Exploring Reaction Mechanisms from Atomistic Simulations: New Insights in Crystal Nucleation, Phase Transitions and Segregation Processes

Recent advances in molecular dynamics simulations of complex processes opened new perspectives for the exploration of phase transitions and the segregation of phases at the atomistic level of detail. Along this line, we investigated the nucleation and growth of new structures such as vapor bubble formation during the boiling of water[1] and the morphogenesis of domains and grain boundary formation in pressure-induced phase transitions[2,3]. Our most recent work is focused on phase transformations in heterogeneous systems. These studies range from very initial aggregation steps to nano-crystal formation from solution[4,5,6]. Moreover, we explore the solidification of multinary melts leading to mixed crystal formation and/or impurity segregation[7].

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