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Multi-Scale Modeling of Structure and Defects in Layered Materials

Systems and Modeling Approaches

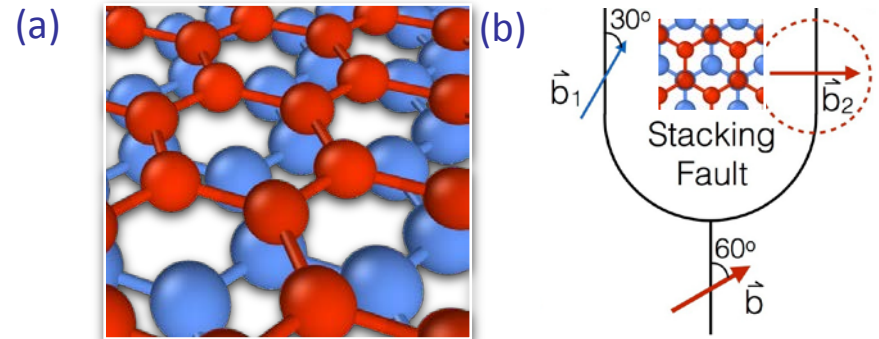
- Dislocations in atomic multilayers
Extended Frenkel-Kontorova models
- Heterophase interfaces in mono/multilayers
Bending and buckling of multilayers
Elastic continuum and Phase Field Crystal

Scope of effort

- Characterize dislocation statics, kinetics, and patterning in atomic multilayers
- Examine grain boundary and heterophase interface properties in mono/multilayers
- Study coexistence and phase transformations between MoS₂ structural polymorphs

Challenges to address

- Model development and solution for new classes of layered materials
- Connections to devices and strain engineering



(a) Atomic representation of bilayer graphene. (b) Characterization of experimentally observed stacking defects as faults and interlayer partial dislocations, b_1 and b_2 , derived from a dissociated perfect 60° dislocation, b .