Spin-density wave in Cr without the nesting property of the Fermi surface

2006 J. Phys.: Condens. Matter 18 2717

(http://iopscience.iop.org/0953-8984/18/9/009)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **18** (2006) 2717–2728 doi:10.1088/0953-8984/18/9/009

Spin-density wave in Cr without the nesting property of the Fermi surface

V M Uzdin[1,2] **and C Demangeat**[2]

[1] St Petersburg State University, ICAPE, 14 linia VO 29, 199178, St Petersburg, Russia
[2] Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, F-67034, Strasbourg, France

Received 31 October 2005, in final form 8 January 2006
Published 17 February 2006
Online at stacks.iop.org/JPhysCM/18/2717

Abstract

Recent *ab initio* calculations have shown that the theory of the spin density wave (SDW) based on the nesting property of the chromium Fermi surface is not able to explain solely the stability of the incommensurate SDW. Using the model Hamiltonian approach, we develop a method which allows self-consistent calculation of SDWs with different wavelengths. The magnetic profile and the energy of the system agree well with *ab initio* results. To check the stability of the SDW we introduce a local external magnetic field which induces transitions towards SDW or antiferromagnetic (AF) states. A very small energy which is enough to create the nodes of the SDW determines the new mechanism of SDW formation without supposition about the nesting property of the Fermi surface. The individual nodes of the SDW are found to be quite stable. They can be considered as low-energy excitations, which do not interact at large distance and annihilate when they approach close to one another. About 10% of non-magnetic Cr atoms randomly distributed in a few (100) layers leads to the formation of the SDW state with the nodal plane inside these layers. A similar trend arises when non-magnetic V impurities are introduced in bulk Cr. The increase of SDW wavelength with temperature and the transition from an SDW to a layered AF state when magnetic impurities (Fe, Mn) are introduced into bulk Cr are discussed on the basis of the developed theory.

1. Introduction

Chromium, one of the most investigated metallic materials, displays very rich magnetic behaviour both in its bulk state and in low-dimensional magnetic structures where it is used as one of the components. It is in the Fe/Cr multilayers that antiferromagnetic interlayer exchange coupling (IEC) and giant magnetoresistance were detected for the first time [1, 2]. Oscillations of IEC in these systems differ essentially from other magnetic multilayers. They show two well defined periods: short wavelength (two monolayers) and anomalous long wavelength (18 Å).

Moreover, biquadratic exchange coupling and non-collinear ordering of Fe magnetic moments across Cr spacer were discovered there [3]. Small Cr clusters supported on the surface of noble metals reveal quite exotic behaviour. In the Cr supported trimer, non-collinear ordering of moments with canting angle depending on the distance between atoms was predicted [4]. At low temperature, in the equilateral Cr trimer, the many-body Kondo-like ground state was found using scanning tunnelling spectroscopy [5]. The typical temperature of transition to this state was found to be hundreds of times larger than for a single supported Cr atom [6]. Therefore, with Cr, it is possible to obtain magnetic nanostructures with very unusual new magnetic properties interesting for applications in nanoelectronics.

To construct low-dimensional magnetic structures in Cr-based systems it is very important to understand the properties of the bulk phase of Cr. Chromium is a typical itinerant antiferromagnet with body-centred cubic (bcc) lattice. The magnitude of the magnetic moments is modulated in the (001) direction in the form of a longitudinal spin density wave (SDW) below 123 K and a transverse SDW between 123 K and Néel temperature $T_N = 311$ K [7–9]. The magnetic moments of the nearest atoms are ordered antiparallel and, as a first approach, the moment M_i on site i can be expressed as

$$M_i = M^*(-1)^{i+1} \sin \frac{a_{Cr}\pi}{\Lambda}(i-1). \tag{1}$$

Here $M^* \sim 0.5\ \mu_B$ and $\Lambda \approx 60$ Å (or 42 interlayer distances) are respectively the amplitude and period of the SDW; $a_{Cr} = 2.884$ Å is the Cr lattice constant. Index i numbers atoms in the (001) direction. In thin films, multilayers and dilute alloys, chromium presents layered antiferromagnetic (AF) structure named sometimes as commensurate SDW.

Qualitative explanation of the SDW in Cr was first proposed by Overhauser [10] and Lomer [11]. They have shown that the nesting property of the Fermi surface of paramagnetic chromium leads to an instability against the formation of the SDW with a period determined by the nesting vector $\boldsymbol{Q}$. The vector $\boldsymbol{Q}$ connects the electron and hole parts of the Fermi surface. Because the hole Fermi surface is slightly larger than the electron Fermi surface the $\boldsymbol{Q}$-vector for the SDW turns out to be incommensurate. Most of the theories developed later for the description of the SDW in chromium are only a petty modification of this original approach. However, state-of-the-art *ab initio* calculations performed in recent years [12–15] have shown that this mechanism cannot solely explain the formation of the SDW ground state in bulk Cr.

Modern density functional theory (DFT) reproduces quite accurately the band structure of bulk chromium and the nesting of its Fermi surface parts. Therefore, it is natural to expect that DFT will give the SDW ground state with an energy gain of order kT_N relative to the non-magnetic state. However, *ab initio* calculations demonstrate another outcome: the SDW proves to be not a ground state and the layered AF ordering has lower energy [12].

