The role of octagonal defects in the electronic properties of graphene nanoribbons and carbon nanotubes

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Abstract

Graphene grown in the laboratory presents structural defects and grain boundaries, which have been observed with various experimental techniques. Topological defects are also common at junctions between different carbon nanotubes. Defects and grain boundaries focus recently a lot of interest because they can strongly influence the transport and magnetic properties of graphene-based products and devices. Here, we investigate the electronic properties of several graphene structures containing defects built of octagonal rings. These rings are commonly present at grain boundaries and defect lines in graphene [1,2], but they also occur at locally isolated and reconstructed divacancies [3,4]. Octagonal defects may also appear at strongly curved graphene or at diagonal junctions between carbon nanotubes.

We summarize our very recent findings concerning octagonal defects at (a) junctions between zigzag graphene nanoribbons [5], (b) diagonal junctions between zigzag carbon tubes [6], and (c) isolated divacancies in graphene ribbons and carbon nanotubes [7]. We work in the π-electron tight-binding approximation and the electron interaction effects are taken into account by the Hubbard model. The junction between zigzag graphene ribbons (case a) has a form of a defect line built of octagons or octagons accompanied by pentagon pairs. We show that the octagon-localized states, with energies at the Fermi level (see Fig.1), can be univocally derived from the edge states of the zigzag nanoribbons [8]. This is because the octagons in defect lines show up only as the result of the specific shape of the joined edges. Additionally, the results of Hubbard calculations reveal that junctions built of octagons may show spontaneous magnetization.

The isolated octagonal defects (cases b and c) also lead to the appearance of states at the Fermi energy. By disconnecting such octagons from the graphene network we are able to explain the origin of the defect-localized states. We prove that they are directly related to the doubly degenerate zero-energy levels of carbon rings forming the octagonal topological defects (see Fig. 2). In the case of isolated divacancies, the octagons are accompanied by a pair of pentagons. Since the pentagons mix the graphene sublattices, the energies of the defect-localized states are shifted from the Fermi level. In the wide-gap semiconducting graphene ribbons or carbon nanotubes tubes, the defect-localized states may appear in the energy gap and can act as acceptor or donor states (see Fig.3).

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Figures

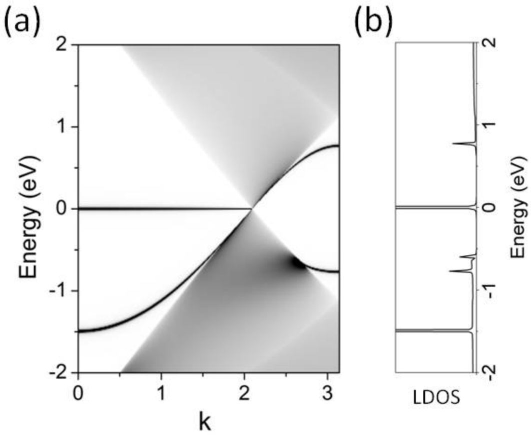

Fig.1. (a) Local density of states (LDOS) at the interface between two zigzag graphene half planes; the junction constitutes a defect line built of octagons and pentagon-pairs. (b) LDOS at the interface between two (8,0) nanotubes with an octagon–pentagon-pair junction. Flat band and peaks at E_F correspond to the states localized at octagons.

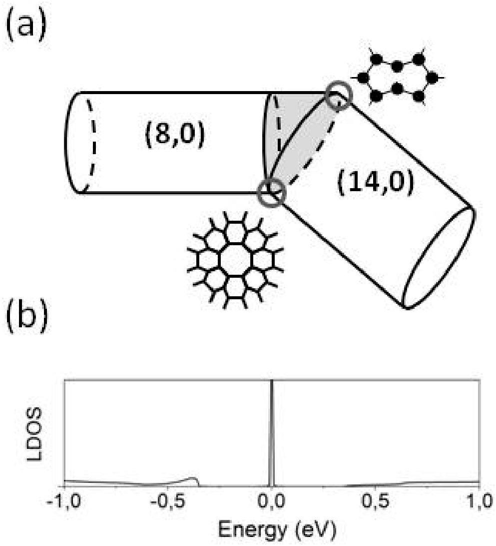

Fig. 2. (a) Schematic diagonal junction between zigzag (8,0) and (14,0) nanotubes. The circles mark the positions of the octagonal defects. (b) Local density of states (LDOS) at the nanotube junction. The peak at E_F is doubly degenerate and corresponds to the octagon-localized states.

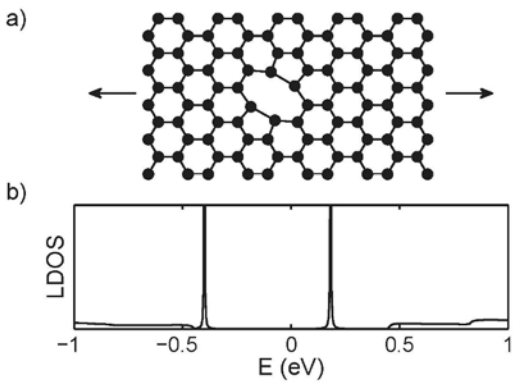

Fig. 3. (a) Geometry and (b) local density of states (LDOS) of the armchair nanoribbon with single divacancy reconstructed to the 5-8-5 defect. The nanoribbon extends horizontally. The gap states originate from octagonal ring. The Fermi level is between the gap states.