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Reorientation of spin-density waves in Cr films induced by proximity effect of vanadium

E Kravtsov[1,2], A Nefedov[1], H Zabel[1], R Brucas[3], B Hjörvarsson[3], A Hoser[4,5] and G J McIntyre[6]

[1] Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany
[2] Institute of Metal Physics, 620041 Ekaterinburg, Russia
[3] Department of Physics, Uppsala University, Box 530, S-75121 Uppsala, Sweden
[4] Institut für Kristallographie, RWTH-Aachen, D-52056 Aachen, Germany
[5] Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany
[6] Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex 9, France

E-mail: evgeny.kravtsov@ruhr-uni-bochum.de

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Abstract
We report on neutron scattering studies from proximity effects of neighbouring vanadium layers on spin-density waves in epitaxial Cr(001) films. We provide direct evidence for long-range effects from the V/Cr interface leading to changes in the polarization and propagation direction of the spin-density waves in rather thick Cr films. The Néel temperature is found to be affected by boundary conditions for the spin-density waves at V/Cr interfaces.

1. Introduction

Bulk chromium is an itinerant antiferromagnet displaying a spin-density wave (SDW) below the Néel temperature of 311 K. The SDW consists of a sinusoidal modulation of the amplitude of the antiferromagnetically ordered magnetic moments, the SDW period being incommensurate with the bcc lattice periodicity of Cr. At the spin-flip transition temperature of 123 K, the SDW polarization changes from longitudinal (LSDW) with magnetic moments aligned parallel to the wave propagation direction to transverse (TSDW), where the magnetic moments align perpendicular to the wave propagation direction. Elastic strains and chemical impurities in Cr may cause the SDW to become commensurate (CSDW). It is well established now that the SDW origin is connected with the peculiar features of the Cr Fermi surface, which provide nesting vectors between electron and hole sheets of similar shape [1]. To date, a substantial body of literature has evolved which traces different aspects of the SDW behaviour in bulk Cr and Cr-based alloys (see reviews [1, 2] and references therein).

The SDW magnetism in Cr films and multilayers is less studied and there are a good number of gaps in our understanding of its nature [3]. Of particular interest are proximity effects from neighbouring films on the SDW magnetism in Cr-based multilayers. These effects are well known for Cr/ferromagnetic metal systems, and for the most part Fe/Cr multilayers, where the interface disorder and exchange coupling are found to be responsible for the SDW behaviour in Cr layers [3–5]. Similar observations have also been made for the SDW behaviour in other Cr/ferromagnet systems, such as Cr/Ni and Cr/Co [3, 6]. There has also been some interest in Cr/paramagnet systems, like Cr/Ag [7], Cr/Cu [6], and Cr/Pd [6]. The main physics in these systems was found to be due to additional strains induced by lattice misfits and frustration effects at interfaces.

Here we address the Cr/V layered system, where proximity effects are provided by hybridization effects between the very similar Fermi surfaces of chromium and vanadium. Almokhtar *et al* [8] have recently shown by using Mössbauer spectroscopy with ^{119}Sn probe monolayers that there is a strong suppression of the Cr magnetic moment and of the SDW near Cr/V interfaces. Whilst the effect is of local nature and it vanishes at distances of about 40 Å from the Cr/V interface, it nevertheless is able to produce a global perturbation of the Cr SDW magnetism, as we have reported earlier [9]. Here we extend our study of the SDW behaviour in a 2000 Å thick Cr(001) film sandwiched between V layers in comparison to that in bulk Cr and in a 2000 Å thick plain Cr(001) film. A preliminary discussion of our observations for the Cr(001) film and the Cr(001)/V bilayer was published previously [9, 10]. We provide direct evidence for the polarization and propagation direction of the SDWs in Cr films being conditioned by V/Cr interface effects.

2. Experimental details

The samples were grown by UHV molecular-beam epitaxy on MgO(001) substrates. The first sample is a 2000 Å thick Cr film grown directly on the substrate without any buffer or cap layers. The substrate temperature was kept at 600 °C to provide good crystalline quality of the sample as monitored by RHEED during the deposition. For the other two samples we have deposited first a V buffer layer of 14 Å thickness, and continued with a 2000 Å thick Cr film. One of the samples was left unprotected, while the third sample was capped with a 14 Å thick V layer and a 20 Å thick Cr protection layer. During the deposition of these two samples the substrate temperature was lowered to 200 °C to avoid interdiffusion at the interfaces.

