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LETTER TO THE EDITOR

The localization of electrons in the band structure of Dy with film thickness

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Abstract. By growing dysprosium films on Cu(100), the electronic band structure of dysprosium metal has been investigated using synchrotron radiation photoemission. We have found that 5d electrons become localized with increasing dysprosium coverage. The localization of the 5d band with increasing thickness leads to changes in the 5p multiplet oscillator strengths.

The study of the electronic and magnetic properties of thin metallic rare-earth films is an area of increasing interest [1-3]. Probing the itinerancy of the 5d band near the Fermi level is important in understanding the magnetic properties of rare earths. The magnetic ordering of the rare-earth metals has been postulated to occur as a result of a polarization of the 5d and 6sp bands at the Fermi level [4]. The RKKY model considers the linear response in the exchange interaction between the local moments and the conduction electrons [5-7].

Both theoretical [8-10] and experimental [11,12] studies of the band structure of rare earths have been undertaken. Dysprosium is of particular interest because the outer electron configuration is different for the atomic and solid states: the divalent ($4f^{10}6s^2$) atomic configuration becomes trivalent ($4f^9 5d^1 6s^2$) in the solid state [13].

In this letter we report the development of the dysprosium band structure with increasing film thickness, mainly the localization of the 5d band. We first discuss the experimental set-up, and then we discuss the results.

The measurements were carried out at the beamline 6mTGM of the Synchrotron Radiation Center (SRC) in Stoughton, Wisconsin, USA. A toroidal grating monochromator was used to disperse the synchrotron light. The photoelectron energies were measured with a hemispherical analyser with an angular acceptance window of $\pm 1.5^\circ$ for angle-resolved photoemission. The crystallinity and the quality of the surface were characterized by low-energy electron diffraction (LEED). The thickness of the dysprosium films was determined using an oscillating-crystal thin-film thickness monitor. We chose Cu(100) as a substrate for the Dy thin-film studies. The Cu(100) surface was cleaned before each deposition; the Cu(100) cleaning procedure is described in detail elsewhere [14]. The sample was mounted on a manipulator that allowed it to be moved in the proper position for LEED or photoemission experiments. This manipulator also allowed rotations around three mutually perpendicular axes, so that photoemission experiments could be done with either s- or p-polarized radiation.

The incidence angle of the light is defined with respect to the surface normal, so that normal incidence (zero degrees) has the vector potential completely parallel to the surface (s polarized) while glancing incidence light has a large component of the vector potential normal to the surface (p polarized), preserving symmetry selection rules. Photoelectrons were collected normal to the surface throughout this work.

The deposition of dysprosium on the Cu(100) substrate was undertaken from metal evaporators after considerable outgassing of the sources. During the evaporation, the base pressure in the system typically rose to 1×10^{-10} – 5×10^{-10} torr.

Figure 1 illustrates photoemission electron energy distribution curves taken at normal emission for 5, 10 and 15 Å films of Dy on Cu(100). There is a wealth of Dy valence features resulting from 4f multiplets, which can be identified by comparison with x-ray photoemission spectra [11, 12]. The various multiplets have binding energies at 4.2 ± 0.1 eV (7F), 7.9 ± 0.1 eV (5L , 5G) and 9.5 ± 0.2 eV (2I , 5H) for thick films.

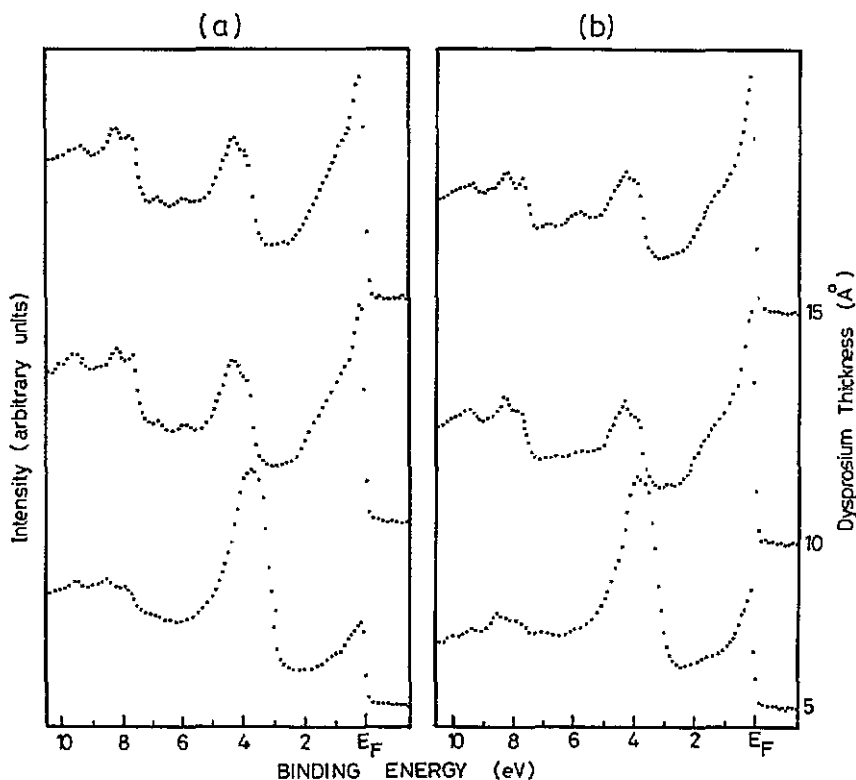


Figure 1. Photoemission spectra of dysprosium overlayers on Cu(100). (a) Light incident angle 34° (s polarized). (b) Light incident angle 64° (p polarized). The photon energy $h\nu = 40$ eV. All photoelectrons were collected normal to the surface.

