Spin-density-wave ordering in chromium-based layered structures with the insertion of nonmagnetic monatomic layers

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The magnetic structure of Cr/*X* layered systems with inserted nonmagnetic monolayer *X* is studied within the Ginzburg-Landau functional approach. The mechanism of the spin-density-wave (SDW) ordering, induced by the plane defect, is proposed. The spatial distribution of the SDW order parameter is described for various temperature regions, different kinds of inserted monolayers *X* and thickness of Cr layer. The obtained results are compared with recently reported data on the Mössbauer spectroscopy measurements in epitaxial *X*/Cr/Sn/Cr multilayers (*X*=V, Ag, or Fe).

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I. INTRODUCTION

The magnetic properties of ultrathin Cr layers incorporated into the layered nanostructures (bilayers, trilayers, superlattices, and so on) are substantially different from those of bulk chromium.[1,2] The rich magnetic phase diagrams and the structural or compositional aspects, which determine the characteristics of these artificial materials, have been the primary focus of both experimentalists and theorists. Since the discovery of oscillating coupling through a Cr layer in Fe/Cr/Fe trilayers, giant magnetoresistance in Fe/Cr multilayers, as well as many other interesting effects, a considerable attention has been paid to the antiferromagnetism (AFM) of Cr in Fe/Cr layered structures; see, e.g., Refs. 2–4.

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.[5–7] They studied the local magnetic states of Cr-based multilayers using the ^{119}Sn Mössbauer spectroscopy. With the probe layer technique, this method is able to study the element-specific and position-selective spin arrangement. 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.[8] The magnetic moments and the Néel temperature of Cr in these systems, as inferred from induced hyperfine fields, were found to change drastically, depending on the sort of inserted metal *X* as well as the Cr layer thickness *t*. In the case of [Cr(*t*)/Sn(1 ML)] superlattices with $t=5-40$ Å, a large hyperfine field (H_{hf}) of 11–13 T 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,[5] and decreases as the Cr layer thickness *t* increases. The large value of H_{hf}, observed at room temperatures, shows that the magnetic ordering temperature for Cr layers, $T_N(t)$, is much higher than the Néel temperature of bulk Cr, $T_N^{Cr}\approx 311$ K. Monatomic-Ag layers tend to increase the magnetic moments of Cr at the interfaces, similar to monatomic-Sn layers.[6] 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.[6,7] The Fe-ML insertions also tend to reduce the magnetic moments of Cr.[6]

It is established that insertions of nonmagnetic (Sn, V, Ag)-ML strongly modify the characteristics of magnetic ordering in Cr thin layers, while the mechanism of these modifications is not still understood. Moreover, in [Cr(*t*)/Sn(1 ML)] superlattices with $t>42$ Å, the spin structure of Cr changes at low temperature from the "normal" to the "exotic" incommensurate spin-density wave (SDW), with complex modulation, whose wavelength is controlled by the artificial periodicity, induced by the embedded Sn-MLs.[9] These facts prompt us to find the reason of the specific magnetic properties of Cr/*X* layered structures (including Cr/Fe) in the features of a microscopic mechanism of the SDW formation in such systems.

It is well known that the AFM of Cr has an itinerant nature. Electron-electron interaction and topology of the Fermi surface determine the SDW type of magnetic structure in Cr and its dilute alloys.[1,10,11] 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 spin fluctuations correlation length in Cr host $\zeta(T)\gg a$, where $a\approx 2.8$ Å is the parameter of the bcc lattice of chromium. Recently, we have suggested a self-consistent model describing the SDW formation inside the spacer in Fe/Cr/Fe trilayer, based on the idea of charge and spin density redistribution near the metal/metal interface.[12,13] This model, called "contact-induced SDW," was successfully used to analyze the formation of both collinear and noncollinear magnetic configurations in terms of short-range order and "local phase transition" towards the state with spatially inhomogeneous SDW amplitude.[14]

Below, the model described in Refs. 12 and 13 will be generalized to analyze systems of type [Cr(*t*)/*X*(1 ML)] with the nonmagnetic ML insertion. In the framework of a continuum approach, we propose a mechanism of the SDW modification caused by nonmagnetic plane defect embedded in an itinerant AFM host. The distribution of the SDW order parameter in layered system [Cr/*X*] with paramagnetic MLs

is analytically described. The spin density amplitude at the Cr/X interface versus the Cr layer thickness and the temperature is evaluated. The results are used to discuss the local magnetic structure of $[X/\mathrm{Cr}(t)/\mathrm{Sn}(1\ \mathrm{ML})/\mathrm{Cr}(t)]$ multilayers that has been investigated within the ^{119}Sn Mössbauer spectroscopy.

II. THE FUNCTIONAL APPROACH

The ideal multilayered periodical structure $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ 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 $t=\mathrm{N}a/2$.

The form of a spin density distribution $\vec{S}(\vec{r})$ in an itinerant electron AFM caused by a plane defect can be understood in the framework of the functional approach. We assume that both quantum and classical thermodynamic fluctuations of spin density are small and all conditions are satisfied to consider the thermodynamics of the system $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ in the mean-field approximation using the Ginzburg-Landau expansion for the thermodynamic potential Ω. The period t along the $\vec{x}$ axis is much larger than the lattice parameter and the effective dimensionless constant of electron-electron interaction is smaller than unity (condition of a weak interaction).

