Interlayer Hopping Effects on Energy Bands in Bilayer Graphene (Boron-Carbon-Nitride) Nanoribbons with Zigzag Edges

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The graphite, multi-layer, and single-layer graphene materials have been studied intensively, since the electric field effect has been found in atomically thin graphene films [1]. These materials can be regarded as bulk systems. On the other hand, nanographenes with controlled edge structures have been predicted to have localized states along the zigzag edges [2]. The presence of the edge states has been observed by experiments of scanning tunneling spectroscopy [3,4]. Thus, the studies of the edge states are one of the interesting topics of the field. The recent atomic bottom-up fabrication of nanoribbons really promotes experimental and theoretical investigations [5].

In this paper, bilayer graphene (and boron-carbon-nitride) nanoribbon with zigzag edge is investigated with the tight binding model. Two stacking structures, α and β, are considered. Their structures are shown in Fig. 1. In the α structure, the upper layer is shift by the bond length downward to the position of the lower layer. In the β structure, the lower layer is shift to the right-down direction. In the boron-carbon-nitride nanoribbons, the upper edge atoms are replaced with borons, and the lower edge atoms are substituted with nitrogens. The band splitting is seen in the α structure, while the splitting in the wave number direction is found in the β structure (Fig. 2). The local density of states in the β structure tends to avoid the sites where interlayer hopping interactions are present. The dependence of the number of states on energy reflects the band structures, and this will appear in quantization of conductance experimentally.

In detail, the energy band structures of the systems with the zigzag line number 10 are displayed in Fig. 2, for the single layer (a), the α structure (b), and the β structure (c). The interlayer interaction strength is t_1=0.1t. In Fig. 2 (b), the split of the energy bands is seen compared with Fig. 2 (a). In contrast, split in the perpendicular direction is negligibly small in Fig. 2 (c). The nearly flat band due to the edge state in $2\pi/3 < |kd| < \pi$ is present at the energy E~0 in Figs. 2 (a-c), where d is the unit cell length of the one dimensional direction of Figs. 1 (a) and (b). The energy bands starts at E=1.0t at $|kd|=\pi$, typical to the graphene structure. Comparing Fig. 2 (b) with Fig. 2 (c), the energy split is not seen in Fig. 2 (c), and split in the wave number direction is found.

References

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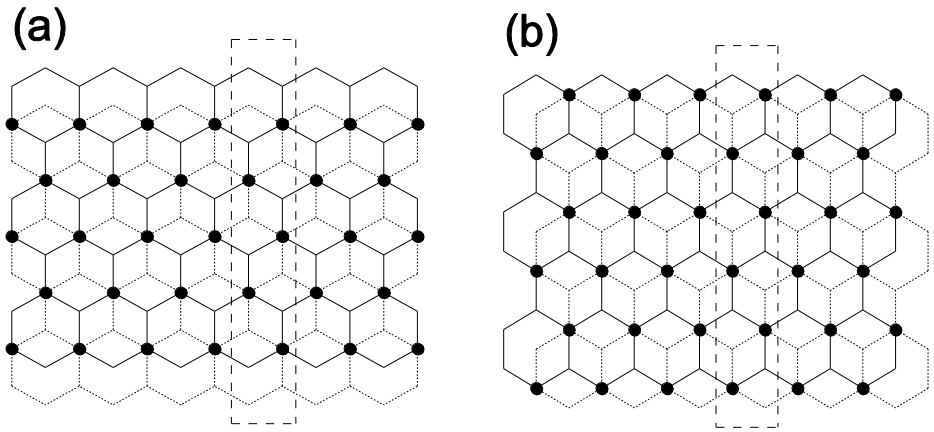
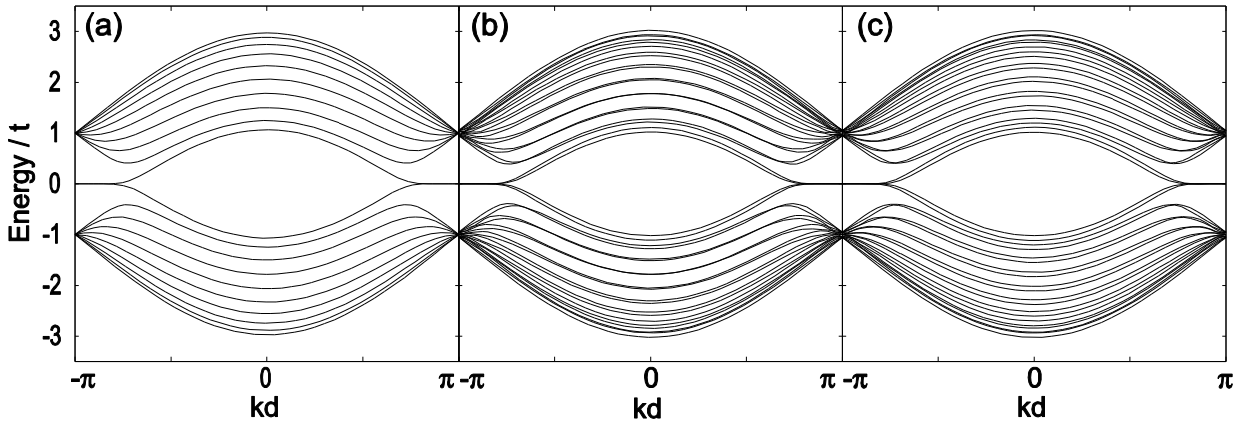
Figure 1



A-B stacked bilayer graphene nanoribbon with zigzag edges. The upper layer is shown by the solid lines,and the lower layer by dotted lines. In the α structure (a), the upper layer is shift by the bond length downward to the position of the lower layer. The region surrounded by the dashed line is the unit cell in the direction of the one dimensional direction. At the circles, two carbon atoms of the upper and lower layers overlap completely, and there is the weak hopping interaction t_1 here. In (b), the β structure is shown, where the lower layer is shift to the right-down direction so the stacking pattern is different from that of the α structure.

Figure 2



Energy band structures in the single layer (a), α structure (b), and β structure (c).