For the structural characterization of the samples we used the x-ray diffractometers at the W1.1 and D3 beamlines of the HASYLAB, Germany. The measurements were performed at room temperature using wavelengths at 1.540 and 0.709 Å. Here we discuss only the main structural parameters of the Cr films as deduced from the x-ray intensity around the Cr(002) and (011) fundamental Bragg peaks. A more extensive structural report on the samples will be published elsewhere. We found that the structural properties of the Cr/V films are identical, irrespective of whether they are capped with another V layer or not. Thus the deposition of the top V layer has no effect on the structure of the Cr underlayer. In the following we distinguish only between samples grown with and without the V buffer layer.

The epitaxial relation between Cr and MgO for all samples was determined to be Cr(001)[100]//MgO(001)[110], which is in agreement with the reports for growth of Cr directly on the MgO(001) substrate [12]. The in-plane Cr lattice parameter was found to be the same for all three samples $a_{\parallel} = 2.889 \pm 0.001$ Å. Furthermore, from the radial width of the Cr(002) peaks we calculate an out-of-plane structural coherence length of about 2000 Å. This value corresponds exactly to the total Cr film thickness, such that all Cr films are completely correlated in the out-of-plane direction.

The out-of-plane lattice parameters vary slightly between the samples: $a_{\perp} = 2.875 \pm 0.001$ and 2.879 ± 0.001 Å for the samples with and without V buffer layer, respectively. The in-plane mosaic spread in the Cr films is significantly different: 0.10° and 0.19° for the Cr film with and without V buffer layer, respectively.

The antiferromagnetic structure of the Cr layers was determined by neutron diffraction studies. The neutron scattering experiments were performed using the triple-axis spectrometer UNIDAS (Forschungszentrum Jülich, Germany) and the four-circle diffractometer D10 (Institut Laue-Langevin, Grenoble, France). In the experiments we used pyrolytic graphite (PG) monochromators to select a neutron beam wavelength of $\lambda = 2.351$ Å together with PG transmission filters to reduce the $\lambda/2$ monochromator contamination. The background radiation was sufficiently filtered out by using PG analyser crystals fixed to zero energy transfer. The measurements were taken at temperatures between 10 and 330 K by using a Displex cryostat (UNIDAS) or a He-flow cryostat (D10) with Al windows.

3. Neutron scattering results

Elastic neutron scattering is a powerful tool that provides very complete information on the SDW state in Cr films. The magnetic moment modulation produces corresponding satellite reflections in the vicinity of forbidden Cr bcc Bragg reflections, which can be detected with neutron scattering. The position and intensity of these satellite reflections contain information on the spin orientation, the amplitude, the period and the propagation direction of the spin density waves. The application of neutron scattering methods to the determination of the SDW parameters has been reviewed in a number of papers. We will not repeat this here, but we refer the interested reader to published papers and reviews for further information [1, 3, 6]. To characterize the SDWs in our Cr films, in each case we performed four scans across the (010) and (001) positions in the in-plane (K) and out-of-plane (L) directions. In the following we show only scans providing non-trivial information on the SDWs.

In figure 1 neutron diffraction scans are plotted for the plain Cr film. The scans are taken in the K direction and cover the vicinity of the Cr(010) and Cr(001) positions. Equivalent scans in the L direction were also performed but are not shown here, since they contain no useful further information except for a high-temperature commensurate peak at the (010) position, which is also seen in the K scan. As follows from the above scans, only one SDW exists in the film. At low temperatures two satellite peaks are present around the (001) position in the K direction. From this we infer that a longitudinal incommensurate SDW exists below 100 K which propagates in the film plane. Above 100 K these satellite peaks completely disappear; instead, a set of new satellite peaks appears around the (010) position. Thus between 100 and 150 K a spin-flip transition occurs from a longitudinal to a transverse incommensurate SDW. The propagation direction remains in plane, but the spins turn out of plane. A commensurate SDW becomes visible in the film at high temperatures close to the Néel temperature of the incommensurate SDW at about 275 K. The Néel temperature of the commensurate phase could not be reached and seems to be well above the bulk Néel temperature. The qualitative magnetic phase diagram for the SDWs in a plain Cr(2000 Å) film on MgO(001) is shown schematically in figure 2.