Below, we analyze only the linearly polarized transverse SDW configurations $S(\vec{r})$, which are varying along $\vec{x}$ direction, perpendicular to ML plane and can be expressed in terms of the order parameter $\Delta(x)$ as

$$\vec{S}(\vec{r}) = \vec{n}\Delta(x)\cos(2\pi x/a)/g, \tag{1}$$

where g is the SDW potential.[10,11]

Let us formulate the above approach on the basis of the Ginzburg-Landau expansion for the thermodynamic potential Ω of the system. In the temperature region under investigation, it is assumed that the order parameter is small, $|\Delta(x)| \ll \pi T$, and varies slowly with the coordinate x, $|\Delta'(x)| \ll \pi T/\xi_0$, so the expansion of the functional $\Omega[\Delta(x),\Delta'(x)]$ in powers of $\Delta(x)$ and $\Delta'(x)$ is valid[12,13]

$$\Omega_V = \tfrac{1}{2}\int (c_1\Delta^2 + \nu_F^2 c_2\Delta'^2 + c_2\Delta^4)dx, \tag{2}$$

where c_1 and c_2 are coefficients that depend on temperature and topology of the band structure of the matrix (in particular, on the deviation from ideal nesting of electron and hole pockets). Besides, c_1 changes its sign at the characteristic temperature T_N^0, $c_1 \sim (T-T_N^0)$. For the present purposes we ignore the fine question concerning the effect of an incommensurate modulation of the SDW texture and assume c_2 to be positive, this assumption is explained in detail in the following.

By theoretical reasons, the incommensurate SDW can appear only if c_2 is negative. In the nesting-type model this coefficient strongly depends on the imperfections of nesting (μ), electron scattering on impurities and lattice strains (ν_{imp}) and temperature (T). The function $c_2(\mu,\nu_{imp},T)$ changes its sign at the hypersurface $\{\mu^*,\nu_{imp}^*,T^*\}$ in the space of parameters (μ,ν_{imp},T) and varies from negative to positive values with increasing T or ν_{imp} and decreasing μ (see calculations and a detailed analysis in Ref. 11). In pure bulk chromium at fixed $(\mu^{Cr*},\nu_{imp}^{Cr*})$ the temperature T^{Cr*} slightly exceeds the Néel temperature $T_N^{Cr} \approx 311$ K, so c_2 is negative in the SDW phase and changes its sign in the paramagnetic phase. Different situations with $c_2>0$ or $c_2<0$ are realized in chromium dilute alloys by varying the alloy composition and temperature (see review[11]). We discuss here the situation in chromium based layered structures, where parameters (μ^*,ν_{imp}^*,T^*) are different from those in pure bulk chromium and condition $c_2>0$ can be fulfilled for two formal regimes: (1) the high temperature regime ($T>T^*$) in which the corresponding bulk system is paramagnetic; (2) the strong scattering ($\nu_{imp}>\nu_{imp}^*$) or strong doping ($\mu<\mu^*$) regime in which the corresponding bulk system has commensurate SDW order. We suppose that both regimes are (or can be) realized in Mibu's experiments in multilayers with inserted nonmagnetic monolayers inside the relatively thin Cr (or Cr dilute alloys) spacers. We can only speculate about the role of uncontrolled impurities or local strains inside the Cr spacer in Mibu's experiments as a possible source of suppressing of incommensurate SDW order. The empirical facts have clearly shown the absence of an incommensurate modulation of the SDW in fairly wide region of the Cr thickness t between the inserted layers X: $t<160$ Å at $T\approx 300$ K and $t<40$ Å at $T=15-20$ K.[5–7,9] Hence, in this situation, it seems that the use of functional in the form (2), at least, as a phenomenological model is entirely proved. An incommensurate SDW order exists in the $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ multistructures with relatively large thickness of Cr layer ($t>40$ Å). But the analysis of the situation $c_2<0$ is a very complex matter and requires the special approach.

Other arguments in favor of applicability of the expansion (2) are the following. In general, the structures under consideration could contain the Cr layer doped with donor-type impurities, which increase the electron concentration into the host and improve the nesting (see Ref. 1). The real epitaxial superlattices containing layers with chromium alloys are well known, for example, $\mathrm{Cr}/\mathrm{Cr}_{97.5}\mathrm{Mn}_{2.5}$ (Ref. 15) and $\mathrm{Fe}/\mathrm{Cr}_{94}\mathrm{Fe}_6$.[16] In such situation, owing to the electron doping the coefficient c_2, being negative for pure bulk chromium, shifts into a side of positive values with the doping,[1,10] and the quantity T_N^0 is formally attributed to the Néel point of the corresponding bulk alloy.

Expression (2) can be derived directly from the microscopic model of SDW by means of the standard Green's functions method using the high-temperature expansion of the diagrammatic series for the thermodynamical potential Ω_V.[11] 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, $c_1<0$. Note, that only a single-domain transverse polarized state, $\vec{n}\perp\vec{x}$, is considered in order to simplify the calculations. The qualitative estimation of the SDW correlation length $\zeta(T)$ in the nesting-type model

gives $\zeta(T)=\xi_0/\sqrt{|T/T_N^0-1|}$, where $\xi_0\approx\nu_F/\Delta^0$ is the coherence length of electron-hole pair, ν_F is the average velocity of quasiparticles at the nested parts of the Fermi surface, T_N^0 is the transition temperature into the commensurate SDW phase and Δ^0 is the amplitude of the SDW order parameter at $T=0$. The relation between characteristic lengths considered here is: $t\geqslant\zeta(T)>\xi_0\gg a$. Thus, the mean-field approach can be regarded as satisfactory for a case of not very thin Cr layers and for relatively high temperatures. The behavior of the SDW order parameter in the vicinity of interfaces on scales smaller than ξ_0 is not described in this approach and will be merely defined through the certain boundary conditions.

