Shock wave in phosphorene under lateral high-intensive loading

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Layered materials composed of weakly bonded rigid layers are of interest in modern material science since they exhibit new mechanisms of deformation when compressed along the layers. High strain-rate dynamics of such materials remains mostly unexplored, while some of potential applications, such as ballistic protection or high frequency loading, dictate the need for such research. This work is devoted to molecular dynamics investigation of the in-plane shock waves inducing in hexagonal lattices of monolayer phosphorene [1]. The mechanisms of energy dissipation by the lattice are analyzed. The results obtained are compared with those obtained earlier for graphene and boron nitride [2]. The damping of a shock wave in phosphorene is stronger than in graphene and boron nitride, since it has a puckered structure and, therefore, more channels for energy dissipation. Overall, our results contribute to understanding the nonlinear dynamics of localized excitations in two-dimensional materials.

[1] Yang N, Xu X, Zhang G and Li B 2012 *AIP Adv.* **2** 041410
[2] Shepelev I A, Chetverikov A P, Dmitriev S V and Korznikova E A 2020 *Comput. Mater. Sci.* **177** 109549