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Strain Localization in 2D Materials: a Challenge for Computational Mechanics

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ABSTRACT

Strain engineering offers a promising approach to tuning the physical properties of 2D materials. In the case of transition metal dichalcogenides (TMDs), strain engineering has been applied to modify band gaps and valley polarization, to induce exciton valley hall effect, to engineer phonon dispersion, and to define locations of quantum emitters. Thus, it is important to understand the strain distribution in 2D materials. However, it remains a challenge to measure the strain distribution experimentally with nanoscale resolution. Multiscale computational models may be used to calculate the strain distribution in 2D materials, but computational challenges also exist. In this talk I will present several examples, including strain localization in twisted bilayer graphene and MoS2 as well as pressurized micro/nano-blisters. First, periodic moiré superlattices form in twisted bilayer graphene or MoS2, with inhomogeneous interlayer coupling and lattice deformation. For a small twist angle (typically < 2°), each moiré supercell contains a large number of atoms (>10,000), making it computationally expensive for first-principles and atomistic modeling. Using a finite element method based on a continuum model, we can simulate the inhomogeneous interlayer and intralayer deformations of twisted bilayer graphene and MoS2. Our simulations show that structural relaxation and the induced strain localization are most significant in a relatively large 2D flake at small twist angles, where the strain distribution is highly localized as shear strain solitons along the boundaries between neighboring domains of commensurate AB stacking. This strain localization poses a computational challenge for modeling large areas of 2D materials (>1000 nm) with sub-nanoscale features such as domain walls. As another example, pressurized micro/nano-blisters of bilayer graphene and MoS2 leads to relative sliding and hetero-strains in the bilayer. Again, the localized strain distribution in a relatively large blister (with a diameter of a few microns) poses a challenge for both computational modeling and experiments.

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