Superlattices and Microstructures 87 (2015) 137–142

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Tuning of zero energy states in quantum dots of Silicene and bilayer graphene by electric field

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ARTICLE INFO

Article history:
Received 17 March 2015
Accepted 11 April 2015
Available online 14 May 2015

Keywords:
Silicene
Bilayer graphene
Zero energy states
Electric field
Energy gap

ABSTRACT

Electronic properties of triangular and hexagonal nano-scale quantum dots (QDs) of Silicene and bilayer graphene are studied. It is shown that the low-energy edge-localized electronic states, existing within the size-quantized gap are easily tunable by electric field. The appearance and field evolution of the electronic gap in these zero energy states (ZES) is shown to be very sensitive to QD geometry that permits to design the field-effect scalable QD devices with electronic properties on-demand.

1. Introduction

Interest to new graphene-like materials is related with the rising quest to develop the nano-scale field-effect transistor [1,2], unifying the remarkable electronic properties of graphene with possibility of easy tuning by electric field. Given that the monolayer graphene itself is not quite sensitive to the applied field, the natural way consists in creations of the multi-layer structure with gate-controlled potential difference between layers. Two systems are promising: the artificial monolayer materials, like Silicene, Germanene, etc. [3–6] and bilayer [7] (and in general multilayer) graphene structures. The principal distinction of the first group (we consider Silicene for definitiveness) is their buckled structure that separates A and B atoms of the honeycomb lattice in the transversal direction (Fig. 1a) and provides the required gradient of potential. As a result, the band structure can be

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http://dx.doi.org/10.1016/j.spmi.2015.04.038
0749-6036/

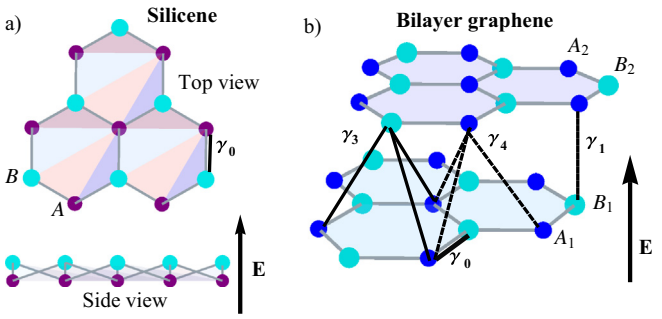

Fig. 1. Structure and coupling parameters for Silicene QD (a) and for graphene bilayer QD (b).

controlled by electric field that tunes the gap and induces transition from a topological insulator to a band insulator [8–11]. The field-provided interlayer potential difference in bilayer graphene (Fig. 1b) also opens a gap between the conduction and the valence bands [7,12], controllable by transistor gate.

Reduction of the lateral dimension of the discussed systems to the size of nanoscale quantum dot (QD) changes however their electronic properties leading to breakdown of the band structure and to enhancement of the role of the edge electronic states [13–21]. Recent studies demonstrated that the electronic properties of QDs in graphene-type materials [22,23] are provided by distribution of the localized edge states in the low-energy spectral region. Depending on the geometrical parameters such as size, shape, edge termination and number of layers the situation can be drastically changed from the uniformly-distributed edge-localized states to the low-energy size-quantized gap with central highly-degenerate peak of zero energy states (ZES) in the middle [23].

In this letter we investigate how the electronic states in Silicene and bilayer graphene QDs can be tuned by the transversal electric field and what impact on the future nanoscale field-effect device engineering can be expected. For calculations we use the standard tight-binding model for clusters with about 450 atoms per layer. We select the most indicative geometries of triangular and hexagonal QDs with zigzag edge termination.

2. Model and density of states

The electronic properties of graphene-type materials in transversal electric field can be calculated using the tight-binding Hamiltonian [7,5],

$$H = \sum_{\langle ij \rangle} t_{ij} c_i^{\dagger} c_j + \sum_i V_i(E) c_i^{\dagger} c_i \tag{1}$$

where $c_i^{\dagger}$ and c_i are the electron creation and annihilation operators, t_{ij} are the inter-site hopping parameters and V_i is the on-site electron potential that depends both on the local atomic environment and on the applied electric field. In cases of Silicene and bilayer graphene the parameters t_{ij} can be written via the nearest neighbor (NN) coupling constants γ_i, as shown in Fig. 1.

Specifying Hamiltonian (1) for the case of Silicene we use the simplified version, appropriate for the low-energy states [10,5]. In this approximation there is only one *in-plane* coupling parameter between sites A and B, $\gamma_0 \simeq 1.6$ eV, whereas the on-site potential, $V_i(E)$ is different for A and B sites and can be presented as $V_i = \xi_i \Delta - \xi_i lE$ where $\xi_i = \pm 1$ for the B and A type of atoms, $\Delta \simeq 3.9$ meV is the effective buckling-gap parameter and lE is the field-provided electrostatic interaction, related to the up/down shift of B and A atoms on $l \simeq 0.23$ Å with respect to the average plane.

For graphene bilayer structure, besides the *in-plane* coupling $\gamma_0 \simeq 3.16$ eV the *interlayer* parameters $\gamma_1 \simeq 0.38$ eV, $\gamma_3 \simeq 0.38$ eV and $\gamma_4 \simeq 0.14$ eV (Fig. 1b) should be also taken into account. The field-dependent on-site potential can be written as $V_i = \eta_i \Delta - \varsigma_i lE$ [7] were $\eta_i = 0$ for A1 and B2 atoms, $\eta_i = 1$ for A2 and B1 atoms and $\varsigma_i = \pm 1$ for atoms, located in the upper (A2, B2) and lower (A1, B1) layers correspondingly (see Fig. 1). The site-environment gap parameter is taken as $\Delta \simeq 22$ meV and the interlayer distance as $2l \simeq 3.5$ Å.