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蚕丝的功能化与丝素蛋白基新材料

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Deformation Mechanism of Nano Layered Solid

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Abstract: Graphite consists of carbon atoms arranged in layers of hexagonal lattice. In this research, we aim to obtain the fundamental knowledge about controlling the out-of-plane deformation of graphite with lattice defects. We discuss the simulation result of graphite with arranged lattice defects under compression force using molecular dynamics method. The results of simulation show that out-of-plane deformation like delamination and kink deformation occur. The positions of out-of-plane deformation correspond to the location of dislocations. The out-of-plane deformation is not only affected by the positions of dislocations but misorientation angle due to dislocation array. Compressive stress-compressive strain curve of the simulation shows that maximum compressive stress becomes relatively higher as increasing the number of dislocations. We investigate the mean curvature of each layer of graphite to discuss the amplitude of out-of-plane deformation. We use dip isogon method which is often used to study the folding mechanism of strata in geology to classify the deformation of adjacent layers. From the obtained results, there is possibility of controlling compressive deformation of graphite by arranging dislocations.

Keyword graphite; lattice defect; kink deformation; mean curvature.

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