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Edge stacking dislocations in two-dimensional bilayers with a small lattice mismatch

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ABSTRACT

Incomplete stacking dislocations are predicted to form at edges of the shorter upper layer in two-dimensional hexagonal bilayers upon stretching the longer bottom layer. A concept of the edge Burgers vector is introduced to describe such dislocations by analogy with the Burgers vector of standard bulk dislocations. Analytical solutions for the structure and energy of edge stacking dislocations in bilayer graphene are obtained depending on the magnitude of elongation and angles between the edge Burgers vector, direction of elongation and edge. The barrier for penetration of stacking dislocations inside the bilayer is estimated. The possibilities to measure the barrier to relative motion of graphene layers and strain of graphene on a substrate by observation of edge stacking dislocations are discussed.

1. Introduction

Dislocations associated with a variation in stacking of two-dimensional hexagonal layers (Fig. 1a) and manifested through incommensurate boundaries between commensurate domains have been recently in focus of extensive experimental [1–4] and theoretical [3,5–7] research. Similar to in-plane defects, such stacking dislocations affect electronic [8–12] and optical [13] properties of bilayer and few-layer systems and, therefore, have implications for development of nanoelectronic devices.

In addition to stacking dislocations occasionally present in bilayer and few-layer samples, it has been proposed that they can be intentionally generated by stretching of one of the layers. While at small external strains the interlayer interaction keeps the layers commensurate, increasing the strain to some critical value leads to a release of the excessive elastic energy through formation of dislocations. It has been shown that this is the second-order phase transition characterized by the density of stacking dislocations as the order parameter [14,5]. Predicted theoretically for hexagonal bilayers [5,7] and nanotubes with commensurate walls [15,16], this new phenomenon, commensurate-incommensurate phase transition, is still waiting for the experimental validation. In the meanwhile, the crossover from the structure with commensurate domains separated by incommensurate boundaries to the fully incommensurate state has already been observed for the layers with a small mismatch of the lattice constants upon changing the relative orientation of the layers [17].

Furthermore, physical phenomena where stacking between two-dimensional hexagonal layers is different from the ground-state one and is related to the interaction between the edges have been observed recently. Bilayer graphene with the AA stacking and common folded edge where adjacent layers form a curved closed loop has been fabricated by heat treatment [18]. Lock-in positions of a graphene flake on the underlying graphene layer with the stacking different from the AB stacking and resulting from the edge-edge interaction have been studied by high-resolution electron microscopy [19].

In the present paper we propose yet another edge phenomenon which could be observed in two-dimensional hexagonal bilayers with a strained layer. Different from the previous studies dealing with stacking dislocations inside bilayers, we consider evolution of stacking at the edge of the shorter layer on top of the longer layer that is being stretched (Fig. 2). We suggest that any non-zero elongation of the bottom layer results in formation of an incomplete stacking dislocation at the edge of the upper layer (Fig. 1b), hereafter referred to as an edge stacking dislocation (ESD). The consideration of the edge evolution also allows us to estimate the barriers for penetration of complete stacking dislocations inside the layers and, therefore, to get an insight into kinetics of dislocation generation. Similar to transmission electron microscopy studies of pre-existing dislocations in few-layer graphene that resulted in an experimental estimate of the barrier to relative sliding of graphene layers [1], experimental investigation of ESDs

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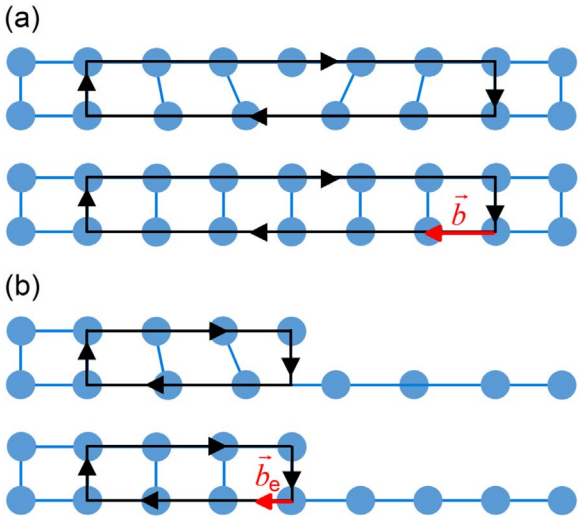

Fig. 1. Schematic representation of stacking dislocations inside (a) and at the edge (b) of a bilayer. The standard bulk (a) and edge (b) Burgers vectors $\vec{b}$ and $\vec{b}_e$ are indicated.

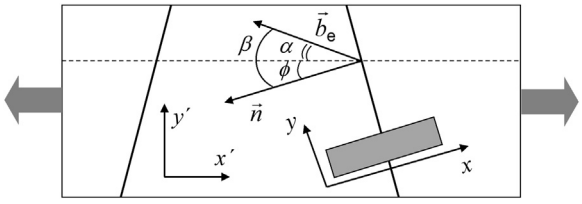

Fig. 2. Scheme of formation of stacking dislocations at edges (inclined lines) of the upper layer of bilayer graphene upon elongation of the bottom layer (rectangular). The normal $\vec{n}$ to the edge and edge Burgers vector $\vec{b}_e$ are shown. The direction of elongation is indicated by the thick arrows and dashed line. α is the angle between the direction of elongation and edge Burgers vector $\vec{b}_e$. ϕ is the angle between the normal $\vec{n}$ to the edge and direction of elongation. $\beta = \alpha + \phi$ is the angle between the normal $\vec{n}$ to the edge and edge Burgers vector $\vec{b}_e$. The coordinate systems $x - y$ and $x' - y'$ associated with the edge and elongation applied, respectively, are shown.

could help to validate the theoretical predictions and learn more about interaction of atomically thin layers. Particularly we suggest possible experimental schemes using edge stacking dislocations for measurements of the barrier to relative motion of graphene layers, strain of graphene on a subtrate and average lattice constants of graphene membranes chemically modified at one side.