Notice, that in the general case we should use instead of the rather simple expression (2) the more complex expression containing the higher-order terms proportional to Δ^6, $(\Delta'')^2$, and $(\Delta\Delta')^2$. This is associated with specific features of the microscopic nesting-type model, in which the coefficient c_2 may change its sign with temperature and doping. Therefore, in the temperature and doping regions, where the coefficient c_2 is either negative or rather small, it is necessary to hold the above mentioned higher-order terms in the expansion for Ω_V. On the basis of such expansion, the incommensurate SDW state, which exists in the pure Cr below the Néel temperature $T_N^{Cr}\approx 311$ K, was exactly described in form of the "soliton lattice."[10,11] In the high-temperature region $T>T_N^0$, the coefficient c_2 becomes positive and it is enough to hold only terms up to $\sim c_2\Delta^4$ and the lowest gradient $\sim c_2(\Delta')^2$ in the functional. This is a principal reason, why we use functional (2) to describe the phase transition into the state with "commensurate," but inhomogeneously modulated SDW in the layered structures of type Cr/X at temperature higher than the Néel temperature of bulk chromium.

Interaction of electrons, which are participating in the SDW formation, with X-ML inserted into bulk Cr is modeled by means of the short-range potential $U(x)\approx\Sigma_m U_0\delta(x-x_m)$, where x_m is the coordinate of the mth impurity ML, $m=0,\pm1,\pm2,\ldots$, U_0 is the effective potential of an interface, defined in the model of plane defect embedded into the SDW host (see Ref. 11). Since the order parameter $\Delta(x)$ is a slowly varying function of x on the length scale of $U(x)$, one can write the functional of the system $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ as the sum of "volume" (Ω_V) and "plane defect" (Ω_{ML}) components

$$\Omega=\Omega_V+\Omega_{ML}, \tag{3}$$

$$\Omega_{ML}=\frac{\nu}{2}\sum_m\Delta^2(x_m),\quad x_m=\frac{t}{2}(2m+1), \tag{4}$$

$$\nu\sim-\frac{U_0\bar{N}^2}{n_0},\quad \bar{N}\sim\frac{a}{\nu_F}, \tag{5}$$

where n_0 is the difference in filling of electron and hole pockets forming the nesting part of the Fermi surface of Cr, $\bar{N}$ is their average density of states at the Fermi level. Note that within the scope of the approximation (2)–(4) the behavior of $\Delta(x)$ is not well described in the vicinity of X-ML, on the length scale smaller than ξ_0, and will be simply taken into account through the interface boundary conditions under certain reasonable assumptions. We shall suppose in the follows that the period of the $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ superlattice t, i.e., the distance between adjacent X-MLs, is much larger than the coherent length ξ_0.

The physical meaning of plane defect component (4) is the following: within several atomic Cr planes which are sandwiching X-ML, the electron susceptibility, the quasiparticle spectrum, and the filling of band states are changed as compared to those in bulk Cr due to hybridization between Cr and X valence bonds. Hence, the conditions of the paramagnetic phase instability towards SDW formation are also changed locally, i.e., in a range of the order of few lattice constants a around X-ML. According to the theory,[12,13] the additional term of type (4) appears, because of the charge redistribution on length scale of order of the Debye screening length $l_D(\approx 3-5$ Å) near the Cr/X interface. In pure bulk chromium, where $n_0<0$, the electron transfer from X-ML to Cr host may be interpreted as the local restoration of nesting of electron and hole pockets, and vice versa, the electron transfer from Cr host to X-ML is thought to make worse this nesting near plane defect.

On the other hand, the aspect of mechanical adaptation of ML to Cr crystalline lattice is fairly essential for the epitaxially grown nanostructures of type Cr/X. The distortion with relative magnitude of some percent in the relaxation region of scale $l_S(\approx 3-5$ Å) near a plane defect is produced by difference in the lattice parameters between the Cr host and the X-ML. It is believed that the epitaxial strain could be the reason for the change of the SDW onset conditions. It may be thought that the local structural imperfection carries its own contribution to the effective potential $U(x)$.

III. THE SELF-CONSISTENT EQUATIONS AND THE SPATIAL STRUCTURE OF SDW

In the continuum mean field model of the multilayer structure $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$, the spatial profile of the order parameter $\Delta(x)$ can be obtained by solving the minimized equation for the functional $\Omega[\Delta(x),\Delta'(x)]$ (2)–(4):

$$\nu_F^2c_2\Delta''-c_1\Delta-2c_2\Delta^3=0, \tag{6}$$

completed by the boundary conditions

$$\Delta(x_m+0)=\Delta(x_m-0), \tag{7}$$

$$\Delta'(x_m+0)-\Delta'(x_m-0)=\frac{\nu\Delta(x_m)}{\nu_F^2c_2}, \tag{8}$$

at each point $x=x_m$. The system of Eqs. (6)–(8) is exactly solvable in the class of the Jacobi elliptic functions, since the first integral of Eq. (6) 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 $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ structure. Therefore, we shall restrict ourselves to analyze the solutions that satisfy the requirement: $\Delta(x)=\Delta(x+mt)$.