Next we present results on the SDW state in a V(14 Å)/Cr(2000 Å) bilayer structure grown on a MgO(001) substrate. In figure 3 are reproduced the neutron scattering data from the bilayer. Again, the satellite reflections due to the incommensurate SDW were detected only in the K direction in the vicinity of the (001) and (010) positions. We also performed scans in the L direction around the (001) and (010) positions but we do not show them, since these scans detected no useful signal except for peaks at the (010) and (001) positions, that were also seen in the K-scans. In addition, satellite reflections were also observed up to 100 K at $H = 0.05$ in the H direction in the vicinity of the (010) position, the projections of which

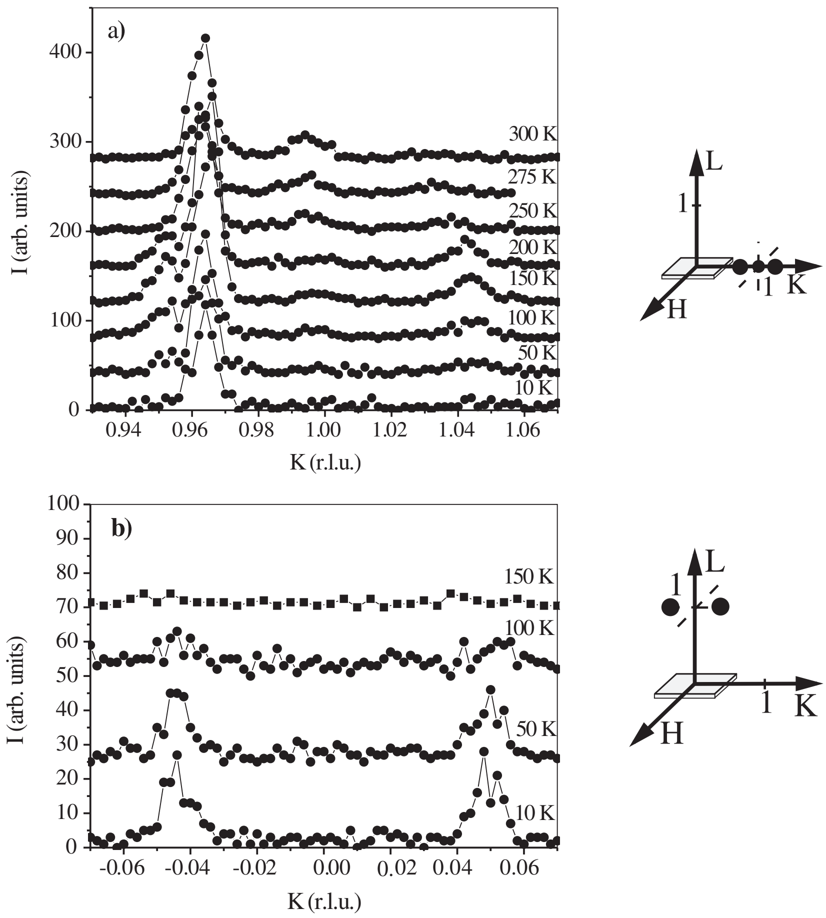

Figure 1. Neutron scattering scans for the plain Cr(2000 Å) film on MgO(001) taken in the K direction at (a) the Cr(010) and (b) the Cr(001) positions. The scans recorded at different temperatures are depicted with an offset in the vertical direction for clarity. The strong temperature-independent peak at $K \sim 0.97$ rlu in (a) is due to the MgO(022) reflection for the $\lambda/2$ harmonic.

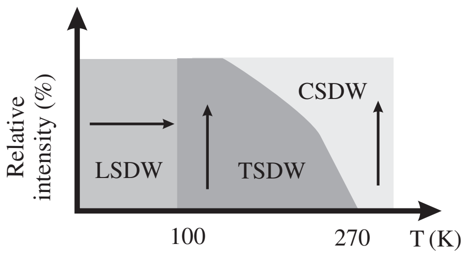

Figure 2. Qualitative magnetic phase diagram for the spin density waves in a 2000 Å thick Cr(001) film deposited on a MgO(001) substrate. The phase diagram is the result of neutron-scattering experiments shown in figure 1.