A comparison of the results obtained using different *ab initio* codes was reported recently by Hafner *et al* [12]. Their analysis demonstrates that, within DFT, SDW modulation can be obtained for different wavelengths Λ and that the profile of the magnetization depends essentially on Λ. The SDW is sinusoidal only for small wavelength. The calculations for large wavelength show that the magnetic profile consists of regions with pure AF order and regions where the moments are reduced because of the frustration near the node sites in SDW. Each reduction of the magnetic moments near the nodes *increases* the total energy of the system. Therefore, as was concluded in [12], neither of the DFT variants predicts a stable SDW of Cr.

Attempts to reconcile the results of DFT with the experimentally observed stability of the SDW were undertaken by different authors. Hirai, using the local spin density approximation and the Korringa–Kohn–Rostoker Green's function method [13], found the minimum of energy for the SDW state with a period close to the experimentally incommensurate wavevector (40 monolayers). Nevertheless, the gain in energy was found to be very small, so that the difference

between the energies obtained for AF and SDW solution looks even below the accuracy of his method [12].

Marcus *et al* suggested another mechanism of SDW formation [14]. They suggested that the modulation of the moments in AF phase compensates the strain energy of the lattice expansion. However, accurate calculations with the Vienna *ab initio* simulation package (VASP), which includes structural relaxation in the SDW, have shown that the stress relaxation has no significant effect on the energetics of the SDW phase [12].

Cottenier *et al* [15] conjectured that the widely varying results of *ab initio* methods with different forms of exchange–correlation functional can be scaled by the size of the calculated magnetic moment. They suggest a fitting of the lattice constant as a free parameter in order to correctly reproduce the magnetic behaviour. Such a theory is not *ab initio*, but by setting only a single parameter several different aspects of the magnetic behaviour come out right [15]. However even in this semiphenomenological model there is no explanation of the stability of the SDW.

Here we investigate the problem of stability of the SDW in bulk Cr on the basis of a very simple tight binding approach based on the periodic Anderson model (PAM) with Coulomb repulsion on site taken into account in the Hartree–Fock approximation [16, 17]. This theory, applied for calculation of the bulk metal, contains only three parameters, which determine the position of the d level relative to the Fermi level E_0 (and consequently the number of d electrons), Coulomb repulsion on site U and hopping integral V between nearest neighbour sites. Below we will describe the method which allows us to find an SDW solution with preassigned wavelength and to check its stability. It allows the new scenario of SDW formation without any premise about nesting of the Fermi surface.

2. Self-consistency in the external local magnetic field. SDW solution for the bulk Cr

We will use the PAM together with real-space recursion methods for self-consistent calculations of the Cr magnetic structure. On-site Coulomb repulsion will be taken into account in the Hartree–Fock approximation. The model assumes the existence of two bands, one corresponding to the quasilocalized d electrons and the other one to the itinerant s electrons. The on-site s–d coupling is presupposed to be stronger than d–s–d interaction of d electrons on different sites. In this case one should construct resonant d states with finite width Γ first and only after that introduce the electron hopping between different sites. All the energy parameters of the model are measured in units of Γ. The hopping integrals V_{ij} include contributions from direct d–d transitions between atoms i and j as well as the contributions from d–s–d transitions via a conductivity band. The model contains very few semiempirical dimensionless parameters, which have to be chosen to reproduce the data of *ab initio* calculations for model systems. These parameters determine the position of the d states relative to the Fermi level $(E_0 - \varepsilon_F)/\Gamma$, the onsite Coulomb repulsion U/Γ and the hopping integrals between nearest neighbours V/Γ.

Self-consistent calculations within the PAM were used recently for the explanation of the phase of short wavelength oscillations of interlayer exchange coupling in Fe/Cr/Fe trilayers [16] and for the interpretation of hyperfine field distribution in Fe/Cr multilayers [17]. It was shown that the model captures the main peculiarities of the complex magnetic behaviour of Cr. Values of the parameters were adjusted to reproduce *ab initio* results for various ideal systems. For the bulk Cr we have $(E_0 - \varepsilon_F)/\Gamma = -3.37$; $U/\Gamma = 6.745$; $V/\Gamma = 0.9$.

The self-consistent calculations of electronic structure often lead to different magnetic solutions in dependence on the initial distribution of charge and spin. In some cases the symmetry constraint allows the separation of a solution with required properties. When

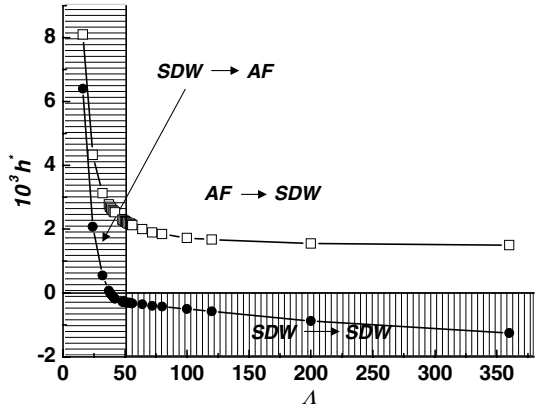

Figure 1. The threshold magnetic field for AF → SDW transition (empty squares), for SDW → AF transition (solid circles in hatched horizontally region) and for SDW → SDW transition (solid circles in hatched vertically region) as a function of the wavelength of applied field Λ.