Various modifications of the order parameter, strongly dependent on the sign of parameters ν and $c_1 \sim (T-T_N^0)$, are caused by embedding the single nonmagnetic defect into the SDW host:[11] (1) the induced SDW at $\nu<0$, $T>T_N^0$; (2) the enhanced SDW at $\nu<0$, $T<T_N^0$; and (3) the partially suppressed SDW at $\nu>0$, $T<T_N^0$. If $\nu>0$ and $T>T_N^0$, the spin order is not possible. In the temperature region under consideration, such modifications has spread over on a macroscopic scale of the order of the SDW correlation length, $\zeta(T) \sim |T-T_N^0|^{-1/2}$. One may thus expect that even small changes of the electron properties on the relatively short-range length scale, $\{l_D, l_S\} \ll \zeta(T)$, should significantly influence the magnetic state of the nanostructure $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ with finite thickness of Cr layer.

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

$$\Delta(x) = \frac{\nu_F k'}{\zeta_k} nc\left(\frac{x}{\zeta_k}, k\right), \tag{9}$$

where k is the modulus of the elliptic function defined from the boundary conditions (7) and (8), $k'=\sqrt{1-k^2}$, $\zeta_k = \zeta\sqrt{2k^2-1}$, $1>k^2>1/2$; $\zeta=\nu_F\sqrt{c_2/c_1}$ is the correlation length of the spin density fluctuations. Here and in the following we are employing the standard notations for the elliptic functions and integrals.[17] The parameter k is related to the characteristic lengths of the system by the following equation:

$$dc\left(\frac{t}{2\zeta_k}, k\right) sn\left(\frac{t}{2\zeta_k}, k\right) = \frac{\zeta_k}{D_-}, \quad \frac{t}{2\zeta_k} < K(k). \tag{10}$$

Equation (10) has been derived from the interface boundary conditions (7) and (8); $K(k)$ is the complete elliptic integral of the first kind. It was also introduced the so-called interpolation length[13]

$$D_- = \frac{2c_2\nu_F^2}{|\nu|}. \tag{11}$$

In our model this length is considered to be almost independent of temperature. Taking the limit $k\to 1$ $(k'\to 0)$ in Eq. (10), we can obtain the instability condition respect to the SDW appearance

$$\frac{\zeta}{D_-} = \tanh\left(\frac{t}{2\zeta}\right). \tag{12}$$

This equation gives the Néel temperature, $T_N(t, D_-)$, for the multilayer $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ with $\nu<0$. If $t \gg D_- \simeq \zeta$ then the value $T_N \simeq T_N^0[1+2\exp(-t/D_-)]$, i.e., $T_N(t, D_-)$ slightly exceeds T_N^0; if $t \ll \zeta < D_-$, then the ratio $T_N/T_N^0 \sim \sqrt{D_-/t}$ may formally become enormous, as long as $t > 2\xi_0$.

Near the transition temperature, $T \simeq T_N$, the expression for the SDW profile can be simplified

$$\Delta(x) = \frac{\nu_F k'}{\zeta} \cosh\left(\frac{x}{\zeta}\right), \tag{13}$$

$$k'^2 = \frac{\left[\frac{\zeta}{D_-}\coth\left(\frac{t}{2\zeta}\right) - 1\right]}{f\left(\frac{t}{2\zeta}\right)}, \tag{14}$$

$$f(y) = 1 + \frac{1}{4}\cosh(2y) + \frac{3y}{2\sinh(2y)}. \tag{15}$$

(2) For $\nu<0$ and $T<T_N^0$, the form of SDW is different from that in Eq. (9). At $T_S<T<T_N^0$, where T_S is the below evaluated characteristic temperature, the dependence $\Delta(x)$ is described in the interval $|x|<t/2$ by the formula

$$\Delta(x) = k'\Delta_k nc\left(\frac{\Delta_k x}{\nu_F}, k\right). \tag{16}$$

Now, $k'=\sqrt{1-k^2}$, $\Delta_k = \sqrt{2}\Delta_0/\sqrt{1-2k^2}$, $0<k^2<1/2$, the value $\nu_F/(\sqrt{2}\Delta_0)$ is the correlation length at $T<T_N^0$ and $\Delta_0(T) = \sqrt{|c_1|/(2c_2)}$ is the order parameter amplitude in the homogeneous itinerant AFM. Inserting the function (16) into the interface boundary conditions, Eqs. (7) and (8), one obtains the equation determining the modulus k:

$$sn\left(\frac{\Delta_k t}{2\nu_F}\right) dc\left(\frac{\Delta_k t}{2\nu_F}\right) = \frac{\nu_F}{D_-\Delta_k}, \quad \frac{\Delta_k t}{2\nu_F} < K(k). \tag{17}$$

For a relatively short period of the superlattice, $t \ll 2\nu_F/\Delta_k$, Eq. (17) can be simplified

$$1 - 2k^2 = \frac{D_- t\Delta_0^2}{\nu_F^2}. \tag{18}$$

For the case of weak perturbation, induced by the defect potential $U(x)$, when $D_- \gg \nu_F/\Delta_k$, Eq. (17) is reduced to

$$\frac{\nu_F}{D_-\Delta_k}\left[K(k) - \frac{t\Delta_k}{2\nu_F}\right] = k'. \tag{19}$$

For a further decrease of temperature, the form of the SDW changes, so that, in the temperature region $T<T_S$, the function $\Delta(x)$ is the following:

$$\Delta(x) = \Delta_k dc\left(\frac{\Delta_k x}{\nu_F}, k\right), \tag{20}$$

where $\Delta_k = \sqrt{2}\Delta_0/\sqrt{1-k^2}$, $0<k<1$, $|x|<t/2$. Here, the equation for the modulus k has the form

$$k'^2 sc\left(\frac{\Delta_k t}{2\nu_F}\right) nd\left(\frac{\Delta_k t}{2\nu_F}\right) = \frac{\nu_F}{D_-\Delta_k}, \quad \frac{\Delta_k t}{2\nu_F} < K(k), \quad k' = \sqrt{1-k^2}. \tag{21}$$

