Abstract

Structural phase transitions in crystals, induced by pressure or temperature, are interesting for fundamental and practical reasons. Transforming the structure and all related physical properties, they offer a possibility of creating new materials with unusual properties, as demonstrated by the well-known graphite-to-diamond transformation in carbon. In spite of substantial progress in their modelling during past two decades, there is still a significant gap in our understanding of the transformation pathways, especially under realistic conditions, such as the presence of defects, non-hydrostatic stress, metastability, etc. This gap in fundamental understanding is clearly seen in our inability to predict the experimental outcome of structural transitions when strong kinetic effects are involved, such as, e.g. decompression of the β-tin phase of Si. Perhaps even more importantly, from the practical point of view, the gap also directly impacts possible technological applications such as steering the transition towards the creation of a desired phase with interesting/useful properties. This thesis consists of six parts: (a) in the first part, we show an already published metadynamics scheme which can induce a nucleating regime in the solid-solid phase transitions and demonstrate it for the B1-B2 transition in NaCl, (b) in the second part, we move from the homogeneous nucleation and apply this scheme to the case of the nucleation on grain boundaries, (c) in the third part, we apply this scheme to the graphite to diamond transition in carbon, also studying dislocation loops, (d) in the fourth part, we show preliminary results of the application of the scheme to the post-diamond phases of carbon aiming to answer the question of how the BC8 phase can be synthesized and outline the construction of machine learning CVs aiming to answer this question, (e) in the fifth part, we apply a similar scheme to the α-ω and ω-α transitions in titanium, and finally (f) in the last part, we present an algorithm for the quantitative assessment of the suitability of the CVs in the metadynamics simulations.

Key words: structural transformations • metadynamics • metastability