different solutions are close in energy, as happened with AF and SDW states in Cr, it is very useful to have a regular procedure which allows us to obtain one particular solution, for example an SDW with given wavelength. Such a procedure, developed for PAM, presupposes switching on the external magnetic field H_i, individually on each atomic site i in the lattice and performing self-consistency with it. The magnetic field shifts, in the opposite directions, the energy E_0 of electrons with spins 'up' ($\sigma = 1$) and 'down' ($\sigma = -1$): $E_0 \to E_0^\sigma = E_0 + \sigma\mu_B H$. Below we will use, instead of H_i, the dimensionless parameter $h_i = \frac{\mu_B H_i}{\Gamma}$. The self-consistent distribution of magnetic moments depends on the configuration of the field. Therefore, convergence to the required solution can be governed via manipulation of the field. When convergence is achieved, the magnetic field has to be switched off. In some cases the new self-consistent solution (without field) will conserve the structure of the solution with field even if it is not the ground state of the system. Moreover, the change of the amplitude and direction of magnetic field can be used to study the stability of the solution.

In order to obtain the SDW structure with period Λ the field was taken in following form, which almost repeats the distribution of the magnetic moments (1):

$$h_i = (-1)^{i+1} h^* \sin \frac{2\pi}{\Lambda}(i-1), \qquad i = 1, 2 \ldots \Lambda. \tag{2}$$

Here h^* and Λ are the amplitude and period (in the units $a_{Cr}/2$) of the applied field respectively; index i numbers the layers in the (1, 0, 0) direction. We start the calculation from the AF state without field and then at fixed Λ increase h^* from zero to $h^*_{max} = 4 \times 10^{-3}$ with step $\Delta h^* = 2.5 \times 10^{-5}$. The self-consistent solution obtained for each value of h^* was used then as the initial state for calculations with field amplitude $h^* + \Delta h^*$. For all Λ, in large field, we observed the transition to the SDW state with nodes near the sites $i = 1$, $\Lambda/2 + 1$ and $\Lambda + 1$. The dependence of the threshold value $h^*_{AF\to SDW}$ at which this transition takes place, at the wavelength Λ, is shown in figure 1 by empty squares. It is almost constant for large wavelength $\Lambda > 50$ and increases rapidly for Λ smaller than 25 layers. If we start from the SDW solution in magnetic field and step by step (Δh^*) decrease h^*, then the behaviour of the system depends qualitatively on wavelength Λ. For $\Lambda \geqslant 40$, it is possible to decrease h^* to zero and obtain an SDW solution without field. However, comparison of the energies of SDW and AF solutions shows that energy of the AF state is lower, in accordance with *ab initio* results. In figure 2, the difference between SDW and AF energies $\Delta E_{SDW} = E_{SDW} - E_{AF}$

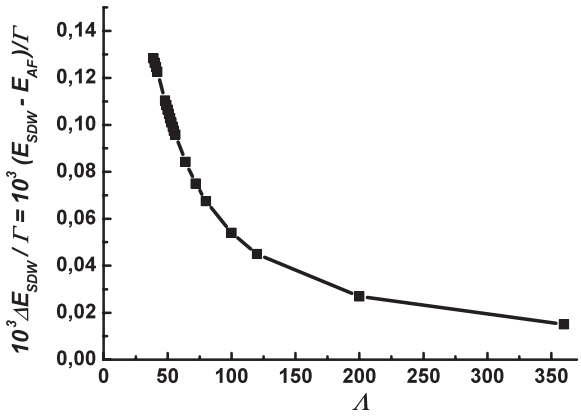

Figure 2. The difference between energies of SDW and AF states per atom (in $\Gamma \times 10^{-3}$ units) versus wavelength of the SDW Λ.

per atom is plotted versus wavelength Λ. As a first approach $\Delta E \sim \Lambda^{-1}$ means that the loss of energy arises from each node in SDW independently because the number of nodes per unit length is also proportional to the Λ^{-1}. In figure 3 the profile of magnetization in the SDW for $\Lambda = 40$, 80 and 120 monolayers is represented. Formation of regions with pure AF ordering inside the SDW, reported in [12] as a result of *ab initio* calculations, is clearly seen. In the regions where the magnetic moment is quenched, the density of states (DOS) is very similar to the DOS of non-magnetic (NM) Cr. Therefore, the energy for the SDW has to lie between the energies of AF and NM states in accordance with [12]. The value of ΔE proves to be quite small. The typical change of the energy associated with the magnetic field is of the order of 1 meV per site. If $\Lambda > 40$ the transition to the AF state occurs before h^* reaches zero value. In this case the SDW state without field does not exist.

