General Method for Determining Atomic Pathways in Reconstructive Phase Transitions: SiC and GaN

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We have developed a general method for determining atomic pathways in reconstructive phase transitions in crystalline materials. Using a computer program COMSUBS, we first collect a large number of possible pathways under a set of constraints determined by the user. Second, we estimate the enthalpy barrier for each pathway by finding the barrier along pathways which are linear in the structural parameters. Third, we use the bow-function method to calculate the enthalpy barrier for the pathways with the lowest estimated barriers. Fourth, we search for possible ways to lower the barrier even further along each pathway by lowering the symmetry and increasing the number of structural parameters. We have successfully applied this method to the zincblende-rocksalt transition in SiC and the wurtzite-zincblende transition in GaN.

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