The size dependence of the mechanical property of the single-layer molybdenum disulfide (MoS_2)

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Abstract

Nowadays, the nanoscale two dimensional materials, such as graphene, black phosphorus, molybdenum disulfide, etc., have attracted considerable attention because of their potential applications in the nanoscale electric and cooling equipment. Understanding the mechanical property of the relevant materials would facilitate their design and application. In this work, the elastic properties including the elastic modulus, Poisson's ratio, shear modulus and bending modulus of the single-layer molybdenum disulfide (MoS2) are investigated based on the nanoscale computational methods. For the elastic modulus, Poisson's ratio and shear modulus, the analytical expressions are derived based on the molecular mechanics framework. Moreover, the molecular dynamics (MD) method is adopted to verify the obtained analytical results. The results indicate that the elastic property of the single-layer MoS2 exhibits pronounced chiral dependence and size effect: as the characteristic size increases, the elastic modulus for armchair direction and zigzag direction increases and decreases, respectively, and gradually approach the same value 178.9 GPa; the Poisson's ratio for two directions decrease monotonously and gradually approach the same value 0.22; the shear modulus increases monotonously and gradually approach the same value 73.32 GPa. As for the bending modulus, a skillful computational method for the nanoscale two dimensional materials is proposed on the basis of the MD simulation. Similarly, the bending modulus exhibits obvious size and chiral dependence. The present results on the mechanical property of MoS2 provide an important reference for the design of the nanoscale product on the basis of this material, and also have an insight into the researches on the mechanical property of the other two dimensional materials. The supports from NSFC (11672063, 11672062, 11772082, 11472117 and 11232003), Young Science and Technology Star Program of Dalian (2016RQ018) and Fundamental Research Funds for the Central Universities are gratefully acknowledged.

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