To investigate the stability of the SDW solutions we have built the 'hysteresis loop' of the system. As before we start from the AF solution without magnetic field, increase field from zero to $h^*_{\max}$, then with the same step Δh^* decrease h^* to $-h^*_{\max}$ and again increase it to $h^*_{\max}$. For large negative and large positive h^*, for all wavelengths of applied field Λ, there is a saturation and the system goes to the SDW states which differ only by the opposite directions of the moments on each site. The transition from one SDW state to another versus h^* occurs in different ways depending on Λ.

The magnetic moments on the node site of applied field and the energy of the system as a function of h^* are plotted in figure 4 for a few typical wavelengths Λ. Parts of the curves, which were obtained when h^* was varied from zero to $h^*_{\max}$, from $h^*_{\max}$ to $-h^*_{\max}$ and from $-h^*_{\max}$ to $h^*_{\max}$ are shown by the solid line, short dotted line and dash–dot line respectively. For $\Lambda < 40$ (upper panel), the transition from SDW to AF with decrease of h^* takes place at positive values $h^* = h^*_{\mathrm{SDW}\to\mathrm{AF}}$. However, there is a hysteresis: $h^*_{\mathrm{SDW}\to\mathrm{AF}} < h^*_{\mathrm{AF}\to\mathrm{SDW}}$ and for h^* in the interval $(h^*_{\mathrm{SDW}\to\mathrm{AF}}, h^*_{\mathrm{AF}\to\mathrm{SDW}})$ the SDW state is metastable. For negative value of h^* the transitions from the AF to the SDW solutions and back occur at the same modulus of h^* as for positive ones.

For $40 \leqslant \Lambda < 51$ the hysteresis loop has similar shape (middle panel) but the AF zone is narrower and the transition from the SDW to AF state takes place only when h^* changes sign. In the region h^* near zero the metastable SDW state remains. The behaviour of the system changes qualitatively when Λ exceeds 52 layers (lower panel). Now the transition from one SDW state to another avoids the AF state. Although the SDW is not the ground state, the

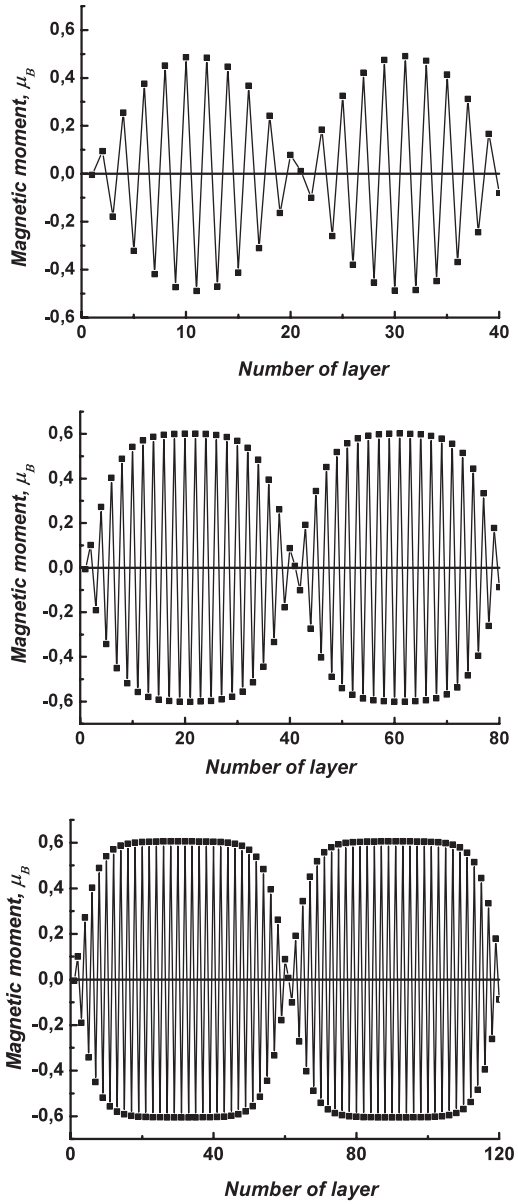

Figure 3. Magnetization profile in the SDW with $\Lambda = 40$, 80 and 120 atomic layers.

threshold energy for transition to the AF state proves to be larger than that between two SDW states. Taking into account that if the wavelength exceeds 51 layers the profiles of the SDW near the nodes are very similar, we can conclude that the nodes placed at such a distance are quite stable and the recovery of the AF structure from the SDW will be more difficult than a slight change of the SDW wavelength or a shift of the node position. We would like to underline that 52 layers is the typical wavelength of the SDW in the bulk Cr which in dependence on the temperature lies between 42 and 54 layers. Magnetic nodes are similar to the creases on the rumpled surface: when we try to sleek one of them locally it simply moves to a neighbouring

