Short-range atomic and magnetic orders in substitution binary alloys and nanosize regions of corresponding orderings

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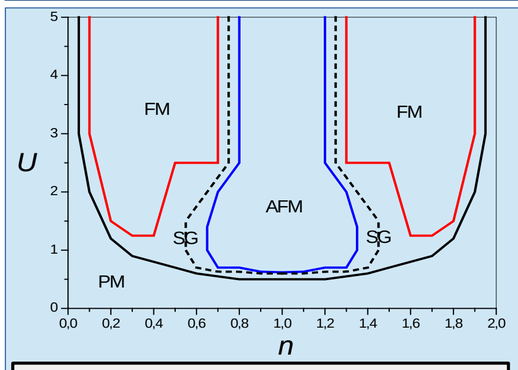
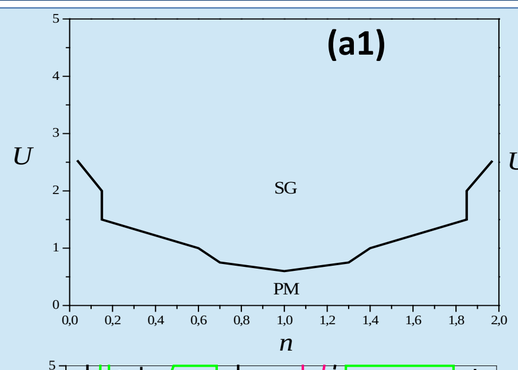
Actuality. Modern nanotechnologies require new materials, the properties of which change radically with relatively small external influences. The most promising from this point of view are systems with strong electron-electron correlations (SECs), in which with changes in temperature, external magnetic field, electron concentration and other external parameters the significant changes in the electronic structure are observed. They cause a wide range of phase transitions: between magnetic ordered and disordered or metal and dielectric states, to the superconducting state and to the modes of charge or spin transports.

Predicting the properties of such systems is inhibited due to the complexity of their theoretical description — it is common to describe only fully ordered or disordered systems. Only cluster methods for calculating the electronic structure allow us to partially advance in the sphere of incomplete magnetic and atomic orders. In this work, within the framework of the cluster expansion method for the one-particle Green's function and the single-band Hubbard model for alloys, the mutual influence of short atomic and magnetic orders and their joint influence on electronic and magnetic characteristics of systems with strong electron correlations are investigated as well as their exhibiting in extent of regions of corresponding orderings.

Model. The substitution binary alloys A_xB_{1-x} at x=0.5 and temperature of 0 K, at the same values of Coulomb repulsion potentials of electrons with opposite spins on one site for atoms of different types ($U_0=U_0^A=U_0^B$) for the value of the impurity scattering potential $W_0=W_0^B-W_0^A=-0.2$ is considered in the semi-elliptic model for the density of states. Energy is measured in units of half-width of the energy zone of a one-component crystal, and localized magnetic moments are measured in Bohr magneton μ_B. For the absence of a magnetic field, the probabilities of finding the projections of localized magnetic moments ($\mu^{\pm}$) in the selected site are the same ($P_0^{\mu+}=P_0^{\mu-}=0.5$). Equilibrium values of magnetic moments and orders parameters are found from the condition of free energy minimum. The parameters of short-range atomic and magnetic orders determine the sizes of regions of corresponding orderings in the investigated strongly correlated alloys.





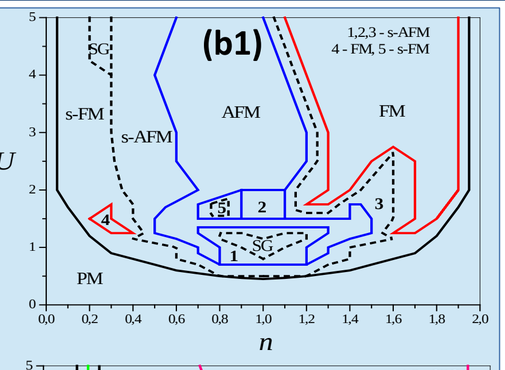
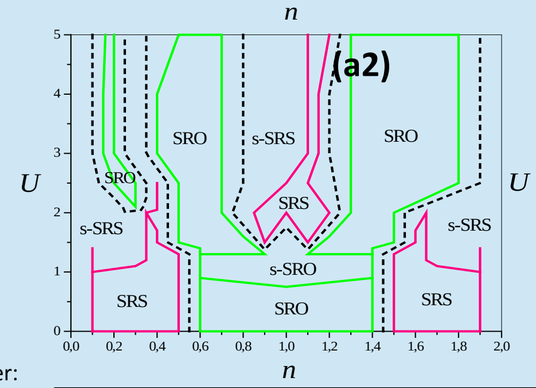
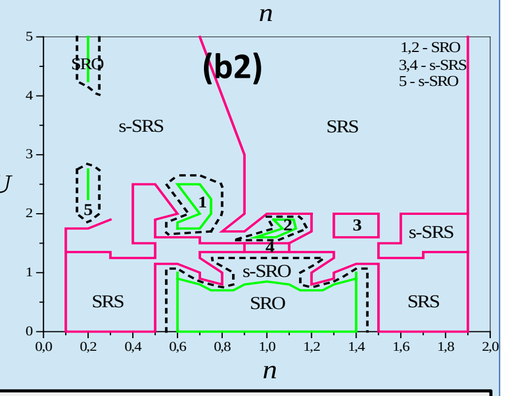


