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Folding and fracture of graphene grown on a Cu(111) foil

A single-crystal graphene film grown on a Cu(111) foil by chemical vapor deposition (CVD) has ribbon-like fold structures. These graphene folds are highly oriented and essentially parallel to each other.^[1] We found Cu surface steps underneath the graphene are along the $\langle 110 \rangle$ and $\langle 211 \rangle$ directions, leading to the formation of the arrays of folds. The folds in the single-layer graphene (SLG) are not continuous but break up into alternating patterns. A “joint” (an AB-stacked bilayer graphene) region connects two neighboring alternating regions, and the breaks are always along zigzag or armchair directions. We are able to *perfectly* reproduce the structures of the fractured folds by paper kirigami. Once we learned this we realized we can present a really clear picture about how the graphene is fractured that consists of several steps including wrinkling, initiation of cracks, propagation of cracks during folding over, and sliding-induced further propagation of cracks. Folds formed in bilayer or few-layer graphene are continuous with no breaks. Molecular dynamics simulations show that SLG suffers a significantly higher compressive stress compared to bilayer graphene when both are under the same compression, thus leading to the rupture of SLG in these fold regions. The fracture strength of a CVD-grown single-crystal SLG film is simulated to be about 70 GPa.^[2] We appreciate support from Institute for Basic Science (IBS-R019-D1).

References

- [1] Luo, D., Wang, M., Li, Y., Kim, C., Yu, K. M., Kim, Y., Han, H., Biswal, M., Huang, M., Kwon, Y., Goo, M., Camacho-Mojica, D. C., Shi, H., Yoo, W. J., Altman, M. S., Shin, H.-J., Ruoff, R. S., *Advanced Materials*, 31 (2019) 1903615.
- [2] Luo, D., Choe, M., Bizard, R. A., Wang, M., Su, H., Huang, M., Jin, S., Li, Y., Kim, M., Pugno, N. M., Ren, B., Lee, Z., Ruoff, R. S., *Advanced Materials*, 34 (2022) 2110509.

Figures

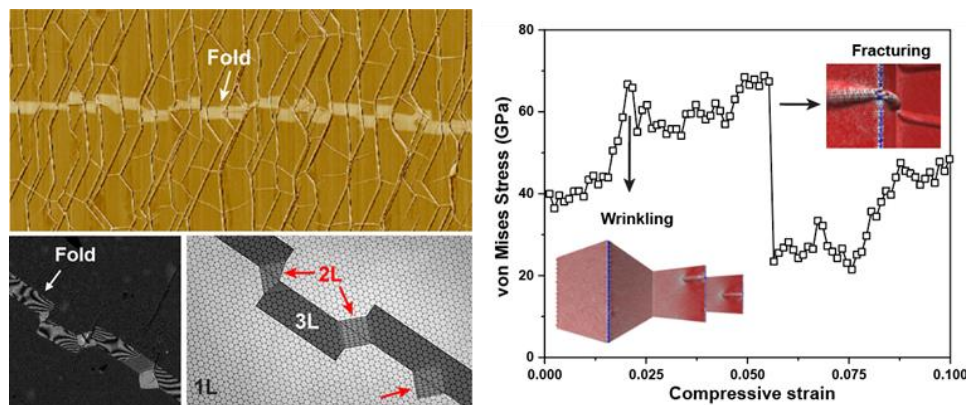


Figure 1: The structure of fold and molecular dynamics simulations showing the fracture of fold.