Nucleation and Growth Mechanisms in Solid-Solid Phase Transitions

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We present a recent powerful strategy[1-4] to elucidate the mechanistic details of reconstructive phase transitions at the experimental temperature and pressure. We implement molecular dynamics simulations, starting from putative intermediates worked out with a topological approach[2,5], and obtain a first dynamic trajectory. A path sampling scheme [6] is applyed on top of this, which allows driving the system towards the most probable transition route.

With this scaffolding we are able to discriminate between many mechanisms suggested for the B1-B2 transition in ionic compounds. For NaCl we find the Hyde&O'Keeffe mechanism to be favored. Furthermore, the process starts at a single ionic site , followed by layer displacement and setup of an interface of B33 structure between regions of B1 and B2 structure. With many variations on the form and on the propagation of the interface, the mechanism dominates in the compound class of alkali halogenides.

The approach opens new simulation scenariois at a level of detail that was not accessible up to now. Furthermore it allows discriminatingbetween many possible mechanisms in favor of the most probable, real mechanism.

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