Fig. 1. The magnetic phase diagram (MPD) of a completely atomically disordered (ε_a = 0) substitution binary alloys (*n* is the average electron density per one site).





The sizes of regions with homogeneous magnetic order:

$$\frac{d}{a}=2k=2\cdot\begin{cases}\ln(1/2)(\ln P_{j\,0}^{\mu_\lambda^-/\mu_\lambda^-})^{-1}, & \text{for } \varepsilon_m>0 \text{ (s-FM, FM)},\\ 1, & \text{for } \varepsilon_m\cong 0 \text{ (SG)},\\ \ln(1/2)(\ln P_{j\,0}^{\mu_\lambda^+/\mu_\lambda^-})^{-1}, & \text{for } \varepsilon_m<0 \text{ (s-AFM, AFM)},\end{cases} \quad (1)$$

$$P_{j\,0}^{m_{\lambda'}/m_\lambda}=P_j^{m_{\lambda'}}\pm\varepsilon_{j\,0}^{\mu_{\lambda'}^-\mu_\lambda^-}/P_0^{m_\lambda}\quad(\varepsilon_{j\,0}^{\mu_{\lambda'}^-\mu_\lambda^-}\equiv\varepsilon_m,\lambda=[A,B],m_\lambda=\mu_\lambda^{\pm}).$$

For atomic order one can replase $\mu_\lambda^+\to A$, $\mu_\lambda^-\to B$, $\varepsilon_m\to\varepsilon_a$).

Fig. 2. MPDs for magnetically completely disordered (ε_m = 0) alloys (a1) and alloys with equilibrium values of parameters of atomic (ε_a) and magnetic (ε_m) short orders (b1); (a2, b2) — corresponding to the above MPDs (Figs. a1 and b1) atomic phase diagrams (APD) of substitution binary alloys with SECs.

Results of numerical calculations. The regions on the magnetic phase diagrams (MPDs) (Figs. 1 and 2,a1,b1) are selected according to the following rules: under the condition $\mu^{\pm}\neq 0$ the value of $\varepsilon_m=-0.25$ corresponds to the complete antiferromagnetic (AFM) and $\varepsilon_m=0.25$ — complete ferromagnetic (FM) short orderings; at lower correlations in the orientation of the magnetic moments at neighboring sites we have the states with incomplete antiferromagnetic (s-AFM) ($-0.25<\varepsilon_m<0$) or with incomplete ferromagnetic (s-FM) ($0<\varepsilon_m<0.25$) orderings, which form the transition regions between FM and AFM states, separated by a dotted lines corresponding to the state of the spin glass (SG) ($\varepsilon_m=0$ at $\mu^{\pm}\neq 0$); the paramagnetic (PM) phase is characterized by the values of $\mu^{\pm}=0$.

Similarly, for atomic phase diagrams (APDs) (Figs. 2, a2, b2), the next notations are used: for complete short atomic ordering and stratification — SRO ($\varepsilon_a=-0.25$) and SRS ($\varepsilon_a=0.25$), respectively; for regions with incomplete atomic ordering and stratification — s-SRO and s-SRS, respectively; the dotted line corresponds to the boundary between these phases ($\varepsilon_a=0$).

MPD for the semi-elliptical model for atomically disordered alloys (see Figs. 1, 4,a) agrees qualitatively with the MPD for the real law of electron dispersion [1], but with much smaller violations of electron-hole symmetry. A much larger asymmetry (relative to n=1) is demonstrated by the APD of a magnetically disordered alloys (Fig. 2, a2). The transition to the equilibrium values of both order parameters ε_a and ε_m leads to a significant adjustments of the electronic structure of the alloys (Fig. 3) and changes in their magnetic properties as well as in nature of the magnetic and atomic orders (Figs. 2,b, 4,c).

