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On the valence fluctuation phenomena in SmS compounds

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Résumé. — La transition métal non métal et les fluctuations de valence observées dans SmS sont formulées dans le cadre de l'analogie d'alliage. L'importance du couplage électron-phonon dans ces phénomènes est discutée.

Abstract. — The valence fluctuation phenomena, together with the description of the metal insulator transition of SmS are formulated within the alloy analogy picture for correlated d and f electrons. Emphasis is made on the relevance of electron-phonon coupling in these phenomena.

The valence fluctuation phenomena exhibited by the SmS compound, when submitted to pressure, as well as the insulator-metal transition have been extensively discussed in the literature [1, 2]. A treatment using alloy analogy ideas [3] to describe the valence fluctuation regime was developed by Ghatak et al. [2]. In that work the volume dependence of the d and f levels energies was included. The system is described as an alloy \( A_{1-x}B_xS \), where \( x \) denotes the concentration and the species A and B correspond to \( S^{2+} \) and \( S^{4+} \) respectively.

In a recent work [4], it was shown, within a Hartree-Fock treatment for an extended Anderson model, that the electron-phonon interaction could play a central role in the valence fluctuation of europium compounds. Based on that work [4], we intend to qualitatively discuss within the proposed alloy analogy approach [2], how the electron-phonon coupling may be relevant to SmS also.

Starting from a non-degenerate 4-f level, we describe the system by the same Hamiltonian as in ref. [2], but including now an electron-electron interaction among the d-electrons mediated via phonons, in the same way as in ref. [4].

Within the allow analogy approach, the Hamiltonian reads:

\[ H = \sum_i [\varepsilon_i^{(f)} + (U_{ff} - C)n_i^{(f)} + \sum_f (\varepsilon_f^{(d)} + (U_{dd} - C)n_f^{(d)} + U_{df} n_i^{(f)} n_f^{(d)}) + \sum_{i,j,\sigma} T_{ij}^{(d)} d_{i\sigma}^+ d_{j\sigma} + \sum_{i,j,\sigma} T_{ij}^{(f)} f_{i\sigma}^+ f_{j\sigma} + \sum_{i,j,\sigma} \left[ \gamma_{ij} \{ d_{i\sigma}^+ f_{j\sigma} + C.C \} \right]. \]  

The following considerations are behind equation (1). Firstly we assume \( U_{ff} \gg kT \), so the only Coulomb parameter involving the f electrons is \( U_{ff} \). Contrary to reference [2], we do not include implicitly the volume dependence of the energy levels \( \varepsilon_i^{(f)} \) and \( \varepsilon_f^{(d)} \). So the energy levels corresponding to species A and B read:

\[ \varepsilon_A^{(f)} = \varepsilon_f^{(f)} + (U_{ff} - C)n_f^{(d)} + U_{df} n_i^{(f)} \]  

\[ \varepsilon_B^{(f)} = \varepsilon_f^{(f)} + (U_{ff} - C)n_f^{(d)} + U_{df} n_i^{(f)} + C' \]  

We consider \( C' = U_{dd} - C \) as an effective interaction among d electrons. In equation (2), \( U_{df} \) and \( U_{dd}^{(m)} \) stand as expected for the different values of the Coulomb parameters in the insulating and metallic regions of SmS. In fact, screening effects tend to make \( U_{df}^{(m)} \) smaller than the corresponding one in the insulating phase. Consequently, the levels \( \varepsilon_A^{(d)} \) and \( \varepsilon_B^{(d)} \) are separated by a small quantity \( U_{dd}^{(m)}/2 \). In order to ensure the possibility of stabilizing the B species, one needs to overcome in the d levels the contribution \( U_{dd} \), and this can be performed by the dominance of the phonon coupling \( C' \) over the Coulomb interaction \( U_{dd} \), thus making \( C' \) an attractive interaction. Note that \( U_{dd} \) is expected to be small since the d-band is constructed from rare
earth 5d states. On the other hand, the relevance of the coupling between d-states and the lattice is indicated by the large volume effects observed in the metallic phase of SmS. A very crude description of the transition can be obtained neglecting hybridization effects. Firstly introduce $E_g$ as the distance between the f level $E_f^{(0)}$ and the bottom of the d-band in the insulating phase. From equations (2), and adopting a natural band width $\Gamma_0$ for the f band, it will exist a critical distance $E_g^{\text{crit}}$ to have a solution corresponding to a B configuration ($\text{Sm}^{3+}$). For $E_g \approx E_g^{\text{crit}}$ one has only a solution with $n_f = 1$ ($\text{Sm}^{2+}$). The critical value $E_g^{\text{crit}}$ depends on the model parameters. For $E_g \ll E_g^{\text{crit}}$ one finds the solution $n_f = 0$ ($\text{Sm}^{3+}$). For intermediate values of $E_g$, a crossover region can be obtained. In order to improve the agreement with experimental results [5] which predict a first order transition from $n_f = 1$ to $n_f = 0.23$, one has to switch on the hybridization term $\gamma_{ij}$ in order to transfer some occupied d-states to the empty f level in the B configuration. Note that electron-phonon interactions involving f $\leftrightarrow$ d transitions will have also the same effect. Again one can see the importance of electron-phonon interaction on the transition [6].

References