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Size dependent spinodal decomposition in Cu-Ag nanoparticles

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Nanoparticles are of considerable interest, owing to their size-dependent properties, different from those of bulk materials. For revealing internal atomic processes in them, individual nanoparticles of Cu-Ag alloys were grown by direct current (DC) magnetron sputtering. Phase-separation during growth in Cu-Ag particles was found to be size- and composition-dependent. Particles below 5 nm in diameter grow as a solid solution of the components for all compositions (15–80 at% Ag). In the low Ag content range (15 and 30 at% Ag) phase-separation occurs only for particles above 5 nm in diameter. The separation into Cu-rich and Ag-rich domains, when observed, takes place by spinodal decomposition for all particle sizes. In particles undergoing incomplete coalescence, phase-separation occurs even if the diameter of the colliding particles is below 5 nm. In the higher Ag content range (60-80 at%), however, no phase-separation is observed until coalescence sets in. Lattice parameter measurements in alloy particles of 30 at% Ag revealed that the miscibility gap in individual particles varies between 70 and 90 at%. Calculation of the composition dependence of the critical length for spinodal decomposition based on the Cahn-Hilliard theory provided quantitative explanation for the observed phenomena. [1] Besides, computer simulations using the Stochastic Kinetic Mean Filed model (skmf.eu, open source) [2] have also been performed which confirmed the results of the analytical calculations.

[1] G. Radnóczi, E. Bokányi, Z. Erdélyi, F. Misják, ACTA MATERIALIA 123: pp. 82-89. (2017)
[2] Erdélyi Z, Pasichnyy M, Bezpalchuk V, Tomán JJ, Gajdics B, Gusak AM, COMPUTER PHYSICS COMMUNICATIONS 204: pp. 31-37. (2016)

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