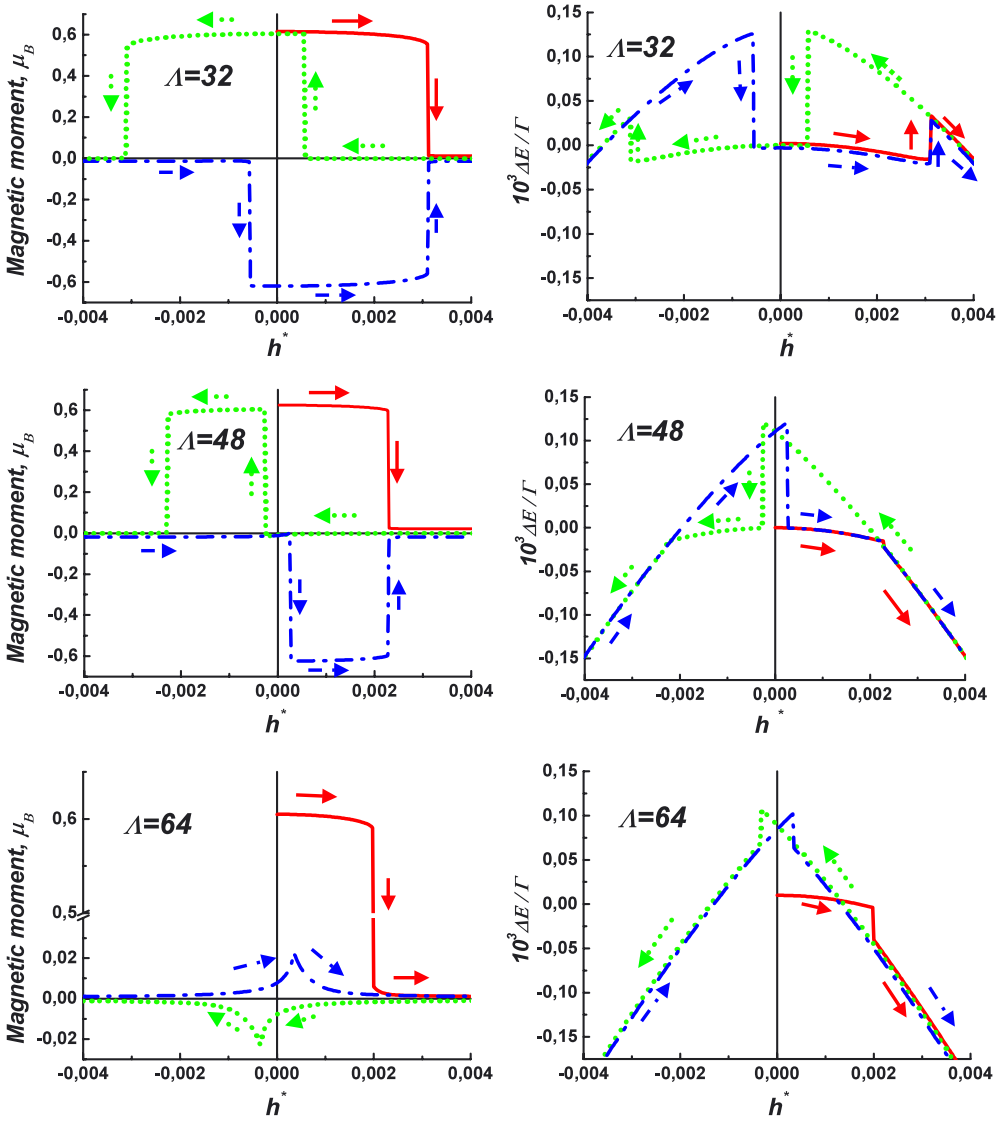

Figure 4. Magnetic moment at the node site of applied field (left panel) and the energy per atom relative to the energy in the AF state without field (right panel) as a function of applied field amplitude h^* for different values of Λ. Solid (red), dotted (green) and dot and dash (blue) curves correspond to the change of h^* from 0 to $h^*_{\max}$, from $h^*_{\max}$ to $-h^*_{\max}$ and from $-h^*_{\max}$ to $h^*_{\max}$ respectively. Arrows show the direction of the change of applied magnetic field amplitude h^*.

(This figure is in colour only in the electronic version)

location, and only when two creases conjugate on a small distance does it lead to the smoothing of the surface in that place. It is worth noting that in applied field with large amplitude the SDW has lower energy than the AF state and the AF $\rightarrow$ SDW transition also occurs with hysteresis, as seen from the right panel of figure 4.

In figure 1 the threshold amplitude for transition between SDW states or from SDW to AF state is shown versus wavelength Λ by black circles. The SDW state without field exists when

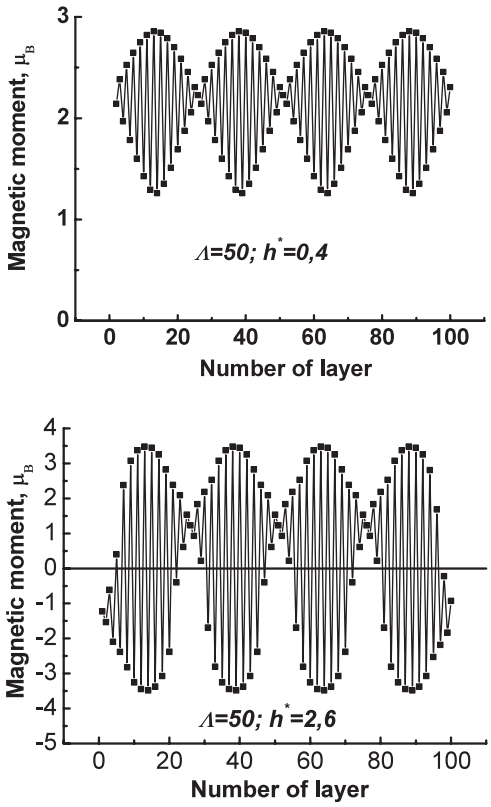

Figure 5. Magnetization profile in the bulk Fe in the local external magnetic field (2) with $\Lambda = 50$ and $h^* = 0.4$ (upper panel) and $h^* = 2.6$ (lower panel).

