AB INITIO SIMULATION OF SURFACE EFFECTS IN METALIC NICKEL USING THE CONCEPT SUPERCELL

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This paper presents the results of computer modeling of electronic and magnetic ordering in the surface areas of nickel particles carried in the ab initio *DFT*-approach that takes into account the spin polarization of electron states. Using the computer code *"ESPRESSO"*, based on the methodology of the pseudopotential, the energy spectrum of the hypothetical structural FCT- nickel polytype, constructed in the form of a films "sandwich" has been calculated. Film packs

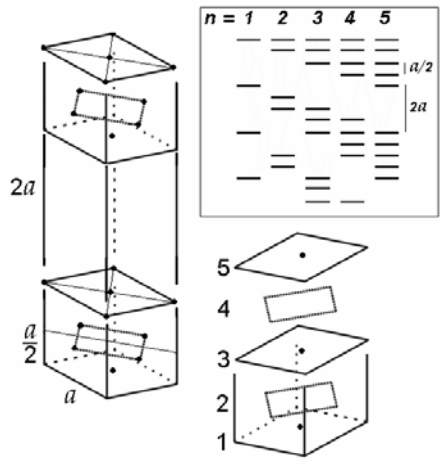

Fig. 1. Building a supercell of nickel

contain n = 1-6 atomic layers and are separated from each other as far as the interaction between atoms of different films can be considered weak. In Fig. 1 shows the method for choosing supercells, the relative position of the films and structure of contained atomic layers.

The data on the electronic spectrum and the density of electronic states of an ideal fcc nickel structure and family its tetragonal polytypes can be understood in a uniform hybridization pattern of strongly and weakly bound electron states for high and low density areas. Using these data, the dependencies the total internal energy (E_{tot}), electronic density of states at the Fermi level $N(E_F)$ and the total magnetization (M_{tot}) on the "capacity" of the layers in supercells (n) are determined. These dependencies are shown in Fig. 2, display the trends both convergence properties of the polytypes with those for an ideal metal (for large n) and the rise of quasi-two-dimensional effects in the system of "weakly interacting layers or films" (for small n). The growth of the share of the

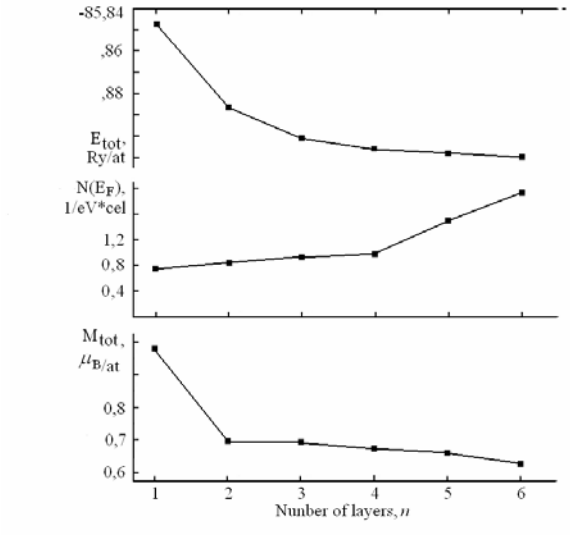

Fig. 2. The properties of nickel polytypes

interlayer spacing in the structure of polytypes with a small number of layers in the package (n = 1-2) leads to a sharp decrease in the effective width of the zones ΔE and to a decrease in the stability of nickel polytypes. At the same time the restriction zones favors the stabilization of the magnetic state with respect to non-magnetic and leads to an increase in the total magnetization, as the effects of spin polarization determined by the parameter $\Delta J/E$, where intra-atomic exchange parameter J varies slaightly in the of family polytypes.

The observed dependence can be used to interpret the features of the electron field dynamics in the nickel cermet in the region of percolation conductivity and superparamagnetic ordering. In the thick-film cermet of Ni-B_2O_3 directional variation in the size of metal particles and the structure of interparticle contacts can reach a maximum value of the anomalous magnetoresistance.