Spinodal decomposition in binary alloys in bulk materials and nanoparticles

B. Gajdics1, J. Tomán1, G. Demange2, H. Zapolsky2, Z. Erdélyi1

1Department of Solid State Physics, University of Debrecen, P.O. Box 400, H-4002 Debrecen, Hungary
2Normandie Univ, UNIROUEN, INSA Rouen, CNRS, Groupe de Physique des Matériaux, Rouen, France

In the framework of EXMONAN, we have developed a new 3D atomistic computer simulation technique, called stochastic kinetic mean field (SKMF). [1,2] In this contribution we compare the SKMF to phase field (PF) for the case of spinodal decomposition in bulk materials. We emphasize their similarities and differences and also compare the results to analytical calculation based on the classical Cahn-Hilliard theory. Then we show the advantages of SKMF through an example: spinodal decomposition in nanoparticles. This is motivated by the experimental finding that the decomposition of bimetallic particles depends on not only their size but also their composition. [3]