

Molecular Dynamics Study of Ripples in Graphene and Bilayer Graphene

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Transmission electron microscopy experiments have shown that suspended graphene is not perfectly flat, but displays ripples such that the surface normal of graphene varies by several degrees [1, 2]. For multi-layered graphene, the ripples are suppressed with increasing numbers of layers. Recent experiments demonstrated that ripples in suspended graphene can also be controlled by mechanical and thermally induced strain [3]. Knowledge of and control over the ripples in graphene is desirable for fabricating and designing of strain-based devices. We show using molecular dynamics simulation that thermally induced ripples in suspended single and multi-layer graphene at room temperature result in deviations of the local surface normal by $\pm 7^\circ$ and $\pm 4^\circ$ over regions of 3\AA for single and bilayer graphene, respectively. These angular deviations are in excellent agreement with transmission electron microscopy results [2] and confirm that these ripples can be dynamic in nature. We find scaling relationships for the average angular deviations as a function of size of the graphene layer L and the size of the region over which the angle is averaged R , corresponding to the spot size in transmission electron microscopy. For single layer the average angle scales with R/L and for bilayer it scales as $R/L^{5/4}$. The scaling relations show that, for the same spot size, the measured angular deviations are larger for larger graphene or bilayer graphene sheets. We also study how these angles change as a function of temperature, applied tensile and compressive strain and number of layers in n -layered graphene.

[1] J. C. Meyer *et al.*, Solid State Commun. **143**, 101 (2007).

[2] J. C. Meyer *et al.*, Nature **446**, 60 (2007).

[3] W. Bao *et al.*, Nat. Nanotechnol., **4**, 562 (2009).