Spin ordering in chromium layered structures with inserted nonmagnetic monolayers

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Available online 16 March 2005

Abstract

The magnetic structures of Cr/X nanomultilayer systems with nonmagnetic monolayer X are studied in the framework of the Ginzburg-Landau functional approach. A mechanism for spin-density-wave ordering induced by the impurity plane defect is proposed. The spatial distribution of the antiferromagnetic order parameter within the superlattice [Cr/X] is described for various temperatures, for different kinds of inserted monolayers X, and for different thickness of Cr layer. Our results are compared with those recently reported from Mossbauer spectroscopy measurements on epitaxial X/Cr/Sn/Cr multilayers (X = V, Ag, or Fe).
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Keywords: Nonmagnetic monolayers; Mossbauer spectroscopy; Superlattice

1. Introduction

Recently, Mibu and his colleagues succeeded in synthesizing novel epitaxial layered systems of Cr/Sn and X/Cr/Sn/Cr (X = Fe, V, Ag, or Au) with Sn monolayer (ML) embedded in a bcc Cr(001) layer [1–3]. They studied the local magnetic states of Cr-based multilayers using ^{119}Sn Mossbauer spectroscopy. The size of the magnetic hyperfine field induced at the Sn sites is thought to be reflecting the size of the magnetic moments of the surrounding Cr atoms [4]. The magnetic moments and the Neel temperature of Cr in these systems, as inferred from the induced hyperfine fields, were found to change drastically, depending on the nature of the inserted metal X. In the case of [Cr(t)/ Sn(1ML)] superlattices with $t = 5$–40 Å, a large hyperfine field of 11–13T at the ^{119}Sn nuclear sites was observed, which is twice as large as that of a single Sn impurity in a single-crystal bulk Cr. Monatomic Ag layers tend to increase the magnetic moments of Cr at the interfaces, similar to monatomic Sn layers. On the other hand, the V layers appear to suppress the magnetic order within Cr layers, so that the hyperfine field at the Sn sites is almost

zero at room temperature when the Sn–ML is located at 10 Å from the V/Cr interfaces. The Fe layers also tend to reduce the magnetic moments of Cr. It is well known that the antiferromagnetism (AFM) of Cr has an itinerant nature. Electrons at the Fermi surface and its topology determine magnetic structure of Cr and its dilute alloys in the form of spin-density wave (SDW) [5,6]. Hence, any local disturbance of their properties, such as the proximity to paramagnetic or ferromagnetic layers, strain in the film, variations in the crystalline order, etc., should be transmitted over long distances of order of the AFM correlation length $\zeta \sim 10$–15 Å. In this paper, in the framework of a continuum approach, we propose a mechanism of the SDW modification caused by plane defect embedded in an itinerant AFM host. The distribution of the SDW order parameter in layered system [Cr/X] with paramagnetic ML's is analytically described.

2. The functional approach

The ideal multilayered periodical structure [Cr(t)/X(1ML)] can be regarded as the single crystalline Cr host in which each Nth atomic plane (counting along one of the cubic axes) is perfectly replaced by atoms of nonmagnetic metal X. Let us formally assume that the system is not restricted along any direction and denote its period by $t = Na$. The form of a spin density distribution $\vec{S}(\vec{r})$

in an itinerant electron antiferromagnet caused by a plane defect can be understood in the framework of the functional approach. Let us formulate the above approach on the basis of the Ginzburg-Landau expansion for the free energy of the system [Cr(t)/X(1ML)]. We shall analyze only SDW configurations which are inhomogeneous along $\vec{x}$-direction, perpendicular to ML plane, and can be expressed in terms of the order parameter as: $\vec{S}(\vec{r}) = \vec{n}\Delta(x)\cos(2\pi x/a)/g$, where g is an effective potential [7]. In the temperature range under investigation, it is assumed that the order parameter is small, $|\Delta(x)| \ll \pi T$, and varies slowly with the coordinate x, $|\Delta'(x)| \ll \pi T/\xi_0$. Here, ξ_0 is the coherence length, so the expansion of $\Omega(\Delta)$ over $\Delta(x)$ and $\Delta'(x)$ is valid. The interaction of itinerant electrons with the impurity ML inserted into the bulk Cr, is modeled by means of an effective potential U_0. The magnetic functional of the system [Cr(t)/X(1ML)] can be written as the sum of 'volume' and 'impurity' ['ML'] components:

