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Field emission properties of graphene nanostructures under the lateral electric field

Graphene has high structural aspect ratio, high mechanical stiffness, chemical stability, and excellent conductivity arising from its covalent honeycomb network of sp^2 C atoms, which make it a potential material for field emission devices. Indeed, it has been reported that the graphene shows excellent field emission property from its edges, implying that the emission efficiency depends on the edge morphologies of graphene. However, experimentally fabricated graphene-based field emission devices may possess rich variation in their edges morphologies, such as the edge shape variations, functionalized edges, and step structures, depending on the fabricating conditions. In this work, we aim to investigate the electrostatic properties of graphene nanoribbons (GNRs) with various edge morphologies using the density functional theory combined with the effective screening medium method. To investigate how the field emission properties depend on the detailed edge shape, we consider the monolayer graphene nanoribbons (GNRs) with the edge angles of 0º(armchair), 8º, 16º, 24º, and 30º(zigzag). We also consider monolayer zigzag graphene nanoribbon (ZGNR) and armchair graphene nanoribbon (AGNR), whose edges are terminated by H, O, COH, COOH, NH, and OH functional groups. In addition, to clarify thickness effect, we investigate the bilayer and folded GNRs.

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. Structural models studied here are shown in Figs. 1(a), 1(b), and 1(c) for monolayer, bilayer, and folded GNRs. Electric field is applied by the counter electrode using the effective screening medium method.

Our calculation showed that the field emission property of monolayer GNR depend on the edge shape. The armchair edge possesses lower potential barrier and larger field emission current than edges with other shapes due to its small work function. [Fig. 2(a)] Furthermore, edge hydrogenation decreases the potential barrier by introducing an edge dipole moment, causing an increase in the field emission current. [Fig. 2(b)] In addition, for chiral GNRs, the electron emission is primarily attributed to the zigzag portion of edges because of the concentration of electrons arising from either the dangling bond state or the edge state.[1] Aside from the edge shape, the field emission property of monolayer GNR is also sensitive to the functional groups attached the edges. The O and CHO groups increase the potential barrier, decreasing the emission current, while other functional groups decrease the potential barrier, causing the increase in the emission current.[Fig. 2(c)] The potential barrier basically decreases with increasing the electric field, except the case of ZGNR terminated by OH. The anomalous phenomenon for the case of ZGNR terminated by OH is caused by the electrons in the nearly free electron state in the vacuum.[2,3]

For bilayer GNRs, we found that field emission property depends not only on the edge shape but also on the lateral edge displacement. Bilayer armchair GNRs have higher field emission current than those with zigzag edges due to their lower potential barriers for the emission. Moreover, the potential barrier for bilayer GNRs decreases with increasing the lateral displacement irrespective of the edge shape, so that the field emission current from bilayer GNRs increases with increasing the lateral displacement [Fig. 3(a)]. For the folded GNRs, we found that the field emission property is sensitive to the atomic arrangements in the folded moiety. Folded zigzag GNRs have lower potential barrier, producing higher field emission current, compared with folded armchair GNRs [Fig. 3(b)].

References

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[2] Y. Gao and S. Okada, Carbon **142**, 190-195, (2019)
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Figures

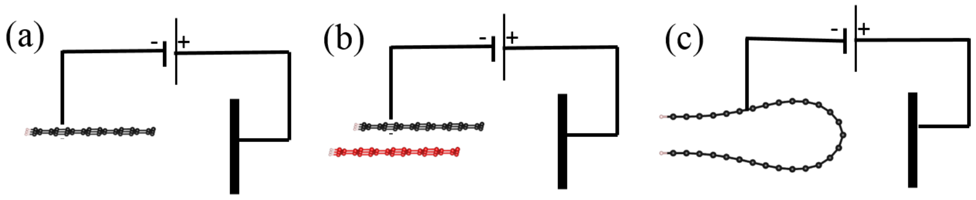

Figure 1: Structural models of (a) the monolayer GNR, (b) bilayer GNR, and (3) folded GNRs under the electric field.

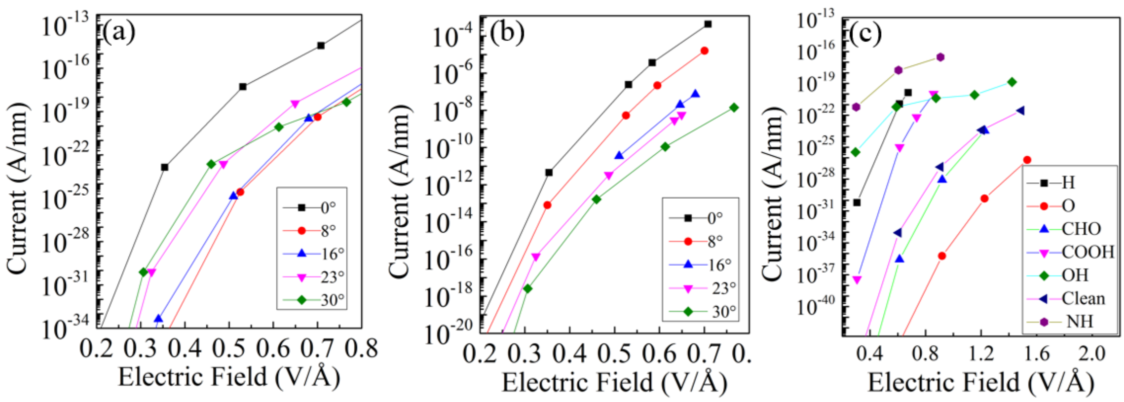

Figure 2: Field emission current of GNRs with (a) clean and (b) hydrogenated edges with various shapes. (c) Field emission current of GNR with functionalized zigzag edge.

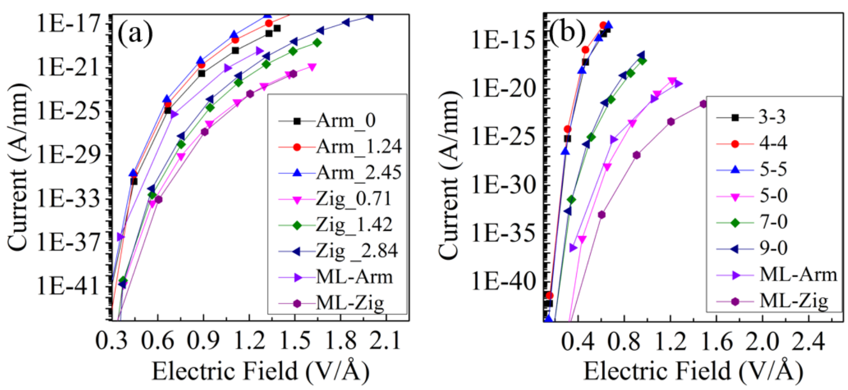

Figure 3: Field emission current of (a) bilayer and (b) folded GNRs.