Influence of the lattice strain on the Mott-Hubbard ferromagnet characteristics at various shape of the unperturbed density of electronic states

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Under the external pressure the correlation effects if a narrow-band material can be consistenlty described if electron transfer parameters are appropriately renormalized, taking the lattice strain into account. Relative volume change $u = \Delta V / V_0 \sim p$, with p being the pressure and V_0 being unit cell volume causes the bandwidth renormalization $w = w_0(1 + au)$, $a = (V_0 / w_0) \cdot (\partial w / \partial V) < 0$ [1], where w_0 is unperturbed halfbandwidth. Therefore, the transfer integrals in a model of Mott-Hubbard material with non-equivalent subbands [2] are to be also renormalized $t \to t(1 + a_1 u)$, $\tilde{t} \to \tilde{t}(1 + a_2 u)$, with a_1, a_2 analogous to a, for corresponding subbands. Similar renormalization is to be done for other matrix elements describing electron transfer. Below, we assume that subbands are expanding coherently, $a_1 = a_2$.

To analyze the influence of lattice srtain on the magnetic properties of Mott-Hubbard material we calculated, within the Green function formalism, quasiparticle energy spectra in the strong Coulomb repulsion limit. These spectra were used in ground state energy minimization and in magnetization calculation for arbitrary temperature at various shape of the unperturbed density of states (DOS). Details of the applied method can be foung in paper [3]. In case of lattice strained under the external pressure or anion subsysten doping (which can be equivalent to pressure application) the character of ferromagnetic order parameter (magnetization, Curie temperature) appears to be determined by the DOS shape. In particular, in the case of semi-elliptical DOS stability of ferromagnetic order is just slightly improved in whole concentrational interval of spontaneous magnetic ordering and the difference of ground state energies for ferro- and paramagnetic configurations ΔE^{FM} has maximum in this region. For simple cubic (sc) latice close halfbandfilling the magnitude of ΔE^{FM} increases as well but for electron concentration $n<2/3$ ferromagnetic ordering stability weakens which leads to slightly lower magnetization and Curie temperature T_C at increasing strain factor au. Note in this connection that for the narrow-band system $CoS_{2-x}Se_x$ with cubic lattice, in which doping by Se is equivivalent to the external pressure application and expansion of the energy bandwidth a decrease of T_C is also observed [4]. The obtained results for model parameter values $zJ_{eff}/w=0.1$, $2w=1$ eV) reproduce qualitatively correct dependence of T_C on the external pressure and quantitatively agree with the experimental data.

References

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