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Strain and strain relief in Gd(0001) films on Mo(112)

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Strain and Strain Relief in Gd(0001) Films on Mo(112)

Takashi Komesu, C. Waldfried, and P. A. Dowben

***Abstract*—The electronic structure of strained and unstrained Gd(0001) has been studied with spin-polarized photoemission spectroscopy and spin-polarized inverse photoemission spectroscopy. In this work, we observed that relaxation of the expansively strained in-plane crystal lattice constant, of Gd(0001) on Mo(112), significantly diminishes the differences in the electronic structure from that observed for Gd(0001) grown on W(110). The defects that are incorporated in the Gd films, with increasing film thickness, lead to an in-plane lattice relaxation. Such thickness dependent strain relief results a loss of net polarization for Gd(0001) grown on Mo(112) compared to the relatively unstrained Gd(0001) films grown on W(110).**

***Index Terms*—Rare earth magnetism, spin-polarized inverse photoemission, magneto-striction, strain relief and misfit dislocations.**

I. Introduction

STRAIN is known to affect magnetism, with possible dramatic effects as suggested by the theoretical calculations of Moruzzi and Marcus [1] and experimental results of Shinde and coworkers [2], Bartholin and coworkers [3], and others. There is a general acceptance of the strong influence of magneto-elastic interactions on the Curie temperature and other magnetic properties. For the rare earth metals, the magnetic-elastic interactions are large [3]–[6]. For gadolinium compression is seen to lead to a suppression of T_c [3], [6] while expansion leads to an increase of T_c [7], [8]. Not only does strain affect the magnetic properties but it has long been established that the lattice constant has a profound influence on the electronic structure, even for the thinnest of thin films [9], [10].

Gd(0001) grown on W(110) surface has been heavily investigated over the past decade [11]. For Gd(0001) grown on W(110), the hexagonal close pack (hcp) film has been observed to be strained (2–3%) for film thickness of 10–50 Å [12]. The Gd grown on W(110) then relaxes toward the bulk lattice constant with increasing film thickness, so that with sufficient deposition of Gd, the bulk Gd lattice parameter, (3.63 Å), is reached at 100 Å to 1000 Å [12]. Gd(0001) grown on Mo(112) exhibits substantial in-plane expansive strain compared to a similar thickness of Gd(0001) on W(110) [9]. For the Gd grown on Mo(112), the lattice is expanded by 4% for a film thickness of 30 to 150 Å [9].

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The mechanism of strain relief with increasing film thickness which is observed for Gd(0001) on W(110) [12] should be applicable to Gd(0001) on Mo(112). The effects of elastic strain are more pronounced for Gd(0001) on Mo(112) than for Gd(0001) on W(110) because of the lager misfit of the Gd versus Mo(112) lattice parameters compared to Gd versus W(110), as defined below,

$$f = \frac{a-b}{a} \tag{1}$$

where a refers to the lattice constant of the sublayer, and b is for the lattice constant of the overlayer. Comparison of misfits for systems with nonconservation of the point group or noncubic lattice constants is, of course, more complicated than is indicated by the above equation, but misfit clearly plays a role.

The crystal growth mode of thin films is often determined by a value of a misfit, f, between substrate and overlayer materials. With the initial growth of the Gd film, there is a great difference of lattice constants, between the Gd and Mo(112), giving rise to large misfit, f, and creating expansive in-plane strain [9] and seen, to some lesser extent, for Gd(0001) on W(110) [12].

The expansive 4% in-plane strained Gd(0001) on Mo(112) results in a quite different electronic structure and altered magnetic properties compared to the strain relieved Gd(0001) grown on W(110), as has been noted elsewhere [8], [13]. In this work, we show that the relief of the strain in Gd(0001) on Mo(112) with increasing film thickness results in a spin-polarized electronic structure that is increasingly similar to the largely unstrained Gd(0001) films grown on W(110).

II. Experiment

We investigated the unoccupied electronic structure of thin films of strained and unstrained Gd(0001) grown on Mo(112) surface. Spin-polarized inverse photoemission spectra (SPIPES) were obtained in a UHV system in the isochromatic mode ($\hbar\omega = 9.4$ eV) with a Geiger-Müller tube and a spin-polarized electron gun based on the Ciccacci design (with a GaAs photocathode) [14]. The results were complemented by spin-polarized photoemission (SPES) experiments were carried out at the U5A undulator beamline of the National Synchrotron Light Source (NSLS) at the Brookhaven National Laboratory in Upton, NY. The details of the experimental setup(s) are described elsewhere [15]. All spectra shown in this work are taken for normal electron incidence (inverse photoemission) or normal emission (photoemission) so that $k_{||} = 0$. The surface and bulk character of the valence bands has been determined from chemisorption studies and photon energy dependence.