these circles are located below the line $h^* = 0$. Horizontally and vertically hatched regions in figure 1 correspond to transitions SDW $\rightarrow$ SDW and SDW $\rightarrow$ AF respectively. We believe that the same results can be obtained within other model Hamiltonians or *ab initio* methods. However, at some points of the hysteresis loop the number of iterations which was necessary to achieve self-consistency was above 20 000, that makes it difficult to perform calculations in the *ab initio* approach.

3. Fe and V in the SDW-like magnetic field

In the previous section we used the method of self-consistent calculations of the system in the external local magnetic field to obtain the SDW solution and to study its stability in the bulk Cr. Now we will present results of similar calculations for two other 3d metals—Fe and V. Both of these elements have bcc structure like chromium and can be described in the PAM by the same formulae. The values of the phenomenological parameters for Fe and V are known from previous calculations and comparison with *ab initio* results [16–18].

In the limit of large magnetic field amplitude h^* in (2) all metals have to transfer into the SDW state with nodes coinciding with the nodes of applied field. These transitions, however, take place for Fe and V at different h^*. Without magnetic field Fe is a ferromagnetic material with spin magnetic moment 2.2 μ_B. In figure 5 the magnetization profiles obtained at $h^* = 0.4$

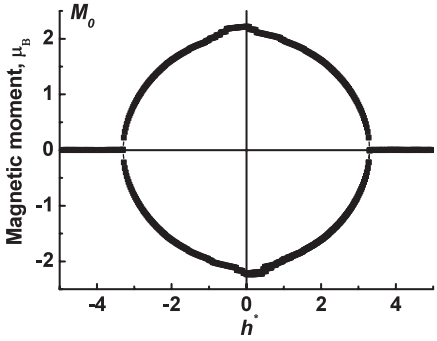

Figure 6. Magnetic moment at the node site of the applied magnetic field (2) with $\Lambda = 50$ for bulk Fe as a function of field amplitude h^*.

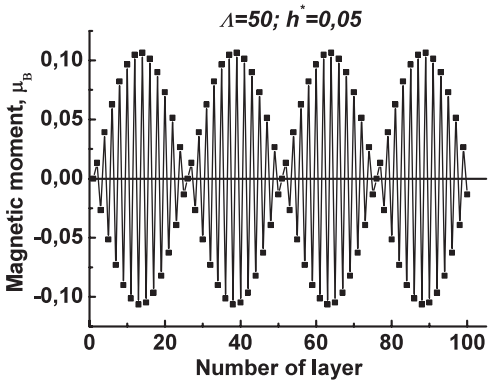

Figure 7. SDW solution for bulk V in the external local magnetic field (2) with $\Lambda = 50$ and $h^* = 0.05$.

and $h^* = 2.6$ are shown. They demonstrate the evolution of magnetic structure versus the strength of applied magnetic field h^*. The small magnetic field perturbs the ferromagnetic state only slightly without change of the magnetic moment's directions. However, when magnetic field increases, modulated AF structure appears first near the antinode of the applied field. The value of magnetic moment at the node site of the applied field as a function of the amplitude h^* is presented in figure 6. The SDW state, which repeats the profile of the applied field, arises only if $h^* > 3$. This field is thousands of times larger than the field which induces the transition to the SDW state in the bulk Cr. After switching off the external field, the system returns to the ferromagnetic state. Thus for the bulk Fe the SDW without external field does not exist for any wavelength Λ.

Another behaviour demonstrates V in the external field (2). Without field V is a non-magnetic metal and there is no threshold field for transition to the SDW state. A typical magnetic profile obtained at $h^* = 0.05$ and $\Lambda = 50$ is shown in figure 7. The dependence of the SDW amplitude on the amplitude of the applied field is linear, as illustrated in figure 8. Obviously, here also, the SDW disappears after switching off the magnetic field. It is worth noting that at $h^* = 0.05$ the amplitude of the SDW is only about 0.1 μ_B, whereas for Cr the transition to the SDW state takes place at $h^* \sim 0.002$ (see figure 1) and the SDW remains after switching off the magnetic field.

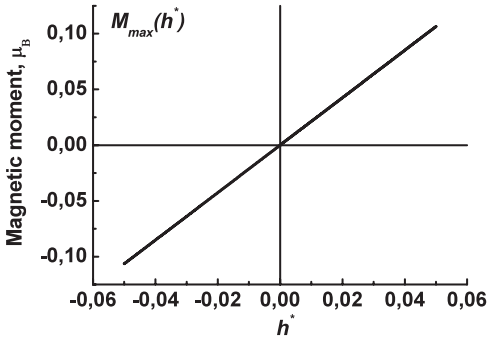

Figure 8. Magnetic moment at the antinode site of the applied magnetic field (2) with $\Lambda = 50$ for bulk V as function of the field's amplitude h^*.

