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Spinodal decomposition in binary alloys in bulk materials and nanoparticles

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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]

[1] Erdélyi Z, Pasichnyy M, Bezpalcuk V, Tomán JJ, Gajdics B, Gusak AM, Stochastic kinetic mean field model, *COMPUTER PHYSICS COMMUNICATIONS* 204: pp. 31-37 (2016)

[2] Open source code: <http://skmf.eu>

[3] G. Radnóczy, E. Bokányi, Z. Erdélyi, F. Misják, Size dependent spinodal decomposition in Cu-Ag nanoparticles, *ACTA MATERIALIA* 123: pp. 82-89 (2017)