MONTE CARLO SIMULATIONS OF EQUILIBRIUM PHASE DIAGRAM OF FE-PT SYSTEM

Dominika Wieczorek[1], Rafał Abdank-Kozubski[1]

[1] Department of Solid State Physics, Faculty of Physisc, Astronomy and Applied Computer Science, Jagiellonian University in Cracow, Poland
dominika.wieczorek@student.uj.edu.pl

The iron - platinum system is characterized by high magnetic anisotropy, thanks to which it became the object of special interest of the technology industry as a candidate for applications in the technology of high density magnetic recording media. [1] The high surface activity and strength of Fe-Pt nanoparticles enables their potential applications in the domain of catalysis. [2] The source of these properties is the internal structure of the alloy - the existence of the $L1_0$ superstructure from low to moderately high temperatures and the presence of the "order - disorder" transition during which the superstructure is lost to a structurally disordered face centered cubic structure. [3]

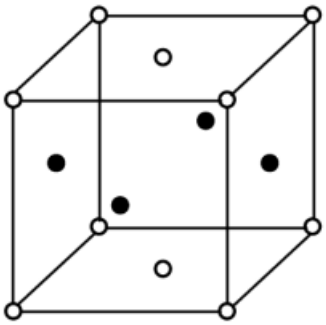

Fig. 1. $L1_0$ superstructure

Computer simulations of the atomic ordering process were carried out in the Fe-Pt system using the Monte Carlo method. The applicability of existing pair interaction parameters in this system for its modeling in a wide range of concentration has been verified by determining the order-disorder transition temperatures for three stoichiometric intermetallic compounds: $FePt_3$, FePt and Fe_3Pt by simulation in a closed system using the "direct exchange" Monte Carlo algorithm. The obtained results were compared with experimental data. The moment of order – disorder transition was identified on the basis of temperature changes of the long range atomic order parameter. Then simulations of the same alloy were performed in a semi-open system using the SGCMC (Semi-Grand Canonical Monte Carlo) method to determine the stability ranges of the superstructures and to create a partial Fe-Pt equilibrium phase diagram. By determining the equilibrium configurations for systems with different platinum concentration at several given temperatures and calculating the long-range atomic order parameter for them the order - disorder transition temperatures were obtained. The results were consistent with the literature data within the limits of uncertainty of calculation.

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[3] S. Brodacka, M. Kozłowski, R. Kozubski, Ch. Goyhenex, G.E. Murch, *Phys. Chem. Chem. Phys*., 2015, **17**, 28394.