4. Discussion

Introduction of external local magnetic field on each atom and enforcement of the self-consistency of the system in this field allows us to find a specific solution from the number of self-consistent solutions existing in the system. If the spatial configuration of the field is taken in accordance with equation (2), the solution at large h^* will always have the form of an SDW with wavelength Λ. Although the transition to the SDW state versus h^* takes place for any metal, only for Cr does the SDW solution remain after switching off the field. The profile of magnetization and the energy of the system obtained within the PAM for the SDW in Cr are in good agreement with state of the art *ab initio* calculations [12].

To study the stability of solutions we change the amplitude h^* of the external field and plot the hysteresis loop of the system. When the wavelength of the applied field Λ in (2) exceeds 50 ML, the system transfers to the SDW state and remains there independently of the value and sign of applied magnetic field. The nodes of the SDW can be shifted but cannot be destroyed by this field.

Taking into consideration that the nodes of the SDW in the bulk Cr are quite stable, we can consider them as one-dimensional quasiparticles which do not interact at large distance and annihilate like soap bubbles when they approach close one to another. Using this analogy, it is possible to find very simple mechanisms of the SDW properties and their rearrangement with temperature and alloying. It is well known that magnetic impurities like Mn or Fe lead to the transition from the SDW to the AF state [19]. Mn and Fe impurities polarize Cr atoms around them and nodes cannot appear there. If we increase the number of magnetic impurities the nodes will disappear and AF ordering will be established in the whole crystal.

It is worth noting that, in the SDW in chromium, the amplitude of local magnetic moments is modulated along a (100) direction and is the same in every plane perpendicular to this direction. The node of the SDW is not a point but a plane, that is, a nodal plane. We also performed calculations with a wavevector of applied SDW-like magnetic field $\boldsymbol{Q}$ along the (110) direction. The amplitude of the field necessary for transition to the SDW state (with (110) nodal planes) proves to be several hundred times larger than in the case of SDW with (100) nodal planes. When the external field was switched off the system returned to the AF state with equal values of local moments in (100) planes (or in some cases into the SDW state with (100) nodal planes) and never stayed in the SDW state with (110) nodal planes. Therefore, SDW states with another orientation of nodal planes than (100) are not stable at zero field. This result is not surprising: each Cr atom in particular (100) plane has four nearest neighbours in previous and four nearest neighbours in the next (100) planes. Taking into account the

tendency of Cr magnetic moments to be ordered antiparallel, one can see that the state with equal moments in the (100) plane gives no magnetic frustrations. It is also in good agreement with recent neutron experiments on Cr(16 nm)/Sn(0.2 nm) multilayers [20], where SDW and AF states with constant moments in the plane (100) were detected in Cr(011)/Sn multilayers.

What about the mechanism driving the system into the SDW state? We have seen above that the difference in energy between SDW and AF states is of the order of a few kelvin per atom. Moreover, Cr is very sensitive to appearance of non-magnetic atoms. We introduced non-magnetic Cr atoms (with reduced parameter U/Γ) into the AF matrix by a random procedure and enforced the self-consistency. As little as 3% of such atoms reduces the average magnitude of magnetic moment in the system from 0.6 μ_B to 0.16 μ_B. When 10% of non-magnetic atoms were embedded into the system, the self-consistent solution was totally non-magnetic and even stayed non-magnetic after switching on the Coulomb repulsion on each atom. When 10% of non-magnetic atoms were introduced randomly inside five atomic layers, the SDW solution with a nodal plane inside these five layers was obtained. Thus in the three-dimensional case a relatively small number of non-magnetic atoms forces the transition to the SDW-like state. The same effect produces the non-magnetic atoms like V embedded into the Cr. They pin the node of SDW, and this is in agreement with resent experiments [21], which have shown that the magnetic structure of Cr films can be controlled by periodic insertion of non-magnetic monatomic layers.

For multilayers, however, the key role is played by the interdiffusion. For example, in Fe/Cr multilayers, interdiffusion may lead to strong magnetic frustrations and the suppression of the Cr magnetic moments instead of polarization of the spacer by Fe moments. Therefore, in dependence on the interdiffusion ratio, the Fe layer can pin the node or maximum of polarization in the Cr layer. As a result, alloying at the interface can lead to the formation of an SDW node [22], in contrast to the bulk alloy, where as little as 2.3% of Fe in Cr leads to AF ordering. Our previous calculations of Fe/Cr multilayers with thick Cr layers show that the SDW solution arises only when intermixing at the Fe/Cr interface exceeds a definite value [23].