[1] V. V. Lizunov et al., *Metallofiz. Noveishie Tekhnol.*, **36**, No. 5: 575 (2014).

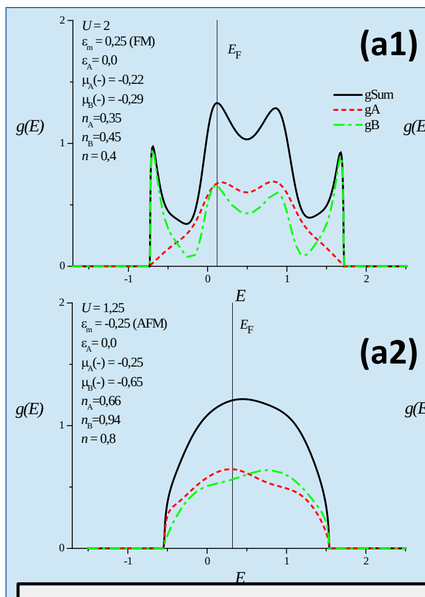


Fig. 3. Densities of electronic states for alloys with ε_a=0 (a1-2) and alloys with equilibrium values of both ε_a and ε_m (b1-2).

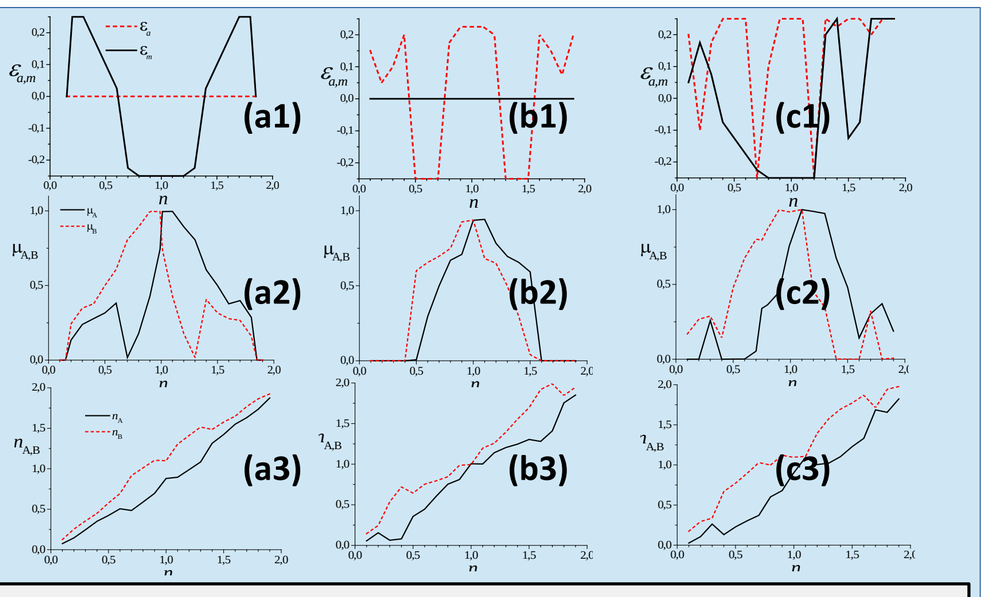


Fig. 4. Dependences of parameters ε_a and ε_m (1), values of magnetic moments (2) and electron concentrations (3) on n (U=2): a — with ε_a=0, b — with ε_m=0, c — with equilibrium values of both ε_a and ε_m , each of them due to Eq. (1) determines the size of region with corresponding homogeneous ordering.

Conclusions. Simultaneous calculation of the equilibrium values of ε_a and ε_m (Figs. 2, b) preserves the general trends in the magnetic ordering of the alloys, but significantly changes the detailed phase distribution of atomic and magnetic ordering everywhere on MPD and APD, except for areas close to PM, where due the small value of U the effect of correlation effects is small. Under the considered conditions, the mutual influence of atomic and magnetic ordering is manifested in the suppression of short range order (SRO) on the APD under the influence of magnetic ordering with the predominance of the tendency to short range atomic stratification. Thereby, according to Eq. (1) and Figs. 2,b, 4,c1, the large domain with atomically ordered structure are suppressed for large range of alloys' parameters due to influence of magnetic ordering, but the different nanosize regions with short-range atomic stratification are predominated.