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Edge orientations of mechanically exfoliated anisotropic two-dimensional materials

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Abstract

Mechanical exfoliation is an approach widely applied to prepare high-quality two-dimensional (2D) materials for investigating their intrinsic physical properties. During mechanical exfoliation, in-plane cleavage results in new edges whose orientations play an important role in determining the properties of the as-exfoliated 2D materials especially those with high anisotropy. Here, we systematically investigate the factors affecting the edge orientation of 2D materials obtained by mechanical exfoliation. Our theoretical study manifests that the fractured direction during mechanical exfoliation is determined synergistically by the tearing direction and material anisotropy of fracture energy. For a specific 2D material, our theory enables us to predict the possible edge orientations of the exfoliated flakes as well as their occurring probabilities. The theoretical prediction is experimentally verified by examining the inter-edge angles of the exfoliated flakes of four typical 2D materials including graphene, MoS_2, PtS_2, and black phosphorus. This work not only sheds light on the mechanics of exfoliation of the 2D materials but also provides a new approach to deriving information of edge orientations of mechanically exfoliated 2D materials by data mining of their macroscopic geometric features.

Keywords: Fracture mechanics, Mode-III fracture, Tearing, Two-dimensional materials

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