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STRAIN AND STRAIN RELIEF IN GD(0001) THIN FILMS ON MO(112)

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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~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].

We investigated the unoccupied electronic structure of thin films of strained and unstrained Gd(0001) grown on Mo(112) surface using spin-polarized inverse photoemission spectra (SPIPES). The results were complemented by spin-polarized photoemission (SPES) experiments. The details of the experimental setup(s) are described in [13]. All spectra shown in this work are taken for normal electron incidence (inverse photoemission) or normal emission (photoemission) so that $k_{\parallel}=0$.

Both occupied and unoccupied spin-polarized electronic structure of strained (bottom) and unstrained (top) Gd(0001) grown on Mo(112) and W(110), respectively, are shown in

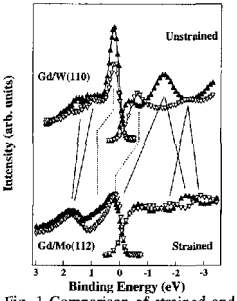

Fig. 1 Comparison of strained and unstrained Gd(0001). Spin-polarized photoemission spectra (left) and spin-polarized inverse photoemission spectra (right) for Gd(0001) on W(110) (unstrained) and Gd(0001) on Mo(112) (strained) at $k_{\parallel}=0$ at nearly 145K. The lines indicate the binding-energy 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 Ref. 14.

Fig. 1. The upward filled triangle (▲) refers to majority band (parallel to external field) and downward open triangle (▽) refers to minority band (antiparallel to external field). 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. 1 indicates that expansive strain has a significant influence on the spin-polarized band structure of Gd(0001).

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 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 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.

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 thicker, d ≈ 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 ML • d • 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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