Special attention has been paid so far to dislocations in graphene [1–5,8–13]. The potential surface of interlayer interaction energy in bilayer graphene has two degenerate inequivalent minima AB and AC. The transition between these two minima corresponds to formation of partial stacking dislocations (PSDs) with the Burgers vector $\vec{b}$ equal in magnitude to the bond length l and smaller than the lattice constant $a_0 = l\sqrt{3}$. In addition to graphene, predictions regarding the properties of dislocations have been also made for hexagonal boron nitride. In particular, it has been suggested that PSDs similar to the ones in graphene could be also found in metastable boron nitride with co-aligned layers (AB stacking in the commensurate state) [6,7], which is only slightly unstable compared to the ground state with the layers aligned in the opposite directions [6] and has been observed experimentally [20]. In the present paper, we consider graphene as an example (Fig. 3). However, our conclusions are qualitatively valid for other hexagonal bilayers, while the results for properties of dislocations in boron nitride with the layers aligned in the same direction and graphene are close even quantitatively [6].

2. Results

We consider the case when the upper adsorbed layer is somewhat

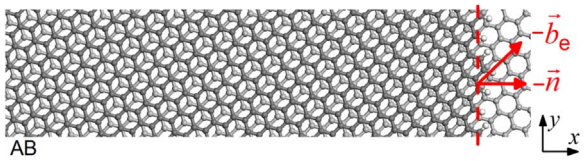

Fig. 3. Atomistic structure corresponding to the stacking dislocation at the edge of the upper layer of bilayer graphene with the angle $\beta = 45°$ between the edge Burgers vector $\vec{b}_e$ and normal $\vec{n}$ to the edge (Fig. 2) for the elongation of the bottom layer of $\epsilon = 6.28 \cdot 10^{-3}$ perpendicular to the edge ($\phi = 0°$ and $\alpha = \beta$). Carbon atoms of the upper and bottom layers and hydrogen atoms are coloured in dark gray, light gray and white, respectively. The magnitude of the vector $\vec{b}_e$ is scaled up for clarity. The coordinate system $x - y$ associated with the edge is indicated.

smaller than the bottom layer to avoid the interaction between their edges. The bottom layer is stretched, while the upper layer is left to relax freely. We assume that there is no difference in the interlayer interaction energy inside the layers and at the edge of the upper layer, which is the case, for example, when edges of the upper layer are terminated by hydrogen (Fig. 3). This ensures that the formalism of the two-chain Frenkel-Kontorova model [15] used previously to study dislocations inside double-walled carbon nanotubes [15,16], graphene [5,7] and boron nitride [6,7] can still be applied. In this model, the upper and bottom layers are represented by two chains of particles connected by harmonic springs and coupled through van der Waals interactions. To consider ESDs we suppose that particle-spring pairs correspond to ribbons of the layers parallel to the edge. The edges are assumed to be straight so that relative displacements of atoms in the layers at each edge of the upper layer depend only of the coordinate x along the normal to the edge. We also restrict our consideration to the case when the density of dislocations is low so that the interaction between ESDs and PSDs inside the layers can be neglected.

Let us first review the main conclusions of the two-chain Frenkel-Kontorova model for PSDs in graphene [5–7]. The first conclusion is that the path of PSDs, i.e. the dependence of relative displacement of the layers $\vec{u}(x)$ on the coordinate x perpendicular to the boundary between commensurate domains that minimizes the formation energy, lies along the straight line between adjacent energy minima AB and AC. Therefore, in this case the dislocation path is parallel to the Burgers vector, which describes the change of the relative displacement of the layers at the final and initial points of the dislocation path (Fig. 1a), at any point along the path. In the limit of an isolated PSD, the magnitude of the relative displacement of the layers $u(x)$ along the dislocation path (or along the direction of the Burgers vector) is determined by equality in the densities of the elastic and interlayer interaction energies

$$\frac{1}{4}K(\beta)l^2|u'|^2 = V(u), \tag{1}$$

where u is in units of the bond length l and changes from 0 to $u_e = 1$, which corresponds to the change in the relative displacements of the layers over the boundary between commensurate domains, $V(u)$ is the interlayer interaction energy per unit area, $|u'| = du/dx$ is the relative strain in the layers associated with formation of the dislocation, β is the angle between the Burgers vector and normal to the boundary between commensurate domains, $K(\beta) = E\cos^2\beta + G\sin^2\beta$ describes the dependence of the elastic constant on fractions of tensile and shear character in the dislocation, $E = k/(1 - \nu^2)$ and $G = k/2(1 + \nu)$ are the tensile and shear elastic constants per unit area, respectively, k=Yd is the elastic constant under uniaxial stress and ν is the Poisson ratio. In the present paper, we use the following parameters for graphene obtained by density functional theory calculations [7] using the vdW-DF2 functional [21]: l=1.430 Å, $k = 331 \pm 1$ J/m^2, $\nu = 0.174 \pm 0.002$ and the barrier to relative sliding of graphene layers $V_{max} = 1.61$ meV/atom (in meV per atom in the upper/adsorbed layer).

It can be noted that consideration of a pair of chains only one of which is infinite and the other one is semi-infinite in the Frenkel-Kontorova model instead of two infinite chains does not change the