are seen partly superposed at the commensurate (010) position in figure 3(a). The SDW thus propagates in the film plane, but its polarization behaviour is different from that in the Cr film

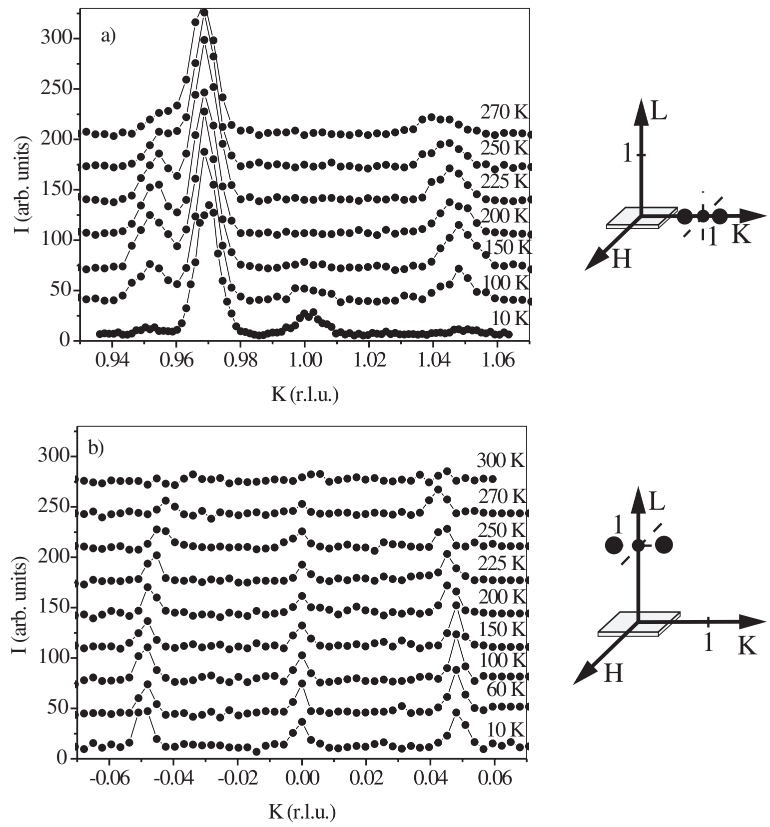

Figure 3. Neutron-scattering scans for the V(14 Å)/Cr(2000 Å) bilayer on MgO(001) taken in the K direction at (a) the Cr(010) and (b) the Cr(001) positions. The scans recorded at different temperatures are depicted with an offset in the vertical direction for clarity. The strong temperature-independent peak at $K \sim 0.97$ rlu in (a) is due to the MgO(022) reflection for the $\lambda/2$ harmonic.

with V buffer. At low temperatures we observe a longitudinal SDW. Above 100 K a spin-flip transition occurs to a transverse SDW with in-plane spins. In addition to the satellite reflections from the incommensurate SDW phase, we also observe the (001) reflection corresponding to a commensurate SDW. The commensurate phase coexists with the incommensurate one at all temperatures up to the Néel temperature. The integrated intensity of the commensurate SDW reflections is about 10% of that of the ISDW satellites. Both the commensurate and incommensurate SDW reflections have the same full width at half maximum (FWHM), which is directly connected with the in-plane SDW correlation length. The Néel temperature for both the commensurate and incommensurate phases is about 300 K. The temperature phase diagram for the V/Cr system is shown in figure 4.

The neutron-scattering results for a trilayer V(14 Å)/Cr(2000 Å)/V(14 Å) structure are represented in figure 5. In this case we observe satellite reflections only in the L direction around the (010) and (001) positions, indicating that the SDW propagates out of the film plane. Scans performed in the K direction around the (010) and (001) positions provided us no useful signal and therefore we do not present them in the picture. At low temperatures below 60 K we observe a longitudinal SDW. The spin-flip transition to the transverse SDW is no longer sharp

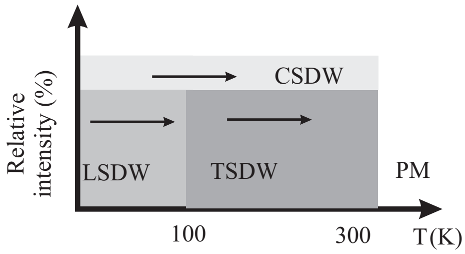

Figure 4. Qualitative magnetic phase diagram for the spin-density waves in a V(14 Å)/Cr(2000 Å) bilayer deposited on a MgO(001) substrate. The phase diagram is the result of neutron-scattering experiments presented in figure 3.

