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An Empirical Description for the Hinge-Like Mechanism in Single-Layer Black Phosphorus: the Angle-Angle Cross Interaction

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Abstract: The single-layer black phosphorus is characterized by its puckered configuration that possesses the hinge-like behavior, which leads to the highly anisotropic in-plane Poisson's ratios and the negative out-of-plane Poisson's ratio. We demonstrate that the hinge-like mechanism can be described by the angle-angle cross interaction, which, combined with the bond stretching and angle bending interactions, is able to provide a good description for the mechanical properties of single-layer black phosphorus. We also propose a nonlinear angle-angle cross interaction, which follows the form of Stillinger-Weber potential and can be advantageous for molecular dynamics simulations of single-layer black phosphorus under large deformation.

Keywords: Black phosphorus, Stillinger-Weber potential, Hinge-like mechanism, Molecular dynamics simulation, Mechanical properties

I. Introduction

The single-layer black phosphorus (SLBP) has anisotropic properties in the two in-plane directions due to its puckered atomic configuration, as shown in FIG. 1. The *x* and *y* axes are in the directions perpendicular or parallel to the pucker. Young's modulus in the *y*-direction is about four times larger than that in the *x*-direction[1-4]. The puckered configuration brings an interesting hinge-like mechanism for the SLBP; i.e., tension along the *y*-direction will generate a strong contraction in the *x*-direction. As a direct result of this hinge-like mechanism, the Poisson's ratio ν_{xy} is much smaller than ν_{yx} [4-5,6]. Furthermore, the Poisson's ratio ν_{yz} is negative owning to the hinge-like mechanism,[3,5,6] which was verified experimentally[7]. The negative Poisson's ratio can typically enhance toughness, shear resistance, and sound absorption. These novel properties will be helpful for medicine[8], fasteners[9], tougher composites[10], tissue engineering[11], national security and defense, e.g. bulletproof vests and armor enhancement[12]. We note that $\nu_{\alpha\beta}=-\epsilon_\beta/\epsilon_\alpha$ is the Poisson's ratio corresponding to the tension of the SLBP along the α-direction, where ϵ_α and ϵ_β are the applied and resultant strains, respectively.

The hinge-like mechanism in SLBP has been discussed based on the structure deformation using first-principles calculations.[3,5] Different from the first-principles calculations, empirical potentials can provide intuitive explanations for physical or mechanical phenomena. In 1982, a valence force field (VFF) model was proposed to describe the interaction for SLBP under small linear deformations[13]. In recent work, we simplified the VFF model by keeping major potential terms, and this simplified VFF model was used to derive the parameters for Stillinger-Weber (SW) potential[14].

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