Compressibility of the high-pressure rocksalt phase of ZnO

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There is a current interest in the derivation of the parameters that define the equation of state (EOS) of polymorphs, that are instable under room conditions [1]. We report the results of a combined experimental and theoretical investigation on the stability and the volume behavior under hydrostatic pressure of the rocksalt (B 1) phase of ZnO. Synchrotron-radiation x-ray powder-diffraction data were obtained from 0 to 30 GPa. Static simulations of the ZnO B 1 phase were performed using the ab initio perubed ion method and the local and nonlocal approximations to the density-functional theory. After the pressure induced transition from the wurtzite phase, we have found that a large fraction of the B 1 high-pressure phase is retained when pressure is released. The metastability of this ZnO polymorph is confirmed through the theoretical evaluation of the Hessian eigenvalues of a nine-parameter potential energy surface. Overall, our results show that the ZnO B 1 phase is slightly more compressible than previously reported. Very good agreement is obtained below 10 GPa. Above this pressure a progressive departure of the theory with the experiment is observed, reaching about 2 % difference at 30 GPa.

Figure 1: Compression curve of the ZnO B1 phase.

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Reference