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Determining Atomic Pathways in Reconstructive Structural Transformations. Dorian M. Hatch[a], Harold T. Stokes[a], Jesse Gunter[a], Jianjun Dong[b], James P. Lewis[a], [a]Brigham Young Univ., Provo, UT, 84602, [b]Auburn Univ., Auburn, Alabama, 36849.

Using a computer program we have developed called COMSUBS, we have theoretically investigated the mechanism of the pressure-induced reconstructive zincblende-to-rocksalt phase transition in SiC. COMSUBS gives us a set of possible pathways under a set of constraints determined by the user. Using an enthalpy barrier estimate along a linear pathway and then using a bow-function method to examine the enthalpy barrier we obtain the lowest estimated barriers. Finally, along each pathway we investigate whether lowering of the symmetry would decrease the barrier height. Starting with an extensive survey of 925 possible transition pathways, we found that those with the lowest enthalpy barriers all have a common mechanism: bilayer sliding of (111) planes. We will also discuss the transformation in GaN.

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