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Electrostatic properties of edge-functionalized graphene nanoribbon under the lateral electric field

Abstract
Nanoscale carbon materials such as carbon nanotube (CNT) and graphene have attracted considerable attention for their potential application as electron emission sources, due to their high structural aspect ratio, high mechanical stiffness and chemical stability, and excellent conductivity produced by sp^2 covalent bonds. It has been reported that CNT and graphene exhibit excellent field emission characteristics.[1, 2]. The field emission phenomenon from these carbon materials strongly depends on their size and shape. Graphene possesses various edge morphologies, which are usually terminated by functional groups depending on the environment [3]. In this work, we investigated the electrostatic properties of edge-functionalized zigzag graphene nanoribbon (ZGNR) by ketone, aldehyde, hydrogen or carboxyl groups to elucidate how the edge functional groups affect the field electron emission from the functionalized edges, using the density functional theory combined with the effective screening medium method.

All calculations were based on the density functional theory with the generalized gradient approximation for describing the exchange–correlation potential among interacting electrons. For the electron-ion interaction, we use ultrasoft pseudopotentials. To apply lateral electric field to ZGNRs, we consider the structural model shown in Fig. 1(a), which is simulated by using the effective screening medium method. The critical electric field for the electron emission from ZGNRs is estimated as the electric field, under which the electrostatic potential at the electrode surface crosses the Fermi level, allowing the tunnelling from nanoribbons to the electrodes [Fig. 1(b)].

Figure 2 shows the critical electric field as a function of the work function of functionalized zigzag edges. The critical electric filed is proportional to the work function of these functionalized edges except the hydroxylated edge. The hydroxylated edge possesses the highest critical electric field, despite the edge possesses the smallest work function among the edges studied here. To clarify the physical orgin of the anormalous behavor of hydroxylaed edge, we show contour and vector plots of electrostatic potential and electric field for functionalized edges of these graphene nanoribbons (Fig. 3). The electric field concentrates at the functionalized edge of graphene, while the field distribution depends on the functional group species. For the hydroxylated edge, we find a potential peak outside the edge and in the vacuum region, leading to an opposite electric field to the external electric field in the vacuum region between the potential peak and the graphene edge. Thus, the potential peak in vacuum region causes the large large critical electric field for field emission, although the hydroxylated edge possesses the smallest work function.

We further studied the potential barrier for field emission from the hydrogenated graphene edge under the external electric field. It is found that the potential barrier decreases with the increase in external electric field at first, and then it increases above the critical electric field at which the electrons are spilled out to the vacuum región. The result indicates that the strong electric field also prevents the electron emission from the hydrogeneated edge (Fig. 4).

References

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[3] R. Taira, A. Yamanaka, and S. Okada, Appl. Phys. Express 9 (2016) 115102

Figures

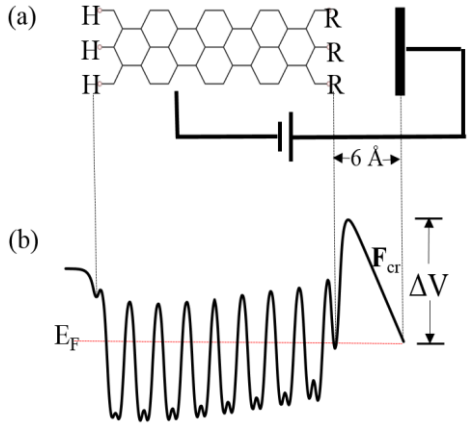

Figure 1: (a) A structural model and (b) schematic diagram of the electrostatic potential for functionalized graphene nanoribbon under the electric field.

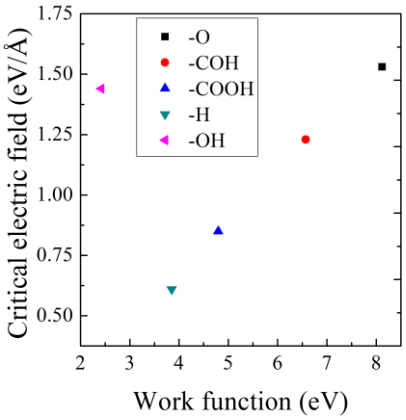

Figure 2: Critical electric field for the electron emission from edge-functionalized ZGNR as a function of work function.

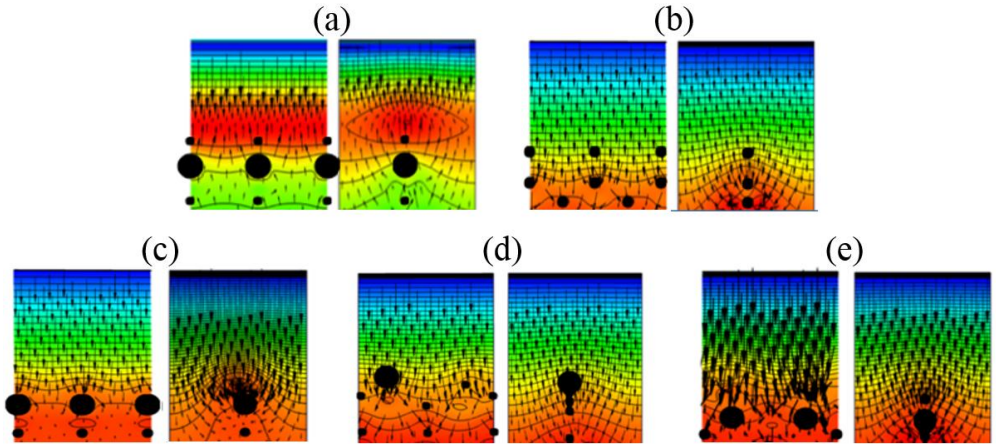

Figure 3: (a) Contour and vector plots of electrostatic potential and electric field, respectively, of ZGNRs functionalized by (a) hydroxyl, (b) H, (c) ketone, (d) aldehyde, and (e) carboxyl functional groups under the critical electric field for the electron emission. The left and right panels in each figure correspond to the parallel and vertical planes of ZGNRs, respectively.

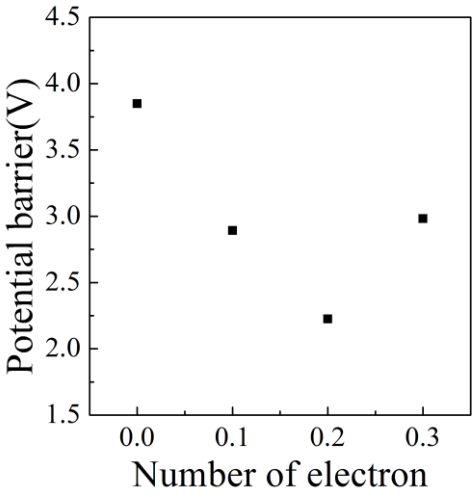

Figure 4: Electrostatic potential barrier (ΔV) in the vacuum region of hydrogenated ZGNR as a function of the number of doped electrons per unit cell.