STUDY OF INTERACTION BETWEEN GRAPHENE LAYERS: FAST DIFFUSION OF GRAPHENE FLAKE AND COMMENSURATE-INCOMMENSURATE PHASE TRANSITION

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The van der Waals corrected first-principles approach (DFT-D) is for the first time applied for investigation of interlayer interaction and relative motion of graphene layers (see [1] for details). The calculated interlayer interaction energy as a function of the relative position of graphene layers and the rotation angle of a graphene flake on a graphene layer are shown in Fig. 1.

Different mechanisms of diffusion in commensurate adsorbate-adsorbent systems are analyzed by the example of a graphene flake on a graphene layer. In addition to diffusion of the flake with the fixed commensurate orientation, a new mechanism through rotation of the flake to incommensurate states is proposed. Due to a significant barrier for rotation of the flake, these events are rare. However, this factor is compensated by long distances passed by the flake before it returns to the commensurate state.

We have performed molecular dynamics simulations to demonstrate that the proposed diffusion mechanism should be dominant at room temperature for the flake consisting of a few hundreds of atoms (see [2] for details). According to analytic expressions derived for the diffusion coefficient of the flake, the relative contribution of the mechanism corresponding to rotation of the flake to incommensurate states is the most significant at temperatures above $kT_{com} = \Delta E_{com}$, where ΔE_{com} is the barrier for transitions of the flake between adjacent energy minima in the commensurate state, and leads to an increase of the diffusion coefficient by more than an order of magnitude. Diffusion coefficients obtained using the analytic estimates and the simulations for the free flake and the flake with the fixed commensurate orientation as functions of temperature are shown in Fig. 2a. The methods of control over the diffusion and drift of graphene components in nanoelectromechanical systems are discussed.

A commensurate-incommensurate phase transition [3] in bilayer graphene is investigated in the framework of the Frenkel-Kontorova model extended to the case of two interacting chains of particles. Analytic expressions are derived to estimate the critical unit elongation of one of the layers at which the transition to the incommensurate phase takes place, length and formation energy of incommensurability defect (ID) on the basis of the DFT-D calculations of the interlayer interaction energy as a function of the relative position of the layers. These

estimates are confirmed by atomistic calculations using the DFT-D based classical potential. The calculated structure of the first ID in the system is shown in Fig. 2b.
The possibilities to measure the barriers for relative motion of graphene layers by study of diffusion of a graphene flake or formation of IDs in bilayer graphene are discussed [4].

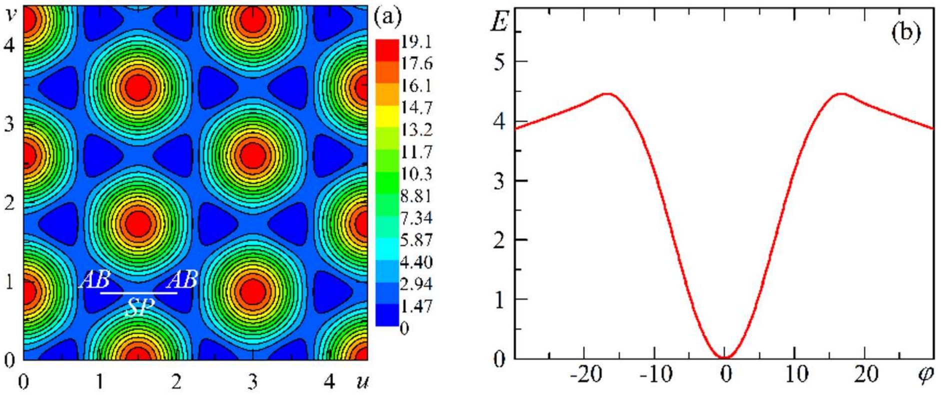

Figure 1: (a) The calculated interlayer interaction energy (in meV/atom) as a function of the relative position of the graphene layers u and v (measured relative to the bond length of graphene l_0=1.42Å u and v axes correspond to the armchair and zigzag directions, respectively). The minimum energy path corresponding to transition between adjacent energy minima is shown by the white line. (b) The calculated interaction energy (in meV/atom) between the graphene flake and the graphene layer for the 54-atom flake as a function of the rotation angle φ (in degrees). The value $\varphi = 0°$ corresponds to the global energy minimum.

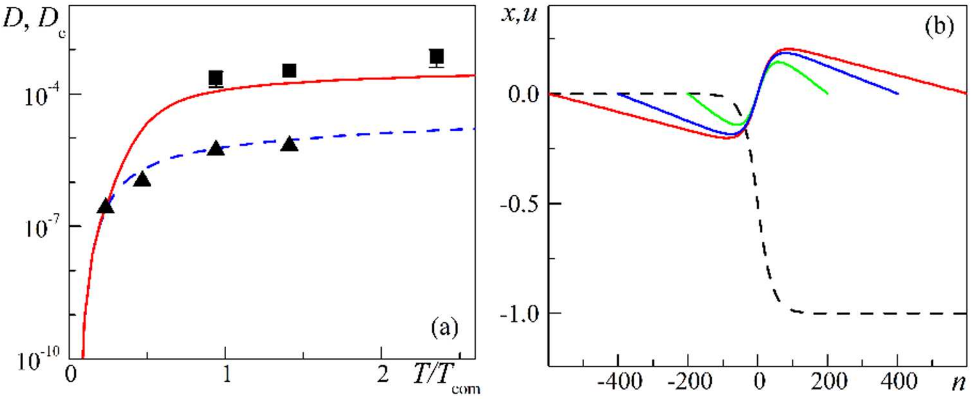

Figure 2: (a) Calculated diffusion coefficients (in cm^2/s): D (red solid line) of the free flake and D_c (blue dashed line) of the flake with the fixed commensurate orientation as functions of temperature T/T_{com} for N=178. The results of the molecular dynamics simulations are shown with black squares for the diffusion coefficient D of the free flake and with black triangles for the diffusion coefficient D_c of the flake with the fixed commensurate orientation. (b) Calculated structure of the first incommensurability defect: displacements $u(n)$ (dashed line) of the particles of the Frenkel-Kontorova model corresponding to the free graphene layer relative to the particles of the tension layer and displacements $x(n)$ (solid lines) of the particles corresponding to the tension layer relative to the perfect graphene lattice along the minimum energy path shown in Fig. 1a for bilayer graphene of length L_0 ≈57, 114 and 170 nm. It is assumed that each "particle" in the model corresponds to a strip of graphene directed perpendicular to the elongation (along the zigzag direction) and of the width equal to the bond length.

References

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