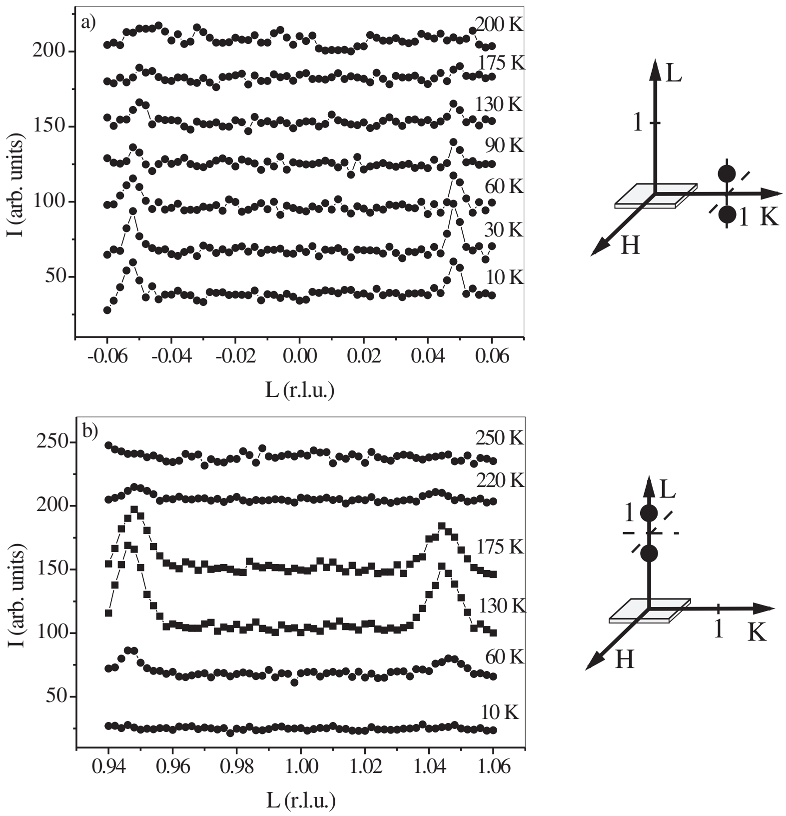

Figure 5. Neutron-scattering scans for the V(14 Å)/Cr(2000 Å)/V(14 Å) trilayer on MgO(001) taken in the L direction at (a) the Cr(010) and (b) the Cr(001) positions. The scans recorded at different temperatures are depicted with an offset in the vertical direction for clarity.

but is spread over a wide temperature interval of about 70 K. No intensity was detected at the commensurate (010) and (100) positions, indicating that the SDW in this sample is completely incommensurate. It is important to note that there is a significant drop in the Néel temperature as compared to the previous samples. The magnetic phase diagram for the V/Cr/V system is depicted in figure 6.

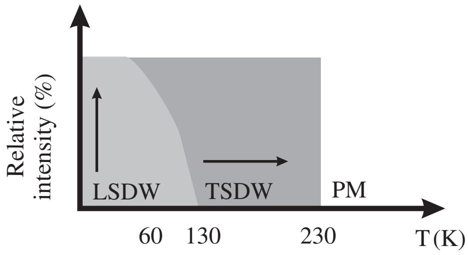

Figure 6. Qualitative magnetic phase diagram for the spin-density waves in a V(14 Å)/Cr(2000 Å)/V(14 Å) trilayer deposited on a MgO(001) substrate. The phase diagram is the result of neutron-scattering experiments presented in figure 5.

4. Discussion

Generally, in bulk Cr there exists a polydomain SDW, with the wavevectors being along the three different [001] crystal axes of the bcc Cr lattice. A monodomain SDW state can be prepared by cooling through the Néel temperature in the presence of a tensile stress applied along a cubic axis. On the other hand, when cooling through the Néel temperature with a compressive stress applied along one cube axis it produces SDWs with the wavevectors along the other two cubic axes [13]. When dealing with Cr thin-film systems, one should distinguish between in-plane and out-of-plane SDW propagation directions and polarizations that are nonequivalent due to the broken symmetry at the interfaces. The SDW behaviour in Cr thin-film systems is conditioned by the competition of different factors, including strains, proximity effects of neighbouring layers, interface disorder and interface exchange coupling, etc. The Cr/V systems under consideration are ideal for concentration on the effects arising only from epitaxial strains and the Cr–V hybridization at interfaces.

