High Performance Calculation of Magnetic Properties and Simulation of Nonequilibrium Phenomena in Co-nanofilms

K. V. Nefedev[1] **and V. Yu. Kapitan**[2]

Abstract: The conditions of phase transition into ferromagnetic state and magnetic hysteresis phenomena of the clustered cobalt nanostructures are studied by method of Monte-Carlo simulation. We used data from scanning tunneling microscope images of submonolayer and monolayer Co-films for the construction of programm model. High performance author supercomputer program package was realized by means of parallel execution algorithms.

The clustered cobalt nanostructures were prepared and then researched experimentally in an Omicron Ultra High Vacuum (UHV) system. The base pressure at the deposition and a scanning tunneling microscope (STM) chambers was $3 \cdot 10^{-11}$ Torr. The pixels on STM-images were differentiated into some clustered cobalt atomic levels over brightness. It was assumed in program model, that the all underlying atomic steps are formed as solid wholly, i.e. without pores and vacancy defects in the process of the epitaxial growth. Therefore Co-clusters were constructed by means of filling of $3D$ space face centered cubic (fcc) lattice. Each pixel and, consequently, each point of the model sample was, approximately, 1.443 atoms of fcc-cobalt with lattice parameter 4,089 Å. Total number of atoms N in sample of 100×100 nm 1.5 ML of Co (111) was $2.7 \cdot 10^5$. We use ranges of the pixel brightness values (0-80, 81-120, 121-150, 151-200, 201-255) of gray scale regime, which ones correspond to the various heights of atomic layers.

There are two possible ways for a parallelization of the calculation scheme in the frame of the proposed model for the purpose of large images processing. The first one is the parallel Monte-Carlo (MC) simulation for several parts of the preconfigured dimension for the one large image in subsidiary process and then the insertion of it in the total massive of the system data (with a binding on a boundaries). The second one is the using of parallel tempering for simulation.

The experimental researches, theoretical estimations and MC simulations of a samples with different number of atomic layers showed, that the Co-samples inclusively up to 1.5 ML at the room temperature were at the cluster ferromagnetism state. The simulation data of magnetisation behavior and hysteresis properties were in agreement with theoretical estimations of critical concentration and with experimental data.

[1] Cathedra of Computer Systems
School of Natural Science
Far Eastern Federal University
690950, Sukhanova street 8-43a, Vladivostok, Russia
knefedev@phys.dvgu.ru

[2] Cathedra of Theoretical and Experimental Physics
School of Natural Science
Far Eastern Federal University
690950, Sukhanova street 8-43, Vladivostok, Russia
kvy@live.ru