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Phase transformation of 2H and 6H-SiC at high pressure: An ab initio constant pressure study MURAT DURANDURDU, University of Texas at El Paso, SITKI EKER, Ahi Evran University — We study the pressure-induced phase transition in the 2H-SiC (wurtzite) and 6H-SiC crystals using a constant pressure *ab initio* technique. A first order phase transition to a rocksalt structure in both SiC polytypes is predicted in the constant pressure simulations. The transformation in 2H-SiC consists of two successive processes. First the 2H-SiC crystal transforms into a fivefold coordinated hexagonal structure with space group $P6_3/mmc$ due to a compression in the direction of the c-axis. Second the hexagonal phase becomes unstable in respect to shear deformation and converts to first a fivefold coordinated orthorhombic intermediate state within the $Cmcm$ symmetry, and then a rocksalt state. The phase change in 6H-SiC also proceeds in two stages: 6H-SiC is first compressed along the c-direction and then it undergoes a shear deformation on the $a-b$ planes. This transformation mechanism is quite similar to that of the 2H-SiC-to-rocksalt observed but there is no metastable phase identified along this path. We also study the 2H-to-rocksalt, zinc blende-to-rocksalt and 6H-to-rocksalt phase transformations of SiC from the enthalpy calculations and find that all SiC polytypes show nearly similar equation of state and transforms to a rocksalt structure about 100.0 GPa, in excellent agreement with experiments.

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