Since the epitaxial strain is of crucial importance in our systems, we estimate first the applied stress from the epitaxial strains as provided by x-ray scattering. For our Cr(001) films the stresses σ_i and the applied pressure p can be estimated by using the relations [14]

$$\sigma_\parallel = (E\epsilon_\parallel + \nu\sigma_\perp)/(1-\nu), \quad (1)$$

$$\sigma_\perp = E\epsilon_\perp + 2\nu\sigma_\parallel, \quad (2)$$

$$p = -(2\sigma_\parallel + \sigma_\perp), \quad (3)$$

where $\epsilon_i = (a_i - a)/a$, a_i being the lattice spacing in the ith direction. E, ν, and a are the Young modulus, the Poisson ratio, and the lattice spacing of bulk Cr (279 GPa, 0.21, and 2.884 Å), respectively.

The results for the samples under consideration are presented in table 1. As follows from the data, the MgO(001) substrate provides an in-plane epitaxial tensile stress on the Cr films. The reference sample, a single Cr(001) film grown directly on a MgO(001) substrate, is an example of a system where the in-plane and out-of-plane strains in Cr are completely due to the epitaxial stress from the substrate. A thin V buffer layer in the Cr/V and V/Cr/V films does not change the in-plane strain but provides an additional out-of-plane strain that significantly decreases the resulting pressure applied to the Cr lattice.

Since the effect of the hybridization between Cr and MgO is almost negligible, the SDW behaviour in the Cr/MgO sample is conditioned fully by the epitaxial strains and dimensional effects due to the limited Cr-layer thickness of 2000 Å. The magnetic phase diagram shown in figure 2 is very similar to that of bulk Cr [1, 11]. The differences are some reduction of the spin-flip and Néel temperatures, as well as a high-temperature contribution from the commensurate

Table 1. Lattice parameters, epitaxial strains, stresses, and resulting pressures in Cr(001) and Cr/V(001) films on MgO(001) substrates.

Sample	$a_\perp$ (Å)	$a_\parallel$ (Å)	$\epsilon_\parallel$ (10^{-3})	$\epsilon_\perp$ (10^{-3})	$\sigma_\parallel$ (kbar)	$\sigma_\perp$ (kbar)	p (kbar)
Cr(001)	2.879	2.889	1.73	−1.73	0.54	−0.26	−0.82
Cr/V(001) and V/Cr(001)/V	2.875	2.889	1.73	−3.12	0.43	−0.69	−0.17

SDW phase observed in the thin-film system and attributed to the dimensional and strain effects. Another reason for the commensurate SDW expansion may be the significant difference in the thermal expansion coefficients of Cr and MgO, especially at temperatures above 200 K. The epitaxial stress from the MgO substrate dictates that the SDWs propagate in-plane. The SDW spin polarization, being in plane at low temperatures and out of plane at high temperatures, seems to be the intrinsic property of the system. Similar results were also reported for a single 4500 Å Cr film on a MgO(001) substrate where Kunnen *et al* [12] observed a transverse SDW with the same propagation and polarization directions as in our case. Surprisingly, in contrast to our results, Kunnen *et al* reported that in their Cr/MgO system there is no longitudinal SDW, even at very low temperatures. The fact that they found no longitudinal SDW in the film is more likely due to a much stronger stress in their sample as compared to our Cr/MgO film. Since the growth conditions vary slightly from laboratory to laboratory, and since the SDWs in Cr are highly sensitive to stress and structural coherence lengths, we often find some disagreement between results from different experimental groups.

