# Precrack fracture behaviors of van der Waals layered materials

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## Abstract

Van der Waals layered materials based on two-dimensional (2D) materials, such as graphene, phosphorene and hexagonal boron nitride, have drawn great attention because of their unique structural, mechanical and optoelectronic properties. However, the existing methods of large-scale production of graphene and other 2D materials as well as their van der Waals layered structures are known to introduce a certain degree of defects in the produced samples. Here, using molecular dynamics (MD) simulations, we investigate the defomration and fracture behavior of defective van der Waals layer materials. Different mechanisms of precrack failure behaviors, i.e., in-plane propagate failure and out of plane propagate failure are systematically studied by regulating the interlayer load capacity of interface. The simulated layered materials include wrinkled graphene, crosslinked graphene, phosphorene, and other 2D materials. A modified deformation tension-shear chain model is proposed by comparing the released energy with fracture energy to describe the failure modes of 2D layered materials. The MD simulation results are in a good consistent with the analytical results.

**Keywords:** Van der Waals layered materials, Precrack, Fracture behavior, MD simulation.