Ion beam modification of single-layer transition metal dichalcogenides

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Ion irradiation techniques have been extensively used for material modification, post-synthesis engineering and imaging purposes. Although the response of bulk targets to ion irradiation has been studied at length, including simulations, much less is known about the effects of ion bombardment on two-dimensional (2D) materials. 2D transition metal dichalcogenides (TMDs) have shown outstanding physical properties which make them intriguing candidates for various nanoelectronic and optoelectronic applications. We have studied the effects of ion irradiation on freestanding and supported 2D TMDs by using analytical potential molecular dynamics combined with Monte Carlo simulations. We characterized the types and assess the abundance of point defects in our structures as a function of ion energy, mass and incident angle. Furthermore, we studied the irradiation with highly charged ions (HCIs) for fabrication of well-defined pores in MoS_2 monolayer. The simulations indic ated a dependence of the pore size on the potential energy of the projectile and suggested an enrichment in molybdenum in the vicinity of the pore edges. These findings help to understand the fundamental physical mechanisms underlying ion irradiation of low-dimensional materials and finding optimum parameters for defect engineering of 2D TMDs with optimized properties.

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