In the case of weak electron-defect interaction $D_- \gg \nu_F/\Delta_0$, or for a relatively long period of superlattice, $t \gg \nu_F/\Delta_0$, the additional modulus is the small quantity

$$k'^2 = \frac{\sqrt{2}\nu_F}{\Delta_0 D_-}\left[\sinh\left(\frac{\sqrt{2}\Delta_0 t}{\nu_F}\right)\right]^{-1} \ll 1. \tag{22}$$

Thus, the order parameter $\Delta(x)$, given by Eq. (20), becomes almost uniform

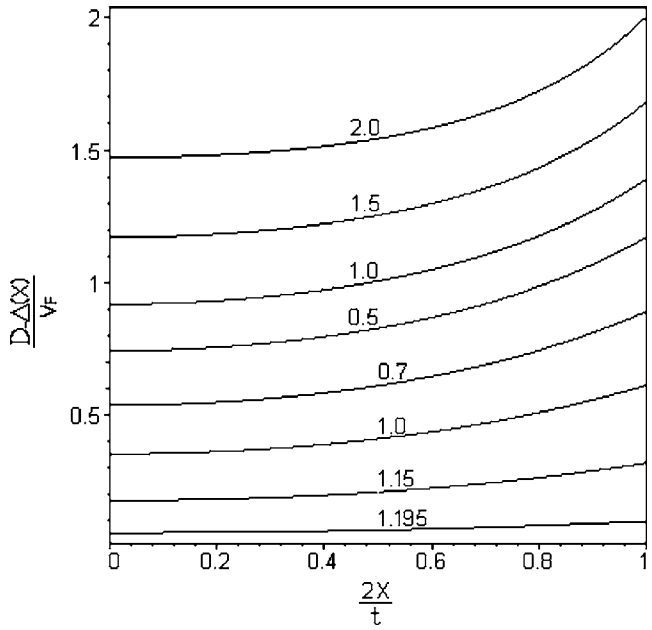

FIG. 1. Space distributions of the order parameter $\Delta(x)$ within Cr layer of middle thickness $t=D_-$ for several values of quantity D_-/ζ (0.7, 1.0, 1.15, 1.195) at $T_N^0<T<T_N$ and $\sqrt{2}D_-\Delta_0/\nu_F$ (0.5, 1.0, 1.15, 2.0) at $T_N^0>T$, in the case of $\nu<0$.

$$\Delta(x)=\Delta_0\left[1+\frac{k'^2}{2}\cosh\left(\frac{2\Delta_0 x}{\nu_F}\right)\right]. \tag{23}$$

At $T=T_S$, the function $\Delta(x)$ in Eq. (16) goes smoothly to Eq. (20). The temperature $T_S(t,D_-)$ can be found from equation

$$\frac{\sqrt{2}D_-\Delta_0}{\nu_F}=\cot\left(\frac{\Delta_0 t}{\sqrt{2}\nu_F}\right),\quad 0<\frac{\Delta_0 t}{\sqrt{2}\nu_F}<\frac{\pi}{2}, \tag{24}$$

which was obtained by using the limit $k\to 0$ in Eqs. (17) and (21).

Figure 1 displays the space distribution of the order parameter $\Delta(x)$ within Cr layer of middle thickness $t=D_-$ in the case of $\nu<0$ for several values of the inverse correlation length: four upper curves are for correlation length at $T<T_N^0$; the next four down curves are for correlation length at $T_N^0<T<T_N$. All of eight curves present united sequence as the temperature changes. The magnetic ordering increases on going along x far from the Cr layer center. The size of the spin density, at the center of Cr layer $\Delta(0)$ (minimum) and at its boundary $\Delta(t/2)$ (maximum), as a function of the inverse correlation length for some thickness values t is displayed in Fig. 2. From the critical point [Eq. (12)], the SDW amplitude increases monotonically as the temperature falls and the Cr layer thickness decreases.

(3) For $\nu>0$ and $T<T_N^0$, the unique periodical solution of Eqs. (6)–(8) exists

$$\Delta(x)=k\Delta_k cd\left(\frac{\Delta_k x}{\nu_F},k\right), \tag{25}$$

where $|x|<t/2$, $\Delta_k=\sqrt{2}\Delta_0/\sqrt{1+k^2}$, $0<k<1$. The equation that determines the parameter k for solution Eq. (25) coincides with Eq. (21) by substituting $D_-\to D_+$, where

