Dislocations in Van der Waals Bilayers

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Bilayer systems, such as homo-bilayer graphene, homo-bilayer boron nitride and hero-bilayer graphene/boron nitride, where there is covalent bonding within each layer and van der Waals bonding between layers, show exceptional promise for applications in electronic nanodevices. Building devices from such materials implies the presence of dislocations between layers in most common cases: e.g., misfit dislocations in the hetero-bilayer case or in low angle grain boundaries in the homo-bilayer case where the layers are rotated with respect to one another. In this talk, I will develop a generalized Peierls-Nabarro model for dislocations in the bilayer case and apply it to the prototypical case of edge dislocations in bilayer graphene. This model is based on a continuum elasticity formulation for the deformation and bending of the individual layers and a first principles calculation of the energy as a function of relative displacement of the two flat layers. The resultant dislocations structures buckle the bilayer through a balance between these out-of-plane deformation, strains within the layers and the displacement of the layers relative to one another. I first develop the model, show first principles results for the energy as a function of relative displacement of the two flat layers, predict the structure of these defects and compare the results with recent molecular dynamics simulations.