



Seminar

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Thursday, 22.02.2011
Beginning 16h00
Bâtiment des Sciences BS 3.04

Crystallization of a binary Lennard-Jones mixture

Transition interface path sampling combined with straightforward molecular dynamics simulation was applied to study the mechanism and kinetics of the crystallization of an undercooled 3:1 binary Lennard-Jones mixture with diameter ratio 0.85 and equal interaction strengths. We find that this mixture freezes via the formation of crystalline clusters consisting of an fcc-rich core and a bcc-rich surface layer, with an excess of large particles and particle species distributed randomly. A detailed comparison reveals that the transition mechanism is similar to that of the pure fluid, but occurs with much smaller nucleation rates even at comparable degrees of undercooling. Also, the growth of the crystalline cluster in the mixture proceeds at a pace about one order of magnitude slower than in the pure system. Possibly, this slow dynamics of the mixture is related to the occurrence and subsequent relaxation of icosahedral structures in the growing crystal.