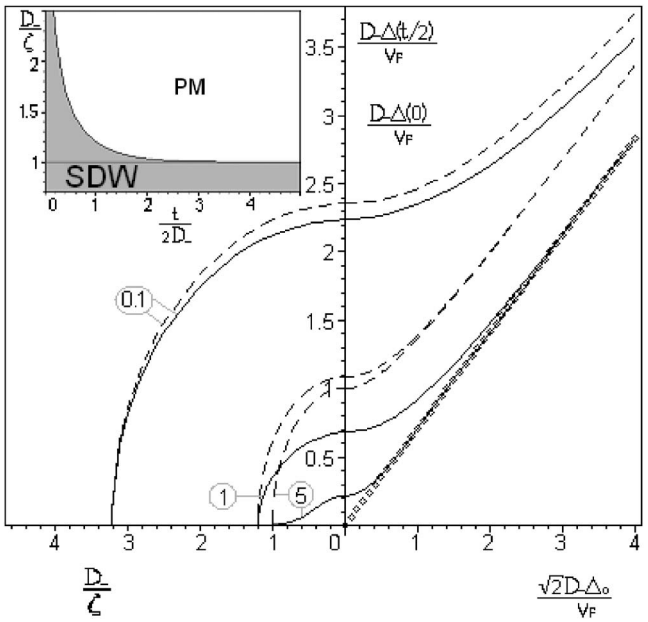

FIG. 2. Size of the spin density at the center of Cr layer $\Delta(0)$ (minimum, solid line) and at the boundary $\Delta(t/2)$ (maximum, dashed line) as a function of the inverse correlation length for three diffent values of thickness $t(t/2D_-=0.1,1.0,5.0)$ in the case of $\nu<0$. The diamond line is the dependence of the SDW amplitude on the inverse correlation length for bulk chromium. The magnetic phase diagram of the $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ multilayer with $\nu<0$ is displayed in the inset.

$$D_+=\frac{2c_2\nu_F^2}{\nu} \tag{26}$$

is the interpolation length in the case $\nu>0$. Therefore, in the limit $k\to 0$, the equation for the modulus k analogous to Eq. (21) is

$$\frac{\sqrt{2}D_+\Delta_0}{\nu_F}=\cot\left(\frac{\Delta_0 t}{\sqrt{2}\nu_F}\right),\quad 0<\frac{\Delta_0 t}{\sqrt{2}\nu_F}<\frac{\pi}{2}, \tag{27}$$

which determines the condition for the SDW formation in the multilayer with $U_0>0$. The Néel temperature of this multilayer is always lower than the bulk one, $T_N(t,D_+)<T_N^0$.

It should be emphasized a peculiar "geometrical" effect. It means, at a given temperature $T<T_N^0$, even a negligibly small parameter $\nu>0$ is sufficient to ensure that a spin ordering shall be suppressed in the whole volume of the superlattice $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ with period t shorter than the critical length $t^*=\pi\nu_F/[\sqrt{2}\Delta_0(T)]$.

Around the ordering temperature, $T_N(t,D_+)$, the SDW profile within the unit cell $|x|<t/2$ has the explicit form

$$\Delta(x)=\sqrt{2}k\Delta_0\cos\left(\frac{\sqrt{2}\Delta_0 x}{\nu_F}\right), \tag{28}$$

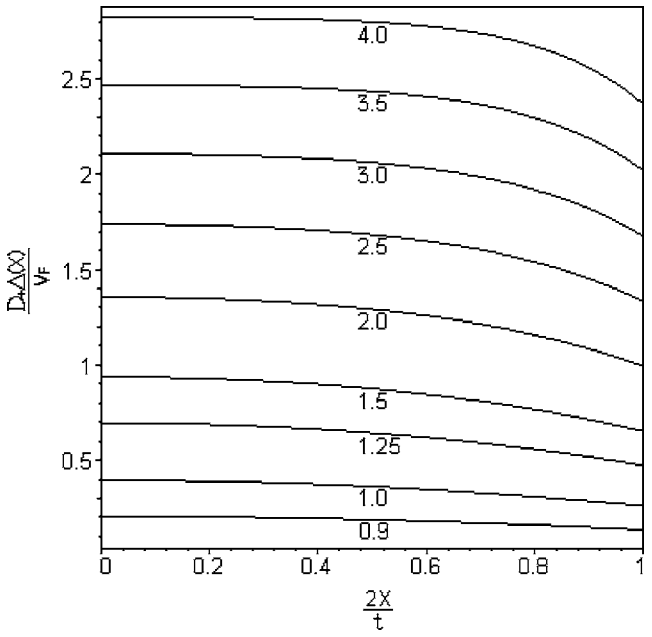

FIG. 3. Space distributions of the order parameter $\Delta(x)$ within Cr layer of middle thickness $t=D_+$ for several values of quantity D_+/ζ (0.9, 1.0, 1.25, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0) in the case of $\nu>0$.

$$k^2=\frac{1-\frac{\nu_F}{\sqrt{2}\Delta_0 D}ctg\left(\frac{\Delta_0 t}{\sqrt{2}\nu_F}\right)}{g\left(\frac{\Delta_0 t}{\sqrt{2}\nu_F}\right)},\quad 0<\frac{\Delta_0 t}{\sqrt{2}\nu_F}<\frac{\pi}{2},\quad (29)$$

$$g(y)=1-\frac{1}{4}\cos(2y)+\frac{3y}{2\sin(2y)},\quad (30)$$

where $k\ll 1$. If the additional modulus k' becomes a fairly small quantity in the sense of Eq. (22), the order parameter distribution tends to be uniform

$$\Delta(x)=\Delta_0\left[1-\frac{k'^2}{2}\cosh\left(\frac{2\Delta_0 x}{\nu_F}\right)\right].\quad (31)$$

In Fig. 3, the space distributions of the order parameter $\Delta(x)$ within Cr layer of middle thickness $t=D_+$ are shown for several values of quantity D_+/ζ in the case of $\nu>0$. The Cr moments increase on going along x far from the Cr/X interface. In Fig. 4, it is plotted the size of the spin density at the center of Cr layer (maximum) and at the boundary (minimum) as a function of the inverse correlation length for three different values of the thickness t. The SDW amplitude decays monotonically when temperature is increasing and when the Cr layer thickness decrease, disappearing at the transition point [see Eq. (27)].

