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Strain-Induced Disorder, Phase Transformations and TRIP in Hexagonal Boron Nitride under Compression and Shear in a Rotational Diamond Anvil Cell: In-Situ X-ray Diffraction Study and Modeling

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It is known that plastic shear significantly reduces the phase transformation (PT) pressure when compared to hydrostatic conditions. Here, a paradoxical result was obtained: PT of hexagonal hBN to superhard wurtzitic wBN under pressure and shear started at the same pressure ~10 GPa as under hydrostatic conditions. To resolve the paradox and to quantitatively study the basic physics and mechanisms, a simultaneous in-situ X-ray diffraction study and modeling of the disorder (the turbostratic staking fault concentration) and PT in hBN were performed. Under hydrostatic pressure, changes in the disorder were negligible. Under compression and shear, a strain-induced disorder was revealed and quantitatively characterized. The strain-induced disorder, in turn suppressed PT; this resolves the paradox. During the strain-induced PT, existence of transformation-induced plasticity (TRIP) was proved. The degree of disorder is suggested as a physical measure of plastic straining which also allows us to quantitatively separate the conventional plasticity and TRIP. TRIP exceeds the conventional plasticity by a factor of 20. In comparison with hydrostatic loading, for the same degree of disorder, plastic shear indeed reduced the PT pressure by a factor of 3-4, as well as caused a complete irreversible PT. Coupled strain-controlled kinetic equations for disorder and PT were derived. The analytical solutions confirm our conclusions and resulted in some predictions. Also, conditions for quasi-uniform pressure distribution were predicted and achieved experimentally. A homogeneous pressure self-multiplication effect was revealed.

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2. V. I. Levitas. Phys. Rev. B. 2004, vol. 70, 184118,1-24.