Temperature properties of the SDW in Cr are more exotic. Except the transition from transverse to longitudinal SDW mentioned above (which is related to spin–orbit interaction not included in our model), there is a temperature dependence of the wavelength Λ. In pure Cr Λ increases from 60 Å at low temperature to 78 Å at room temperature. This is a surprising result because the number of quasiparticle nodes normally has to increase with temperature and therefore the distance between them should decrease. However, if we will take into account very small energy, which is enough to create one single node, we can elucidate the reason for such behaviour. Indeed, already at low temperature, the nodes exist and the distance between them is only slightly larger than the minimal possible equilibrium distance. When temperature increases, due to the fluctuations, new nodes appear between nodes already present in the crystal. The distance between the nodes becomes less than the minimal equilibrium distance (40 monolayers) and the new nodes will annihilate together with nearest neighbouring nodes. Therefore, fluctuations will lead to the destruction of the nodes. Their number will be less and the distance between them larger than at low temperature when creation of a node close to an existing one occurred very seldom.

5. Conclusion

Our suggested theory of SDW formation does not take into account the nesting property of the Cr Fermi surface. Despite this we have seen that the SDW solution becomes stable when the distance between nodes exceeds 25 layers. In this case the threshold between SDW and AF states is larger than the threshold between two SDW states with opposite directions of moment

on each site. This means that the nodes of the SDW can move as quasiparticles and their annihilation needs larger energy than the shift of the nodes. Nodes can be created by thermal fluctuations or by structural defects with magnetic frustrations. Than they can move from the place where they were created along the (100) direction if there are no other nodes around. Thus the nodes of the SDW are low-energy excitations, similar to the usual spin waves—magnons. However, in contrast to the magnons, the nodes annihilate when they approach close to one another. This determines the temperature dependence of the node concentration and therefore the dependence of the SDW wavelength on the temperature.

What is the reason for formation of this large-scale length in the system where only hopping between nearest sites is taken into account? We can now answer this question. The new scale is connected with the typical distance D on which perturbation of magnetic moment decays in bulk Cr. If the distance between two nodes is larger than $2D$, they do not interact. If they approach closer the energy of the system increases and the nodes disappear.

The energy for creation of a single node is extremely low. Transition of several per cent of Cr atoms inside a few (100) layers in the non-magnetic state leads to the SDW state with a nodal plane inside these layers. Therefore, thermal fluctuations and magnetic frustrations can drive the system into the SDW state even at very low temperature.

In our model the nesting property of the Cr Fermi surface is not used. This does not mean that nesting does not exist in the Cr and that the nesting model cannot predict the SDW ground state for other materials. However, agreement between our calculations and results of *ab initio* theories, which take into account the shape of the Cr Fermi surface, supports our scenario of SDW formation in bulk chromium.

Acknowledgments

This work was partially supported by INTAS project 03-51-4778 and RFBR 04-02-16024. The work of VMU in IPCMS (Strasbourg) was supported by a grant from CNRS.

References

[1] Grunberg P, Schreiber R, Pang Y, Brodsky M B and Sowers H 1986 *Phys. Rev. Lett.* **57** 2442
[2] Baibich M N *et al* 1988 *Phys. Rev. Lett.* **61** 2472
[3] Slonczewski J C 1991 *Phys. Rev. Lett.* **67** 3172
[4] Uzdin S, Uzdin V and Demangeat C 1999 *Europhys. Lett.* **47** 556
[5] Jamneala T, Madhavan V and Crommie M F 2001 *Phys. Rev. Lett.* **87** 256804
[6] Kudasov Y B and Uzdin V M 2002 *Phys. Rev. Lett.* **89** 276802
[7] Fawcett E 1988 *Rev. Mod. Phys.* **60** 209
[8] Zabel H 1999 *J. Phys.: Condens. Matter* **11** 9303
[9] Fishman R S 2001 *J. Phys.: Condens. Matter* **13** R235
[10] Overhauser A W 1962 *Phys. Rev.* **128** 1437
[11] Lomer W M 1962 *Proc. Phys. Soc.* **80** 489
[12] Hafner R, Spišák D, Lorenz R and Hafner J 2002 *Phys. Rev.* B **65** 184432
[13] Hirai K 1997 *J. Phys. Soc. Japan* **66** 560
[14] Marcus P M, Qui S-L and Moruzzi V L 1998 *J. Phys.: Condens. Matter* **10** 6541
[15] Cottenier S, De Vries B, Meerschaut J and Rots M 2002 *J. Phys.: Condens. Matter* **14** 3275
[16] Uzdin V M and Demangeat C 2002 *Phys. Rev.* B **66** 92408
[17] Uzdin V M, Keune W, Schrör H and Walterfang M 2001 *Phys. Rev.* B **63** 104407
[18] Uzdin V, Westerholt K, Zabel H and Hjörvarsson B 2003 *Phys. Rev.* B **68** 214407
[19] Fawcett E, Alberts H L, Galkin V Yu and Yakhmi J V 1994 *Rev. Mod. Phys.* **66** 25
[20] Jiko N, Mibu K and Takeda M 2005 *Phys. Rev.* B **71** 014414
[21] Mibu K and Shinjo T 2002 *J. Phys. D: Appl. Phys.* **35** 2359
[22] Fullerton E E, Bader S D and Robertson J L 1996 *Phys. Rev. Lett.* **77** 1382
[23] Uzdin V and Keune W 2001 *Phys. Met. Metallogr.* **91** (Suppl. 1) S82