If the distance between the adjacent ML is much longer than the correlation length, the single plane defect approach is true. Therefore, in the case of $t\gg\zeta$ for $T_N^0<T<T_N$, the magnetic structure of the superlattice with $\nu<0$, can be presented as the superposition of "localized SDW's"[11]

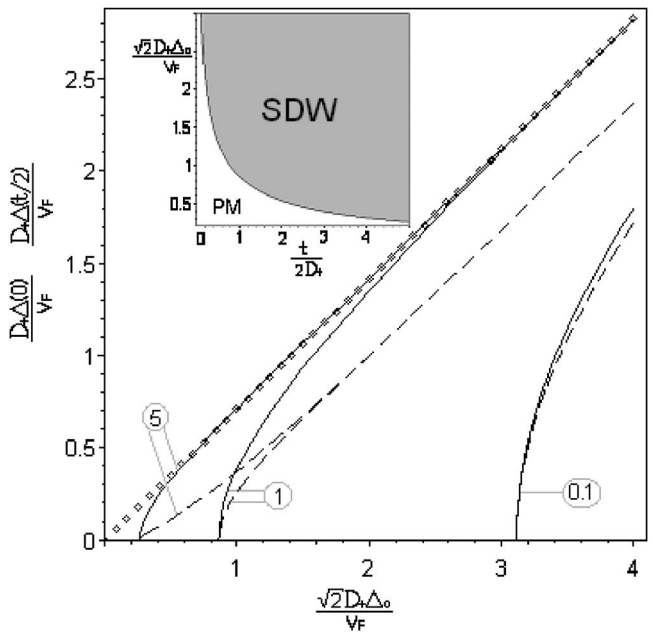

FIG. 4. Size of the spin density at the center of Cr layer $\Delta(0)$ (maximum, solid line) and at its boundary $\Delta(t/2)$ (minimum, dashed line) as a function of the inverse correlation length for three diffent values of thickness $t(t/2D_+=0.1,1.0,5.0)$ in the case of $\nu>0$. The diamond line is the dependence of the SDW amplitude on the inverse correlation length for bulk chromium. The magnetic phase diagram of the $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ multilayer with $\nu>0$ is displayed in the inset.

$$\Delta(x)=\sum_m\frac{\nu_F}{\zeta}\frac{1}{\sinh\left(\frac{|x-x_m|}{\zeta}+\phi\right)},\quad \tanh\phi=\frac{D_-}{\zeta}.\quad (32)$$

Analogously, if $t\gg\nu_F/\Delta_0$, in the region $c_1<0$ we have

$$\Delta(x)=\Delta_0\left(1+\sum_m\left\{\left[\tanh\left(\frac{\Delta_0|x-x_m|}{\nu_F}+\varphi_\pm\right)\right]^\pm-1\right\}\right),\quad (33)$$

$$\sinh(2\varphi_\pm)=\frac{4D_\pm\Delta_0}{\nu_F},\quad (34)$$

where the sign + (−) relates the case of multilayer with $\nu>0$ ($\nu<0$), correspondingly. For the same conditions one can imagine the magnetic configuration of the three-component multilayer of type $[\mathrm{Cr}(t)/X_-(1\ \mathrm{ML})/\mathrm{Cr}(t)/X_+(1\ \mathrm{ML})]$, where monatomic layers of different kind X_- and X_+, with $U_0\{X_+\}>0$ and $U_0\{X_-\}<0$, respectively, are alternately embedded in a Cr(001) host, so

$$\Delta(x)=\Delta_0\left\{1+\sum_{m=even}\left[\tanh\left(\frac{\Delta_0|x-x_m|}{\nu_F}+\varphi_+\right)-1\right]+\sum_{m=odd}\left[\coth\left(\frac{\Delta_0|x-x_m|}{\nu_F}+\varphi_-\right)-1\right]\right\}.\quad (35)$$

Note that similar constructions of order parameter were ap-

plied to model some properties of diluted Cr alloys, both with magnetic and nonmagnetic impurities (see Ref. 11).

In the series of papers[12–14] about the mechanism of interlayer exchange coupling in Fe/Cr multilayers we have already considered the functional [(2) and (4)] in the situation: (1) induced SDW at $\nu<0$, $c_1>0$, but with boundary conditions for the SDW order parameter different from those in the present work. The two others situations: (2) the enhanced SDW at $\nu<0$, $c_1<0$ and (3) the partially suppressed SDW at $\nu>0$, $c_1<0$ have been never analyzed.

IV. DISCUSSION

Let us discuss some interesting experimental results on the magnetic properties of Cr/Sn and Cr/Sn/Cr/X multilayers in the context of presented theory. In order to give a qualitative interpretation of the ^{119}Sn Mössbauer spectroscopy measurements,[5–7] some important assumptions about the sign of the effective potential of the plane defect $U_0\{X\}$ should be made. This phenomenological parameter describes both the effects of charge redistribution and lattice strain near the nonmagnetic X-ML on the SDW ordering in $[\mathrm{Cr}(t)/X(1\ \mathrm{ML})]$ system, it may be either positive or negative, dependent on the sort of inserted metal X. As mentioned above, one can propose a fairly reasonable form for this dependence relying upon the well-established properties of the dilute alloys with corresponding composition $\mathrm{Cr}_{1-x}X_x$.[1] Unfortunately, we are unable to unambiguously interpret the contribution of the induced by X layer strain into the effective potential and, hence, consider $U_0\{X\}$ as a model parameter. Notice, that monatomic V, Fe, Ag, and Sn layers grow epitaxially with the Cr layers in the (001) direction, forming a body-centered-cubic or tetragonal lattice together with the neighboring Cr atoms.[5–7]