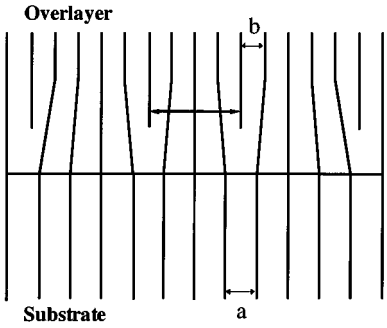

Fig. 1. Schematic representation of misfit of two crystals in the simple case of a one dimensional model with unequal lattice spacings a and b. We propose that unstrained Gd(0001) grows on strained Gd(0001) through such or similar mechanism.

III. Results

Strained and unstrained thin films of Gd(0001), of various thickness, were grown by slow thermal deposition. Strained Gd films of 0.7 monolayers (ML) film thickness, grown on Mo(112), show a 25% larger lattice constant compared to thicker unstrained Gd(0001) films grown on W(110) [9]. For a film thickness of about 10 ML to 40 ML, the strained Gd(0001) thin film on Mo(112) has about 4% larger lattice constant compared to that of unstrained Gd(0001) films [9]. The films were grown at room temperature with the base pressure of 1×10^{-10} Torr and subsequently annealed. The crystal quality of the Gd(0001) films was determined by LEED which was also used to confirmed the expansive strain [9].

There is misfit between the strained Gd(0001) lattice constants (as a sublayer or in the initial stages of thin film growth) and the unstrained Gd(0001) lattice is substantial. With pseudomorphic growth of the Gd(0001) film, the crystal lattice relaxes the strain by means of misfit dislocations that increasingly occur with increasing film thickness [16] so that unstrained Gd(0001) can almost be considered an overlayer on the strained Gd(0001) as schematically indicated in Fig. 1. Misfit dislocations are more likely to appear in the film, the greater the misfit with the substrate, the greater the strain. Misfits will occur in increasing numbers with increasing the film thickness [17]. We have observed regular arrays of such dislocations in LEED in thicker films (>400 Å), manifest as a splitting of the diffraction beam similar to that observed for steps.

Both occupied and unoccupied spin-polarized electronic structure of strained (bottom) and relatively unstrained (top) Gd(0001) grown on Mo(112) and W(110), respectively, are shown in Fig. 2. The upward filled triangle ($\blacktriangle$) refers to majority band (parallel to external field) and downward open triangle (∇) refers to minority band (antiparallel to external field). The SPIPES of unstrained Gd(0001) on W(110) is adapted from the work of Markus Donath and coworkers [18]. Clearly the 4% expansive strain for Gd(0001) on Mo(112) alters the binding energies for both majority and minority bands from that observed for Gd(0001) on W(110) at the surface Brillouin center ($\bar{\Gamma}$). Detailed studies of the spin-polarized band structure indicate that for strained Gd(0001)/Mo(112), the exchange splitting of bands near E_F is larger than is seen for Gd/W(110) at $\bar{\Gamma}$ [13]. Most important, Fig. 2 indicates that expansive strain has a significant influence on the spin-polarized band structure of Gd(0001).

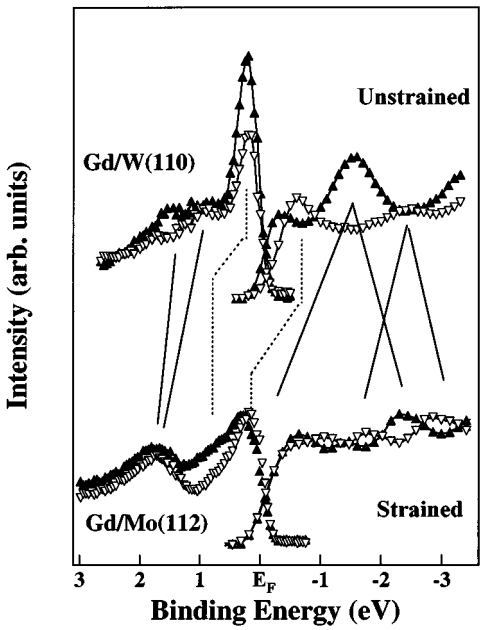

Fig. 2. Comparison of strained and unstrained Gd(0001). Spin-polarized photoemission spectra (left) and spin-polarized inverse photoemission spectra (right) for Gd(0001) on W(110) (unstrained) and Gd(0001) on Mo(112) (strained) at $k_{||} = 0$ or $\bar{\Gamma}$, at approximately 145 K. The lines indicate the binding-energy shifts of the surface (dashed) and bulk (solid) spin subbands as a function of increased expansive strain. The spin-polarized inverse photoemission spectrum for unstrained Gd(0001) grown on W(110) is taken from [18].

