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Journal of Alloys and Compounds 424 (2006) 67–72

Journal of ALLOYS AND COMPOUNDS

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Proximity effects on the local magnetic moments of clusters V_6–V_9 embedded in a Fe matrix

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Received 11 January 2006; received in revised form 16 March 2006; accepted 20 March 2006
Available online 19 May 2006

Abstract

The magnetic behavior of clusters V_6–V_9 in bulk Fe is determined by using an electronic Hamiltonian which includes s, p and d electrons. The spin density distribution is calculated self-consistenly in the unrestricted Hartree–Fock approximation. The local magnetic moments are obtained at V and Fe atoms; the magnetic coupling between Fe and V atoms is antiferromagnetic-like. We consider two cases, the first case correspond to non-interacting clusters, the distance between them is infinity, and the another case, when the clusters are interacting, the separation between them is finite; in the first case, the magnetic order in V_6 is ferromagnetic-like whereas for V_9 the magnetic order is antiferromagnetic-like, in the second case we have found that the magnetic order is not well stablished in V_6. We have found that the magnetic order in the matrix is not broken by the presence of the V atoms, although the local magnetic moments of Fe atoms at the interface cluster–matrix, are reduced respect to Fe bulk magnetization ($2.22\mu_B$) [e.g. $\mu_{Fe}(5) = 1.98\mu_B$ in V_6; $\mu_{Fe}(3) = 1.89\mu_B$ in V_9].

JEL classification: 75.75.+a; 75.50.Bb

Keywords: Local magnetic moments; Magnetic order; Magnetic frustrations

1. Introduction

The ability to continually miniaturizing while at the same time increasing the recording density of hard disk drives requires the synthesis of new advanced magnetic materials that, while exhibiting large magnetization density values, can push the existing technologies beyond the superparamagnetic limit. With these points in view, recent efforts have been concentrated to produce new magnetic materials with novel properties such as large magnetic moments and large magnetic anisotropy energy [1], through the choice of different types of atoms and composition [2].

Most of the attention is focused on the use of transition metals (TM) of the Fe group whose electronic and magnetic properties are very sensitive to the structural and chemical environment of the atoms. When 3d transition metals are combined, the magnetic properties of the interface are influenced by the hybridization of the 3d orbitals. A ferromagnetic material can induce, via these d–d hybridizations, a magnetic order in the former paramagnetic material, like V at the interface with Fe; theoretical [3–6] and experimental [7,8] results confirm this fact. This behavior has motivated the production and experimental study of a large variety of complex magnetic materials involving transition metals in different geometrical arrangements: trilayers [9], superlattices [10], multilayers [11].

The Fe–V systems are one of the most studied because to the fact that the hybridizations between V and a magnetic element, like Fe, could induce magnetic ordering in V: Neutron-diffraction studies [8], first-principles calculations [12] and self-consistent tight-binding calculations [6] displayed sizeable magnetization on V atoms, as well as Korringa–Kohn–Rostoker Green-function studies for V impurities in Fe [13] and absorbate V atoms on Fe substrate [14]. Fe–V interfaces can be produced easily using different techniques like molecular beam epitaxy or sputtering [15]. These systems are interesting, not only from the fundamental point of view, but also for their pos-

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doi:10.1016/j.jallcom.2006.03.052

sible applications in new high-density magnetic storage devices [16].

During the last 60 years the magnetism of fine particles embedded in a non-magnetic matrix has been a topic of interest, from both basic and applied viewpoints [17]. In the last few years, the appearance of new experimental techniques capable of generating samples with controlled nanostructures [18] has led to important advances in the understanding of the behavior of these systems.

In this paper, we study the magnetic behavior of V_6–V_9 as non-interacting embedded clusters as interacting embedded clusters in a Fe matrix, the atoms of the clusters are located as substitutional impurities in the bulk b.c.c. Fe. This specific problem has been chosen not only for its potential technological relevance but for the rich magnetic behavior of Fe/V interfaces in particular this system where the magnetic behavior changes as a function of the cluster size and with the distance between them. The competition between the paramagnetism of V and the ferromagnetism of the Fe matrix offers particularly interesting physical situations for studying the interplay between the magnetic properties of clusters and those of their environment. Moreover, the study of finite clusters embedded stresses the local aspects of the magnetic interactions between ferromagnetic and non-magnetic materials, putting aside the translational symmetry of extended interfaces. Therefore, from the perspective of interface magnetism, this work provides complementary information to investigations on Fe–V systems, such as, superlattices, thin V(Fe) films on Fe(V) substrates, etc.

The remainder of the paper is organized as follows. In the next section we present the details on the electronic calculation and, which parameters were used. In Section 3 we present the discussion of our results, and in Section 4 are presented the conclusions of our work.

