Absorption and temperature effects on the tensile strength of a black phosphorus ribbon in argon environment

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ABSTRACT

Phosphorus has many allotropes [1-3], among them black phosphorus (BP) has the most stable structure via $3sp^3$ bonds within the same layer and van der Waals interaction between layers. In particular, the few-layer BP is a semiconductor material due to its unique electronic properties, e.g., over 10^4 of drain current modulation, up to 10^3 $cm^2/(V.s)$ of charge-carrier mobility, etc. Hence, wide application in nanodevices of the new two-dimensional material becomes possible.

Due to its excellent electrical properties, a few-layer black phosphorus (BP) ribbon has wide potential application in nano-devices. Its strength is essential for fabrication of the nano-devices. However, BP suffers from severe performance degradation in ambient conditions. In the present study, using argon as shielding gas, we investigate the tensile strength of a few-layer ribbon with consideration of both temperature and gas absorption via molecular dynamics simulations. Results demonstrate that the tensile strength of a BP ribbon is weakened at high temperature. If the ribbon has full relaxation before stretching, its tensile strength can be improved slightly by the argon membrane absorbed onto its surfaces. At 300K, the strength is improved obviously due to gas absorption. The conclusions can be used for potential application in fabrication of few-layer BP ribbons.

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