Maximal Symmetry Transition Paths for Reconstructive Phase Transitions

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The transition path of a phase transition with no group-subgroup relation between their phases (as reconstructive phase transitions) can be defined as the set of atomic displacements, and strains that should occur at a local level during the transformation. The maximal symmetry transition paths are characterized by intermediate structural configurations with symmetries given by maximal common subgroups of the space groups of the two end phases. Additional symmetry constraints follow from the compatibility conditions of the occupied atomic positions at both ends of the path. By definition, the symmetry of any possible transition path must be among those maximal symmetry paths, or their subgroups. Recently, we have developed a systematic procedure for the determination of the full set of possible maximal transition paths between two structure types with no group-subgroup relations between their symmetries. A computer program has been implemented at the Bilbao Crystallographic Server (http://www.cryst.ehu.es) [1].

Here we present the results of our search of maximal symmetry transition-paths for some typical cases of reconstructive phase transitions (*e.g.* wurtzite to rocksalt, wurtzite to zincblende or zincblende to rocksalt structure types, *etc.*) [2].

[1] Kroumova E., Perez-Mato J.M, Aroyo M.I., Kirov A., Capillas C., Ivantchev S., Wondratschek H., *Phase Transitions*, 2003, **76**, 155-170. [2] Perez-Mato J.M, Aroyo M.I, Capillas C., Blaha P., Schwarz, *Phys. Rev. Lett.*, 2003, **90**, 4, 049603.

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