$$\Omega = \Omega_V + \Omega_{ML}. \tag{1}$$

$$\Omega_V[\Delta] = \frac{1}{2}\int (c_1\Delta^2 + v_F^2 c_2\Delta'^2 + c_2\Delta^4)\,dx, \tag{2}$$

$$\Omega_{ML} = \frac{\nu}{2}\sum_i \Delta^2(x_i), \quad x_i = \frac{t}{2}(2i + 1), \tag{3}$$

where x_i is the coordinate of the ith impurity ML, $i = 0, \pm 1, \pm 2, \ldots$. The expression (3) for the energy contribution of the nonmagnetic plane defect and the coefficient $\nu \sim U_0$ can be obtained from the microscopic model of SDW [7]. In Eq. (2) v_F is the Fermi velocity of quasiparticles, c_1 and c_2 are coefficients that depend on temperature and some of the characteristic of Cr band structure like the deviation from ideal itinerant electron and hole pockets. Besides, c_1 changes its sign at the Neel temperature, $c_1 \sim (T - T_N^0)$, and $c_2 > 0$. For the present purposes we ignore the question concerning the effect of an incommensurate modulation of the SDW texture. The order parameter corresponding to the minimum of the functional Ω_V vanishes in the paramagnetic region, $c_1 > 0$, and has a constant amplitude $\Delta_0 = \sqrt{|c_1|/(2c_2)}$ in the commensurate SDW phase, $c_1 < 0$. The order parameter $\Delta(x)$ can be found from the self-consistent equation

$$v_F^2 c_2\Delta'' - c_1\Delta - 2c_2\Delta^3 = 0 \tag{4}$$

and the boundary conditions

$$\Delta(x_i + 0) = \Delta(x_i - 0), \tag{5}$$

$$\Delta'(x_i + 0) - \Delta'(x_i - 0) = \frac{\nu\Delta(x_i)}{v_F^2 c_2} \tag{6}$$

at each point $x = x_i$. The system of Eqs. (4)–(6) is exactly solvable in the class of the Jacobi elliptic functions since the first integral of Eq. (4) is well known. However, the number of solutions for the above equations is large. It can be shown

that in the most energetically favorable state of the system, the SDW period coincides with the geometrical period of the multistructure [Cr(t)/X(1ML)]. Therefore, we shall restrict ourselves to analyze the solutions that satisfy the requirement: $\Delta(x) = \Delta(x + it)$.

3. Results and discussion

There are various modifications of the SDW state provided from a non-magnetic defect: (1) The induced SDW at $\nu < 0$, $c_1 > 0$; (2) The enhanced SDW at $\nu < 0$, $c_1 < 0$; (3) The partially suppressed SDW at $\nu > 0$, $c_1 < 0$. If $\nu > 0$ and $c_1 > 0$, the spin order is not possible. In the temperature range under consideration, such modifications appear on a macroscopic scale of the order of the SDW correlation length, $\zeta(T) \approx \zeta_0|T/T_N^0 - 1|^{-1/2}$. One may expect that even small changes of the electron properties should significantly influence the magnetic state of the nanostructure [Cr(t))/X(1ML)] with finite thickness of Cr layer.

In the case of $\nu < 0$ and $c_1 > 0$, the long-range magnetic order induced by regular row of paramagnetic plane defects exists in the region $T_N^0 < T < T_N$, that is above the Neel temperature of bulk Cr. The SDW profile within a unit cell of the superlattice, $|x| < t/2$, is given by