2. Model

In order to study the magnetic and electronic properties of transition metals clusters, we consider a tight binding scheme within the Hubbard Hamiltonian in the unrestricted Hartree–Fock approximation; details about the hamiltonian can be found in [20]. The diagonal elements of the Hamiltonian can be written as

$$\varepsilon_{i\alpha\sigma} = \varepsilon^0_{i\alpha} + \sum_{\beta}\left(U_{\alpha\beta}\Delta\nu_{i\beta} - \sigma\frac{J_{\alpha\beta}}{2}\mu_{i\beta}\right) + z_i\Omega_\alpha \qquad (1)$$

where $\varepsilon^0_{i\alpha}$ stands for the energy level of the orbital α of atom i in the paramagnetic solution of the bulk (e.g., V or Fe). The second term in Eq. (1) takes into account the level shifts due to the redistribution of the spin polarizated density and to the resulting intra-atomic Coulomb interactions. $\Delta\nu_{i\beta} = \nu_{i\beta} - \nu^0_{i\beta}$, where $\nu_{i\beta} = \langle \hat{n}_{i\beta\uparrow} + \hat{n}_{i\beta\downarrow}\rangle$ is the average electronic occupation of the orbital $i\beta$ and $\nu^0_{i\beta\sigma}$ the corresponding average occupation in the bulk. $\mu_{i\beta} = \langle \hat{n}_{i\beta\uparrow} + \hat{n}_{i\beta\downarrow}\rangle$ refers to the spin polarization of the orbital $i\beta$. The intra-atomic direct and exchange Coulomb integrals are denoted by $U_{\alpha\beta}$ and $J_{\alpha\beta}$, respectively. Finally, the last term in Eq. (1) takes into account the environment-dependent energy-level shifts due to non-orthogonality effects and to the crystal-field potential of the neighboring atoms [21], which are approximately proportional to the local coordination number z_i. The average occupations, $\nu_{i\alpha}$, and the local magnetic moments $\mu_{\mathrm{i}\alpha}$ at site i are determined self-consistenly by requiring

$$\langle \hat{n}_{i\alpha\sigma}\rangle = \int_{-\infty}^{\varepsilon_{\mathrm{F}}} \rho_{i\alpha\sigma}(\varepsilon)\,\mathrm{d}\varepsilon \qquad (2)$$

where $\rho_{i\alpha\sigma}(\varepsilon) = (-1/\pi)\,\mathrm{Im}G_{i\alpha\sigma,i\alpha\sigma}(\varepsilon)$ refers to the local density of states (LDOS) at the spin-orbital $i\alpha\sigma$. In the case of finite embedded clusters the Fermi energy, ε_{F}, is given by the matrix (in the present case Fe). The local Green's functions are calculated by using the recursion method. The number of levels, M, of the continued fraction expansion of $G_{i\alpha\sigma,i\alpha\sigma}$ is chosen large enough so that the calculated orbital occupations and magnetic moments are independent of M; in our calculations we used $M = 17$. All the recursion coefficients are determined exactly without spurious boundary effects. Therefore a large number of atoms (about 25,000–40,000) is involved in the real-space expansion. This model has been used in several calculations of this type, for example, in the study of the magnetism of $\mathrm{Fe_1/V_N}$ nanoinclusions embedded in a Fe matrix [3], interacting Cr clusters in a Fe matrix [4], $\mathrm{V_N}$ free atomic clusters [22], free $\mathrm{Co_N}$ atomic clusters with mixed structures [23], and Co clusters on Pd surface [24].

The parameters used in the calculations are determined as follows. The hopping integrals $t^{\alpha\beta}_{ij}$ between atoms of the same element are fitted to band-structure calculations for the pure elements. The heteronuclear hoppings at the clusters–matrix interface are obtained as the geometric average of the corresponding homonuclear hoppings. This procedure has been proved to be a very good approximation in the study of magnetic properties for alloys and multilayers of transition metals [25,26], and in the study of the magnetic properties of Fe clusters embedded in Cr bulk [20]. In the case of Fe, the d-electron exchange integrals are chosen to yield the proper magnetic moment and exchange splittings ($J_{\mathrm{dd}}(\mathrm{Fe}) = 1.05\,\mathrm{eV}$) in the bulk at $T = 0$. For the case of V, $J_{\mathrm{dd}} = 0.72\,\mathrm{eV}$ is obtained from local spin-density approximation (LSDA) [27] by taking into account a reduction of 20% due to correlation effects beyond the LSDA [28]. Exchange integrals other than J_{dd} are neglected. For simplicity, we ignore the differences between s and p integrals (i.e., $U_{\mathrm{ss}} = U_{\mathrm{sp}} = U_{\mathrm{pp}}$ and $U_{\mathrm{sd}} = U_{\mathrm{dd}}$) and we take the ratios between the direct Coulomb integrals U_{ss}:U_{sd}:U_{dd} from atomic Hartree–Fock calculations [29]. With these approximations, the magnetic properties of TM nanostructured systems [6,3,4,22], have been studied and their results are in good agreement with experimental and another theoretical results.

The V atoms are located as substitutional impurities in the Fe b.c.c. lattice, occupying the full shell of neighbors, we neglect the lattice relaxations around the impurities by fixing the neighboring host atoms at the Fe lattice positions. This assumption is realistic because, in V films on Fe, the V atoms adopt the structure bcc of Fe [31]. The lattice structures around the embedded clusters are illustrated in Figs. 1 and 2; the numbers label the