On the valence fluctuation phenomena in SmS compounds
F. Brouers, K. Bennemann, O. De Menezes, A. Troper, A. Gomes

To cite this version:
F. Brouers, K. Bennemann, O. De Menezes, A. Troper, A. Gomes. On the valence fluctuation phenomena in SmS compounds. Journal de Physique Colloques, 1979, 40 (C5), pp.C5-352-C5-353. <10.1051/jphyscol:19795123>. <jpa-00218908>

HAL Id: jpa-00218908
https://hal.archives-ouvertes.fr/jpa-00218908
Submitted on 1 Jan 1979

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
On the valence fluctuation phenomena in SmS compounds

F. Brouers and K. H. Bennemann
Freie Universität Berlin, 1 Berlin 33, F.R.G.

O. L. T. de Menezes, A. Troper and A. A. Gomes
Centro Brasileiro de Pesquisas Fisicas
Av. Wenceslau Braz, 71, Rio de Janeiro, Brasil

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 \( A_{1-x} B_x S \), where \( x \) denotes the concentration and the species A and B correspond to \( S^{2+} \) and \( S^{3+} \) 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 alloy analogy approach, the hamiltonian reads:

\[
\mathcal{H} = \sum_i [\varepsilon^{(0)}_i + iU_{df} \eta^{(0)}_i] \eta^{(0)}_i + \sum_i [\varepsilon^{(0)}_d + (U_{dd} - C)] \eta^{(0)}_d + U_{df} \eta^{(0)}_d \eta^{(0)}_f +
\sum_{i,j,a} T^{(0)}_{ij} d^+_i a^+_j + \sum_{i,j,a} T^{(0)}_{ij} f^+_i c^+_j + \sum_{i,j,a} [\gamma_{ij} \{ d^+_i a^+_j + C.C \}].
\] (1)

The following considerations are behind equation (1). Firstly we assume \( U^{(m)}_{df} \gg kT \), so the only Coulomb parameter involving the f electrons is \( U_{df}^{(m)} \). Contrary to reference [2], we do not include implicitly the volume dependence of the energy levels \( \varepsilon^{(0)}_f \) and \( \varepsilon^{(0)}_d \). So the energy levels corresponding to species A and B read:

\[
\varepsilon^{(0)}_A = \varepsilon^{(0)}_f + U^{(m)}_{df}; \quad \varepsilon^{(0)}_A = \varepsilon^{(0)}_d + U^{(m)}_{df}; \quad \varepsilon^{(0)}_A = \varepsilon^{(0)}_d + U^{(m)}_{df} + C'.
\] (2)

We consider \( C' = U^{(m)}_{dd} - C \) as an effective interaction among d electrons. In equation (2), \( U_{df}^{(m)} \) and \( U_{df}^{(m)} \) 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 metallic phase. Consequently, the levels \( \varepsilon^{(0)}_A \) and \( \varepsilon^{(0)}_B \) are separated by a small quantity \( U_{df}^{(m)}/2 \). In order to ensure the possibility of stabilizing the B species, one needs to overcome in the d levels the contribution \( U_{df}^{(m)} \), and this can be performed by the predominance of the phonon coupling C' over the Coulomb interaction \( U_{dd}^{(m)} \) thus making C' an attractive interaction. Note that \( U_{dd}^{(m)} \) 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 (Sm$^{3+}$). For $E_g \gg E_g^{\text{crit}}$ one has only a solution with $n_f = 1$ (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 $n_f = 0$ (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