The Study of the Mechanical Properties of Silicon Carbide Monolayer

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The mechanical properties of a silicon carbide (SiC) monolayer were studied theoretically based on total energy calculation. The stiffness of the monolayer, the question of whether the system is isotropic/anisotropic, and the issue of linear/nonlinear behavior were studied based on the response of the monolayer to strain in two different directions (zigzag and armchair). Strain values ranging from 0 to 0.3 were applied separately to these directions. It was hypothesized that the system is anisotropic, undergoes a linear to nonlinear transition as the strain increases, and has a 2D Young's modulus (Y2D) less than that of graphene. Based on the change in total energy, the strain energy densities were calculated, from which both Y2D and the 2D third-order elastic modulus (D2D) were derived. The monolayer is found to be very strong and anisotropic, about 12% stiffer in the armchair direction: Y2D was found to be 197.3 Nm-1 and 221.0 Nm-1 in the zigzag and the armchair directions, respectively. D2D was found to be -772.6 Nm-1 and -901.5 Nm-1 in the zigzag and the armchair directions, respectively. Deformation in the armchair direction caused a yield point at strain = 0.225, whereas the monolayer remained elastic for all strain values tested in the zigzag direction. The monolayer undergoes a transition from linear to nonlinear behavior as strain increases. The hypotheses are supported.

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