The comparative analysis of the SDW state in the Cr/MgO and Cr/V/MgO systems allows us to differentiate the effect due to Cr–V hybridization from other effects. The magnetic phase diagram of the SDW state in the Cr/V/MgO sample shown in figure 4 is almost identical to that of the Cr/MgO system. The fact that the contamination from the commensurate SDW phase is not so essential now is well understandable, since the applied pressure from the epitaxial stresses is much weaker. The main but essential difference is the change of the SDW polarization at higher temperatures. The SDW in the Cr/V/MgO sample again propagates in the film plane but the spins are now also oriented in the film plane at all temperatures up to the Néel temperature. The spin reorientation of the transverse SDW from the out-of-plane (Cr/MgO) to in-plane direction (Cr/V/MgO) is no doubt due to the Cr–V interface hybridization effect.

The analysis of the SDW state in the V/Cr/V/MgO(001) system provides new and important information to gain further insight into the Cr–V hybridization effect. We notice in this system two new effects. First, the top Cr/V interface makes the SDW propagate in the out-of-plane direction. Second, we observe a significant drop in the Néel temperatures for the incommensurate SDW. As evident from the comparison of the phase diagrams shown in figures 4 and 6, the Néel temperature in the V/Cr/V film decreases by about 70 K as compared to the Cr/V system. Since there is no essential difference in the Cr structural properties for the Cr/V/MgO and V/Cr/V/MgO samples, the difference in the SDW behaviour is completely due to the Cr–V hybridization at the upper Cr–V interface.

Thus, the effects from strain on the one hand, and the Cr–V hybridization at the interfaces on the other hand, determine the final state of the SDWs in Cr heterostructures, which can be summarized as follows. Stresses arising from epitaxial strains, lattice misfits, structural imperfections in the sample, etc cause additional pressure to be applied to the Cr lattice. This pressure, in turn, suppresses the incommensurate SDW and enhances the commensurate SDW phase with regard to the volume fraction occupied and the temperature range of its existence. In the limiting case of extremely strong strains the incommensurate SDW may be completely suppressed as observed recently by Fritzsche *et al* [15] in Cr/V(110) multilayers on $Al_2O_3(11\bar{2}0)$ substrates. Concerning the propagation direction both (epitaxial) strain and hybridization effects compete. Finally, hybridization effects at the Cr–V interface are mainly responsible for long-range re-orientational effects in Cr/V multilayers. The Cr–V hybridization governs the SDW polarization in Cr/V systems as well as the SDW propagation in V/Cr/V systems. It is important to note that the Néel temperature in Cr/V heterostructures differs significantly for in-plane and out-of-plane propagating SDWs. For the in-plane direction we observe a higher Néel temperature (300 K) than for the out-of-plane direction (230 K).

The strain effects discussed above are fully appreciated and well presented in the literature [1, 13]. In contrast, the global SDW reorientation effects associated with the Cr–V interface hybridization are unexpected and difficult to explain. Recent theoretical predictions concern only short-range local effects arising around the Cr–V interfaces. It is predicted that there should be a strong suppression of the Cr magnetic moment as well as an induced magnetic moment in the V monolayer next to the Cr interface [16, 17]. It was also shown both theoretically [16] and experimentally [8] that for the SDW propagating out of plane in Cr/V multilayers the SDW nodes are pinned near the Cr/V interfaces. However, to the best of our knowledge, currently there is no theoretical consideration of orientational effects caused by the hybridization of Cr with neighbouring paramagnetic layers. All theoretical considerations published so far have assumed a transverse SDW with out-of-plane propagation. It would be highly desirable to have a more complete theoretical understanding of the SDW properties in thin films with different ferro- and paramagnetic boundary conditions.

5. Conclusions

We have studied the proximity effect of vanadium layers on spin-density waves in Cr/V heterostructures grown on MgO(001) substrates. We have found that the MgO(001) substrate provides an in-plane epitaxial tensile stress on the Cr films, so that the SDW behaviour in Cr/V films is conditioned by a competition between strain and Cr–V hybridization effects. The epitaxial stress forces the SDW to propagate in the film plane, it suppresses the incommensurate SDW, and it enhances the commensurate SDW phase in the sample. The Cr–V interface hybridization produces long-range re-orientational effects in Cr/V multilayers. The vanadium proximity hybridization determines the SDW polarization in Cr/V systems as well as the SDW propagation direction in V/Cr/V systems. We have also found that the SDW reorientation from the in-plane to the out-of-plane propagation direction is accompanied by a significant drop in the Néel temperature in Cr/V multilayers. These strong re-orientational effects are unexpected and need to be explained by theory.

Acknowledgments

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