Department of Materials Science and Engineering

PhD Thesis Proposal

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Location: Bossone 302
Zoom
https://drexel.zoom.us/j/9450049634?pwd=dDlQaHhHT1FJTTRBTE9CbERvdmpmZz09

Deformation of Layered Systems

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Abstract

The conventional understanding of how layered crystalline solids (LCSs) like graphite, mica, and the MAX phases deform has centered on basal dislocations. However, this explanation falls short in accounting for various key observations during graphite deformation. These include non-linear elasticity, the pronounced influence of confining hydrostatic pressures on stress-strain curves, and indications of c-axis strain, among other phenomena. In 2015, a novel mechanism – ripplocations - was introduced to understand the deformation in van der Waals solids. Since then, research has been building a case that atomic layers within LCSs, like other layered systems, experience buckling. Molecular dynamics simulations on graphite and MAX phases have provided insights into this process. Buckling gives rise to the formation of multiple ripplocation boundaries (RBs) with opposite signs, which propagate wavelike through the material to create standing waves. The intriguing aspect is the back-and-forth movement of RBs and the associated interlayer friction. When layers are indented along the c-axis, there are notable pileups around spherical indentations, while indentation edge-on results in delamination cracks. Remarkably, stress-strain (SS) curves in this context exhibit fully reversible loops. The goal of this thesis proposal is to elucidate the fundamental atomistics behind the deformation of layered systems, which include graphite, MAX phase ceramics, and composite systems. The primary tools proposed to accomplish this are molecular dynamics, experimentations, and large-scale modeling tools.