IV. Discussion

It has been reported that thin films of Gd(0001) grown on W(110), with a thickness of about 100 Å and larger, provide a strain relieved crystal structure with a lattice constant of 3.63 Å (close to that of bulk) [12]. We can compare such "relaxed" films of Gd(0001) grown on W(110) with films grown on Mo(112) were there is sufficient Gd(0001) film thickness for strain relief to occur via misfit dislocations. Fig. 3 shows the spin-polarized inverse photoemission spectra of Gd(0001) films on W(110) (upper) and Mo(112) (lower), both of sufficient thickness to exhibit some strain relief. The binding energies of the unoccupied bands are very similar (Fig. 3) for both systems indicating that in many respects the electronic structures are comparable—providing the compelling evidence of the strain relief that occurs in both systems in the very thick films.

The misfit dislocations (schematically shown in Fig. 1) are the key to the relaxation of the strained crystal when the film thickness is increased [17] and the explanation for the similarities as well as the differences between the thicker films of Gd(0001) on W(110) and on Mo(112). For Gd(0001) film thickness of about 400 Å, on the Mo(112) substrate, there is a greater number of defects (steps or misfit dislocations) than is the case for Gd(0001) on W(110). This means that the band structure is less well preserved (in the thicker films of Gd on Mo(112)) which leads to wave vector smearing. The weaker band intensities for these "relaxed" Gd(0001) films on Mo(112) could be a

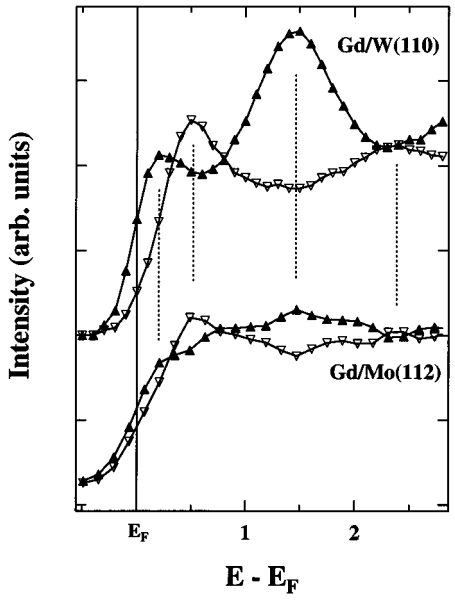

Fig. 3. Comparison of strained and strain relieved Gd(0001). Spin-polarized inverse photoemisson spectra (SPIPES) of unstrained Gd(0001) grown on W(110) (top) and Mo(112) (bottom) at normal incidence or with electron wave vector $k_{||} = 0$ (or $\bar{\Gamma}$). The spectra were acquired at approximately 145 K, well below the accepted thin film Curie temperatures [7]. The solid up-ward triangles (▲) and open down-ward triangles (▽) indicate spin magnetic moment parallel (majority) or antiparallel (minority) to a given magnetic field direction, respectively. The Gd film thickness are 100 Å on W(110) and 400 Å on Mo(112), respectively.

result of such poor conservation of wave vector (in-plane). In addition, in comparing the results for these two Gd film systems, the spin asymmetry of Gd(0001) on Mo(112) is smaller than the that of Gd(0001) on W(110). Misfit dislocations, created by strain relief, might create magnetic defects and hinder complete saturation of the surface magnetization by pinning magnetic domain walls and preventing the magnetic moments from lining up. In this scheme, magnetic domains can be created with the separation of misfit lines. This is similar to creating a "hard axis" as a consequence of shape along the applied field direction in our experiment, as is the case in a "magnetic grating" [19]. Such a model requires further data for confirmation, but is not unprecedented. Such an effect of misfit dislocations on magnetic properties have been previously observed [20].

V. Conclusion

In this paper, we observed that thicker, $d \approx 400$ Å, Gd films grown on the Mo(112) surface are more similar to the spin-polarized electronic structure of "relaxed" Gd(0001) films on W(110) than to that of thinner films of Gd, $10\text{ ML} \leq d \leq 40$ ML, grown on Mo(112). Strain generally decreases with increasing film thickness, which is also the case for Gd on Mo(112). The results of spin-polarized photoemission and spin-polarized inverse photoemission show that the binding energies of both the occupied and unoccupied bands depend on the strain, independent of substrate, but that the substrate choice and initial strain may perturb the magnetic properties through defects that occur with increasing film thickness.

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