Nonlinear elastic properties of bismuth monolayer

Zhe Shi (1st and presenting author)

Department of Material Science and Engineering, University of Toronto
114 – 5795 Yonge Street, Toronto, Canada, M2M4J3
zhe.shi@mail.utoronto.ca

Abstract

The intriguing mechanical properties of graphene have motivated many research groups to investigate mechanical behaviors of other monolayer materials. Besides delving into compound such as MoS_2 [1] or hexagonal BN [2], another class of two-dimensional (2D) materials deserving to be studied are the elemental analogues of graphene. Some moved down the carbon column of the periodic table and studied silicene [3], germanene [4], and stanene [5], while others exploring adjacent Group VA elements scrutinized phosphorene [6, 7], arsenene [8], and antimonene [9]. In our work, we investigate the mechanical properties of a heavy member of the Group VA family, honeycomb bismuth monolayer, by density functional theory (DFT) calculations. Specifically, the response of bismuth monolayer under the nonlinear deformation are investigated and higher order elastic constants (up to 4th order) are obtained by analyzing stress–strain relationships that belong to a continuum formulation. It is found that a bismuth monolayer is able to sustain ~30% uniaxial and ~25% biaxial deformation, which is a superior mechanical behavior to many other 2D materials that guarantees the robustness of potential utilization of 2D bismuth.

References

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Figures

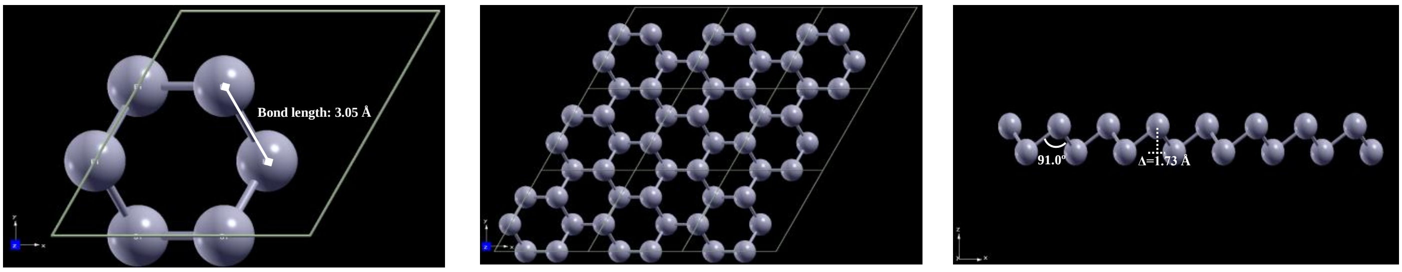

Figure 1. Structural configurations of a buckled bismuth monolayer: (a) a unit cell, (b) top vi

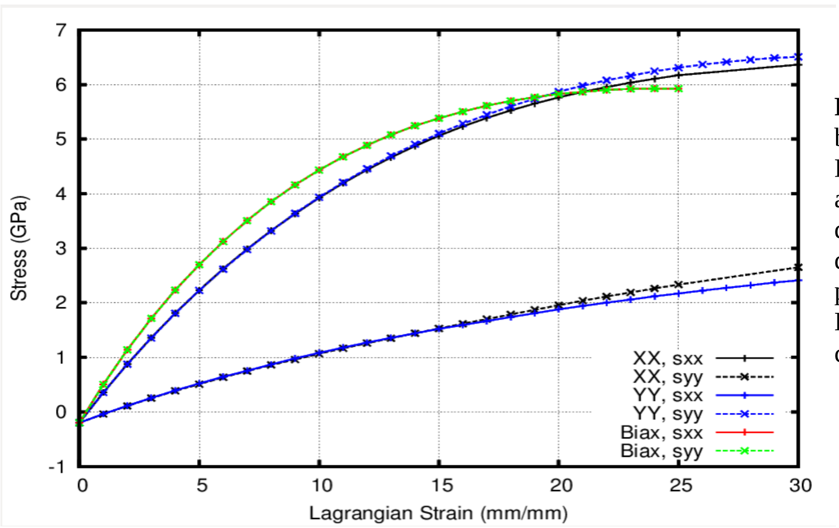

Figure 2. Non-linear stress-strain relationship for bismuth monolayer. The least-squares curve fit to DFT data for two uniaxial (black lines for armchair direction and blues lines for zigzag direction) deformation cases and one biaxial deformation case (green/red). Quantities are plotted in second Piola-Kirchhoff stress (GPa) and Lagrangian strain (mm/mm). Dots represent DFT calculated data and lines depict least-squares fits.