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CHANGES IN THE ELECTRONIC STRUCTURE OF THE $Fe_{a-x}Mn_xAs$ SYSTEM ALLOYS UNDER UNIAXIAL COMPRESSION

On the basis of *ab initio* calculations using a fully relativistic KKR method to study changes in the control panel, electronic density of states is considered, arising under uniaxial compression of alloys of the $Fe_{2-x}Mn_xAs$ system with P4/nmm symmetry group, where spontaneous and magnetic field induced transitions of AF to the non-collinear LFi_1, LFi_2 phases are observed. From the results of ab initio calculations, the most general regularities of changes in the structure of non-magnetic density of electronic states and the degree of electron filling of N_d as a reaction to the corresponding types of deformation were singled out. The uniform or hydrostatic compression (c/a = const, $\omega < 0$) result in a slight decrease in the population of the *d*-band N_d, an increase in the effective width of the filled and empty part of the d-band $\Delta E = \Delta E_{\text{filled}} + \Delta E_{\text{empty}}$. Compression ($P \parallel c$) along the tetragonal axis stronger reduces the population of the *d*-band, narrows the region of the filled states and expands the area of the empty states in a general increase in the band width ΔE. Uniaxial deformation ($P \perp c$), resulting in an increase in the relative volume of the cell ($\omega > 0$), narrows the field of the empty states while increasing the width of the occupied states in such a way that the effective width of the *d*-band narrows with increasing population of the *d*-band. The features of the effect of each of two factors (the form of the density of electronic states and the number of *d*-electrons) on the stability of magnetically ordered states was analyzed in the framework of a two-site model of itinerant electrons. The parameters used in the model were the value of the intra-exchange interaction J and the number of *d*-electrons per a state that were directly evaluated according to *ab initio* calculations of the electronic structure of $Fe_{2-x}Mn_xAs$ for different types of compression of an elementary cell ω. In full agreement with the experimental data, it was demonstrated that hydrostatic compression and compression along the tetragonal axis have a destabilizing effect on the angular phases LFi_1, LFi_2, and compression in the direction perpendicular to the tetragonal axis direction results in stabilization of LFi_1, LFi_2 states in the course of spontaneous and magnetic field induced transitions of AF–LFi_1–LFi_2.

Keywords: antiferromagnetics, ferrimagnetics, electronic structure, density of electronic states

Fig. 1. Temperature dependences of lattice parameters a, c, magnetization σ and critical fields H_{cr1}, H_{cr2} for the single-crystal $Fe_{0.75}Mn_{1.25}As$ sample [9]

Fig. 2. Onset temperature $T_{s1}(T_{s2})$ of ferrimagnetic (LFi) phase of the $Fe_{0.935}Mn_{1.215}As$ sample (a = 2.15) at different types of compression: $P = P_g$ – hydrostatic compression, $P||c$ – uniaxial compression along the tetragonal axis c; $P \perp c$ – uniaxial compression perpendicular to this axis; ○ – T_{s1}, ● – T_{s2} ($P||c$); △ – T_{s1}, ▲ – T_{s2} ($P = P_g$); ◇ – T_{s1}, ◆ – T_{s2} ($P \perp c$)

Fig. 3. Field dependences of magnetization of the single-crystal $Fe_{0.786}Mn_{1.414}As$ sample (a = 2.2) perpendicular to the tetragonal axis ($C||Z$) (*a*) and along the axis (*б*) under uniaxial compression (P, kbar: *1*, *3*, *4*, *5* – 0.001; *2* – 0.52; *6* – 0.48) and at the temperature (T, K:

1 – 321; *2*, *3* – 343; *4* – 313; *5*, *6* – 331 [7]); *1*, *4* – the initial weakly ferrimagnetic state; *2*, *3*, *5*, *6* – antiferromagnetic state

Fig. 4. Densities of the *d*-electron states of some compounds of the $Fe_{2-x}Mn_xAs$ system in the non-magnetic phase, reduced to the single Fermi level: —— – $x = 1.15$, --- – $x = 1.45$. Symbols E_i, D_j mark the characteristic values of DOS(E)

Fig. 5. Relative volume dependence of electron filling and characteristics of the form of the density of electron states DOS_{dNM}: *a* – uniform compression (c/a = const); *б* – uniaxial compression along *c* axis ($\Delta c < 0$, $\Delta a > 0$); *в* – uniaxial compression perpendicular to *c* axis ($\Delta c > 0$, $\Delta a < 0$); □ – ΔE, ■ – M_{FM}, ○ – $D2$, ● – $D5$, ▲ – ΔE_{occup}, △ – ΔE_{empt}

Fig. 6. Model curves of magnetization in the normal state (△ – m_{FM}, $\omega = 0$; ○ – m_0, $\omega = 0$) and in the deformed state (● – m_0, $|\omega| > 0$; ▲ – m_{FM}, $|\omega| > 0$) at $n = 1.2128$ ($x = 1.31$): *a* – compression ⊥ *c*, $\omega = +0.588\%$; *б* – compression || *c*, $\omega = -0.6\%$; *в* – uniform compression, $\omega = -0.8\%$; *б*, *в* are related to curves *6*, *2* in Fig. 3