Interface amorphization: a molecular dynamics approach

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Abstract

A two-dimensional molecular dynamics model is introduced in order to obtain a better understanding of interface amorphization. We start from a monodisperse system of particles arranged on a perfect two-dimensional triangular lattice, which is divided into two separate regions. In one of these regions the particle size is uniformly reduced, while in the other it is enlarged, preserving the total system 'volume'. Using a whole wealth of diagnostic tools, and visualizations of the particle distributions, a clear distinction between the bulk and the interface disordering transition emerges. Several interesting phenomena, such as the formation of defects, hysteresis of the transition, single-layer displacement and grain boundary development in the vicinity of the interface, show up in our simulations.