These dysprosium 4f level binding energies are observed to change with overlayer thickness, particularly the 7F multiplet, which overlaps the substrate Cu 3d [14]. The binding energies will also change with photon energy as a result of the changing oscillator strengths of the different 4f levels [15]. The feature at 5.9 ± 0.1 eV is an intrinsic feature that has been attributed to a many-electron correlation satellite described previously [16].

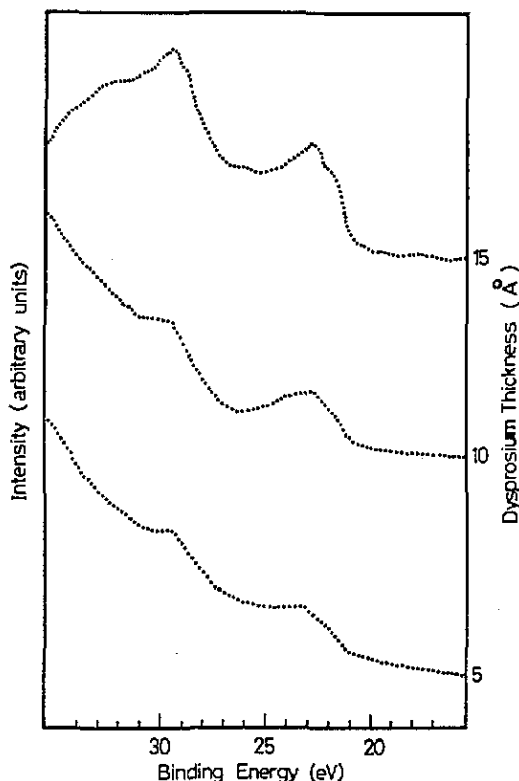


Figure 2. Photoemission spectra from the Dy $5p_{1/2}$ and $5p_{3/2}$ levels with photon energy $h\nu = 50$ eV.

It is clear from figure 1 that the photoemission intensity of the Dy 5d state at the Fermi energy increases with p-polarized light. This is most easily observed by comparing the Dy 5d intensity with Dy 4f. The 4f levels are less likely to have a well defined spatial symmetry axis in one direction [17]. From Fermi's golden rule we can infer that the dysprosium 5d states are largely of $d_{3z^2-r^2}$ character.

We note that the photoemission intensity of the dysprosium 5d band at the Fermi energy increases with Dy coverage (figure 1). This increase is not only due to the finite mean free path of the photoelectrons, but is also a result of the hybridization of the Dy 5d bands of adjacent atoms. Strong 6s to 5d hybridization [18], or hybridization of the 5d levels of adjacent atoms in Dy, could result in a change of electronic structure. Such hybridization is possible because atomic Dy has no 5d electron; the 5d occupation is a result of condensation of the rare earth. As the thickness of the film increases this occupation and the hybridization effect intensify. Such an effect could result in increasing photoemission intensity from the 5d6s band (figure 1).

The photoemission cross section of Dy 4f electrons is low at 40 eV [19], but we could see no effect from 4f multiplets with increasing Dy coverage. This is due to the fact that Dy 4f electrons are very localized [4].

In figure 2 we present the Dy 5p band photoemission feature as a function of Dy film thickness. With strong spin-orbit coupling the Dy 5p band separates into two levels. We see features located at 29.6 ± 0.2 and 22.9 ± 0.2 eV below the Fermi energy. These features originate from $5p_{1/2}$ and $5p_{3/2}$ levels respectively. The binding energies of $5p_{1/2}$ and $5p_{3/2}$ are consistent with the values published in the table of electron binding energies edited by Cardona and Ley [20].

There is a clear indication that the relative 5p multiplet oscillator strengths increase with increasing Dy coverage. This can be correlated with the changes in the 5d band structure as seen in figure 1. Final-state effects must be considered in any photoemission study, particularly of the rare earths. Core-level photoemission studies can exhibit strong exchange interactions. If only the exchange polarization were considered, only two strong 5p features would be observed as a result of the 5d interaction with the 5p hole [21]. There is only one electron in the Dy 5d band, but there are four 5p electrons in the $5p_{3/2}$ level, which makes it understandable that this coupling can occur more strongly with the $5p_{3/2}$ level than the $5p_{1/2}$ level. Photoemission from the 5p levels is strongly influenced by final-state interactions with the 5d levels. The results in figure 2 support this conclusion. Increasing film thickness leads to localization of the 5d band and its strong exchange interaction with the 5p core level. The $5p_{3/2}$ multiplet increases in oscillator strength relative to the $5p_{1/2}$ multiplet with increasing Dy coverage. This is due to the localization of the 5d band structure. It should be noted that 5d states play a major role in the photoexcitation process of the 5p core level.

In summary, we conclude that the rare earths exhibit very different 5d localizations. We base this conclusion upon the observed dramatic changes in the Dy 5d band structure with increasing film thickness. This change in the electronic band structure of dysprosium with increasing thickness results in changes to the photoemission features from the core levels as a result of final-state coupling effects with the 5d bands.

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