reasonable agreement between results obtained with *ab initio* calculations and classical potentials.

Then the determined atomic potentials have been used to simulate the chemical reactions of hydrocarbons at the 4H-SiC surface. Where possible, we compare the results of classical MD with *ab initio* ones observing full consistency of the emerging picture of chemical reactions involving few molecules. This allows us to believe that we have developed valuable simulation tool that provides reliable description of chemical reactions relevant for graphene growth on SiC for systems with tens of reacting molecules. The performed simulations shed light on the microscopic mechanisms leading to graphene layer formation on SiC surfaces.

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[1] for review see, Tao Liang, B. Devine, S. R. Phillpot, and S. B. Sinnott, *J. Phys. Chem. A* **116**, 7976 (2012).

[2] D. W. Brenner, O. A. Shenderova, J. A. Harrison, S. J. Stuart, B. Ni, S. B. Sinnott, *J. Phys.: Condens. Matter* **14**, 783 (2002).

[3] N. Gonzalez Szwacki and J. A. Majewski, *Acta Physica Polonica A* **120**, 964 (2011).