$$\Delta(x) = k'\Delta_k nc\left(\frac{\Delta_k x}{v_F}, k\right), \tag{7}$$

where k is the modulus of the elliptic function defined from the boundary conditions (5)–(6); $k' = \sqrt{1 - k^2}$, $\Delta_k = \Delta_1/\sqrt{2k^2 - 1}$, $1 > k^2 > 1/2$, $\Delta_1 = v_F/\zeta$ and $\zeta = v_F\sqrt{c_2/c_1}$. Here and in the following we are employing the standard notations for the elliptic functions [8]. For $c_1 > 0$ the SDW structure of the system with $\nu < 0$ is described by the formula (7) with $k' = \sqrt{1 - k^2}$, $\Delta_k = \sqrt{2}\Delta_0/\sqrt{1 - 2k^2}$, $0 < k^2 < 1/2$. For $c_1 < 0$, $\nu > 0$ a single periodical solution of Eqs. (4)–(6) exists:

$$\Delta(x) = k\Delta_k cd\left(\frac{\Delta_k x}{v_F}, k\right), \tag{8}$$

where $\Delta_k = \sqrt{2}\Delta_0/\sqrt{1 + k^2}$, $0 < k < 1$.

Let us discuss some interesting experimental results on the magnetic properties of Cr/Sn and Cr/Sn/Cr/X multilayers in the context of our theory. For $Cr_{1-x}V_x$ alloy systems, a linear decrease of the Neel temperature, the SDW incommensurability wave vector, and the SDW amplitude with increasing V concentration were found [5]. From the standpoint of the 'rigid-band' approach [6], it means that V dissolved in Cr host acts as an ideal electron acceptor. On the other hand, the phase diagram of $Cr_{1-x}Sn_x$ alloys has the commensurate SDW region in the interval $T_N^0(311 \text{ K}) < T < 400 \text{ K}$ at $x > 0.5$ at%. This feature indicates that Sn rather plays the role of an electron donor in Cr host, although the 'rigid-band' picture, rigorously speaking, is not applicable to Cr alloys with nontransition metals.

The magnetic peculiarities of the systems with the chemical modulation of Cr/X type, cannot be considered in the framework of the simple band scheme. Nevertheless, the 'charge-induced SDW' conception [9] allows to treat the X-ML embedded into Cr host as a local doping source. Accordingly, the positive effective potential, $v > 0$, is attributed to V-ML (the local acceptor) and the negative one $v < 0$, is attributed to Sn-ML (the local donor). As it has been mentioned above, in the framework of the present calculation scheme, we explicitly reproduce the SDW profile in the 'central' part of Cr layer, ignoring the details of its configuration in a region near the Cr/X interface whose range is of order of the coherence length. It is clear that the trend of the order parameter behavior persists in this narrow region and the spin magnetic moment at the interface Cr site is proportional to the boundary value of the SDW amplitude, i.e. $\sim \Delta(x - t/2)$. Consequently, in multilayers [Cr(t)/ Sn(1ML)] the hyperfine field at ^{119}Sn site is determined by the same value: $H_{hf} \sim \Delta(t/2)$, where the order parameter $\Delta(x)$ may be evaluated from Eqs. (7) and (8). The behavior of $H_{hf}(t,T)$ as a function of the Cr layer thickness and temperature demostrates the considerable enhancement of the Cr magnetic moment at the Cr/Sn interface, as well as the stabilization of the SDW order in very thin Cr layers at temperatures higher than its bulk Neel temperature. The last fact has been established in ref. [1,2] for superlattices [Cr(t)/ Sn(1ML)] with $t \leq 40$ Å, that is in qualitative agreement with the predictions of our theory.

It should be emphasized that the Sn-ML in the layered structures based on Cr is not only an appropriate probe to study magnetic properties of Cr through Mossbauer spectroscopy, but also the source of perturbation of the spin structure in Cr. As far as the three component multilayered system Cr/Sn/Cr/V is concerned, its magnetic properties are affected by the competition between two effective potentials of different sign and value. Of course, to describe the SDW state in this system our theory has to be modified. But some features observed in [2,3] may be also explained in terms of the present model. In particular, our model explains why the order parameter amplitude decreases near V-ML so that SDW collapses and Cr becomes nonmagnetic below a critical thickness t^*. Thus, within the framework of the rather ordinary continuum model of phase transition in itinerant AFM, we have succeeded in understanding the mechanism of the SDW modification caused by the inserted paramagnetic mono-layers in multilayer structures [Cr(t)/X(1ML)].

Acknowledgements

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