For $\mathrm{Cr}_{1-x}\mathrm{V}_x$ alloy systems, a linear decrease of the Néel temperature, the SDW incommensurability wave vector, and the SDW amplitude with increasing V concentration were found. From the standpoint of the "rigid-band" approach,[1,10] it means that V dissolved in Cr host acts as an ideal electron acceptor providing the shift of the Fermi level from the perfect nesting. On the other hand, the phase diagram of $\mathrm{Cr}_{1-x}\mathrm{Sn}_x$ alloys has the commensurate SDW region in the interval $T_N^0(311\ \mathrm{K})<T<400$ 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. It is evident, that systems with the chemical modulation of Cr/X type also cannot be considered in the framework of the rigid-band scheme. Nevertheless, in the contact induced SDW conception[12,13] the X-ML embedded into Cr host is treated as a local doping source. Accordingly, the positive effective potential, $U_0\{X\}>0$, is attributed to V-ML (the local acceptor) and the negative one, $U_0\{X\}<0$, 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 ξ_0. It is clear that the trend of the order parameter behavior persists in this narrow region and, therefore, the magnetic moment at the Cr interface sites is proportional to the boundary value of the SDW amplitude, i.e., $\sim\Delta(x=t/2)$. Consequently, in multilayers $[\mathrm{Cr}(t)/\mathrm{Sn}(1\ \mathrm{ML})]$ the hyperfine field at the ^{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. (9), (15), and (19); the behavior of $\Delta(t/2)$ is given in Figs. 2 and 4. So, our theory qualitatively explains the following experimental results: (a) the variation of the hyperfine field size $H_{hf}(t,T)$ as a function of the temperature and Cr layer thickness; (b) the considerable enhancement of the Cr magnetic moment at the Cr/Sn interface; (c) the stabilization of the magnetic ordered state in very thin Cr layers at temperatures higher than its bulk Néel temperature, which has been established in Refs. 5 and 6 for the superlattices $[\mathrm{Cr}(t)/\mathrm{Sn}(1\ \mathrm{ML})]$ with $t<40$ Å.

It should be emphasized that the Sn-MLs in the layered structures based on Cr are not only an appropriate probe to study the magnetic properties of Cr through the Mössbauer spectroscopy, but also the source of perturbation of the spin structure of 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 Refs. 6 and 7 may be qualitatively explained even in frame of the present approach. In particular, the present model explains why the order parameter amplitude decreases near V-ML so that SDW collapses and Cr becomes nonmagnetic below a critical thickness t^*.

Above we formally described the Cr/X multilayers containing the plane insertions of monatomic thickness with the ideal smooth interfaces. Of course, the obtained results are certainly valid in the case of the bilayers, submonolayers, and other inhomogeneities providing the short-range effective potential on scale of the AFM correlation length. The effects of interfacial disorder such as the roughness and the component interdiffusion are not crucial for the above-proposed model based on the contact induced SDW conception. It is important to mentioned that the present approach can be applied to $[\mathrm{Cr}(t_{Cr})/X(t_X)]$ layered structures with the rather thick nonmagnetic layers, where $t_X\sim t_{Cr}\gg t_{ML}\sim a$.

Although, we have considered the Cr(001)/X structure, the formulation used here can be generalized to study various structures with periodical modulation along any crystalline direction. Recent ^{119}Sn Mössbauer spectroscopy data show with evidence, that not only the Cr(001)/X(ML) multilayers, but also the Cr(011)/X(ML) multilayers have an enhancement of Cr magnetic moments near the interfaces.[18] This experimental fact can be easily interpreted in terms of the local electron doping as well.

It should be noted that the attempt[19] to apply the simplest variational non-self-consistent approach, entirely analogical to that for bulk SDW systems, is unable to explain the magnetic phase diagram of Cr/X multilayers with nonmagnetic MLs even qualitatively, not to mention the fine details of the spin density distribution inside the Cr layer (see discussion in Refs. 12 and 13). The numerical analysis of the magnetization distribution in the multilayers[20] is able, in principle, to

describe the ground state of the system, but it cannot be used for studying the thermodynamics and complex magnetic configurations.

It is worth it to draw attention to the fact that, apart from the Mössbauer spectroscopy, the nonmagnetic ML insertions influence on the spin structure of Cr in the Cr/X multilayers could be found by means of some other methods. For instance, embedding various MLs into the Cr layer, it is possible to vary the amplitude of an exchange coupling between FM layers in the FM/Cr/X(ML)/Cr penta- or multilayers (FM=Fe,Co). The effect must be well noticeable in the case of structures with the perfect FM/Cr interfaces in which the SDW contribution into the interlayer exchange coupling is significant.[3,21] On the other hand, the low-temperature resistivity minimum was observed in several Cr alloy systems.[1] Such phenomenon is associated with the resonance scattering of electrons by the local impurity state lying within the SDW energetic gap. We predict the similar peculiarity in the transport measurement of the superlattices Cr/X(ML) to be possible.

Thus, within the framework of the modified model of contact induced SDW we have succeeded to understand the mechanism of AFM ordering, caused by the inserted paramagnetic monolayers into the multilayered structures [Cr(t)/X(1 ML)]. The behavior of the magnetic structure in this system as a function of the Cr layer thickness and temperature has been qualitatively described for the insertions of various sorts.

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