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COMMENT

Comment on the band effects in the 5p levels of Ho(0001)

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Abstract. The holmium 5p branching ratio is observed to change in angle-resolved photoemission as a result of changes in the photoemission geometry. We suggest that these changes are a result of final state interactions between the 5p hole and the valence 5d band structure rather than a consequence of the initial state band structure of the shallow 5p core levels. The 5d-5p final state interactions are postulated to be wave-vector dependent in angle-resolved photoemission.

Recently Blyth, Patchett, Dhesi, Cosso and Barrett [1] provided evidence that the 5p levels of Ho(0001) exhibit photoemission effects that cannot be understood as typical of a core level. On the basis of their results [1] and band-structure calculations [2] they suggested that the 5p levels of holmium exhibit dispersion more characteristic of band structure than of a core level. According to their results and our previous work on heavy rare-earth metals, we suggest that there may exist an alternative way(s) to interpret their experimental results. We note that the results presented for Ho(0001) do not provide conclusive evidence for the existence of core-level band structure.

Gadolinium and terbium 5p levels exhibit multiplet splittings [3,4], as noted by Blyth *et al* [1]. While the photoemission spectra of the holmium 5p levels do not show this pronounced multiplet splitting of the 5p levels, final-state effects cannot, *a priori*, be excluded even at photon energies well away from a photoemission resonance [5]. Since multiplet splitting is mainly caused by local unpaired spins, virtually all the rare-earth 4f levels exhibit multiplet structures, and magnetic ordering is not a prerequisite for these final-state effects [6]. The multiplet structures of the holmium 5p levels are more complicated than is the case for gadolinium, which has a half-filled 4f level, but many of the final-state effects ascribed to gadolinium are also likely to occur for holmium.

From careful studies of the 5p multiplets, we have been able to demonstrate that the thickness changes of the gadolinium films, and therefore the change of 5d states, has a profound effect on selected multiplet intensities [3]. The 5p multiplet intensities do not solely arise from the j - J coupling with the 4f levels in the final state [4]. There is a significant influence of the 5d levels upon the 5p levels in the photoemission final state [3].

We have observed light polarization effects upon the 5p levels of gadolinium [7,8] and terbium [9-11]. We have proposed that these light polarization effects (which we denoted as the p-level anisotropy) were a consequence of final-state scattering and interactions with the 5d band structure which has different coupling for the

different 5p initial-state eigen-spinors. Ho(0001) is seen to have not only significant 5d occupancy, but also a band structure with fairly pronounced dispersion and changes in oscillator strength of the various symmetry bands with k_{\parallel} [12–14].

If the 5d state couples with the 5p hole in the photoemission final state, then variations in the relative $5p_{1/2}$ to $5p_{3/2}$ photoemission intensities with changes in k_{\parallel} and light polarization should occur, as is seen in the results reported by Blyth *et al* [1]. This is due, not to the 5p band structure, but rather as a consequence of the 5d band structure.

While shallow core levels can exhibit band structure [15], the significant deviation of the 5p-level branching ratio from the statistical value ($5p_{3/2}$ to $5p_{1/2}$ intensities of 1.5) in the results reported for holmium [1] strongly indicates [5] that final-state effects are significant. We cannot and do not exclude the existence of an initial-state 5p band structure, but suggest that final-state effects are more dominant in photoemission from the 5p levels of holmium. Strong dichroism effects are seen with changes in light polarization for the very deep 3d core levels of paramagnetic dysprosium [16]. We believe that interpreting the results of Blyth *et al* [1] in terms of final-state effects results in possible conclusions potentially far more exciting than simple band-structure formation.

Determining initial-state band structure from a shallow core level on the basis of emission-angle-dependent photoemission spectra will not be conclusive. There are two relatively straightforward measurements that can be used to ascertain whether the changes in the 5p-level branching ratios for holmium are final-state effects. First, if the results are not due to final-state effects, the 5p photoemission spectra should be shown to be temperature insensitive. A 5p core-level band structure 20 to 30 eV below E_F should be far more temperature insensitive than a 5d band structure. Second, even with band-structure formation there will exist $p_{x,y}$ (Δ_6 symmetry) and p_z (Δ_1 symmetry) components in both the $5p_{1/2}$ and $5p_{3/2}$ features. If for photoemission at normal emission the dependence on light incidence angle for the $5p_{1/2}$ and $5p_{3/2}$ levels is dissimilar (i.e. the two spin-orbit 5p components exhibit different symmetries) then the final-state effects, rather than initial-state effects such as 5p band structure, dominate the photoemission process. These two checks have been performed for terbium [9, 11], gadolinium [7] and dysprosium [17], and the results are not consistent with initial-state band-structure effects.

References

- [1] Blyth R I R, Patchett A J, Dhesi S S, Cosso R and Barrett S D 1991 *J. Phys.: Condens. Matter* **3** S287
- [2] Temmerman W M and Sterne P A 1990 *J. Phys.: Condens. Matter* **2** 5529
- [3] Li Dongqi, Hutchings C, Dowben P A, Wu Rong-Tzong, Hwang C, Onellion M, Andrews A B and Erskine J L 1991 *J. Appl. Phys.* **70** 6062
- [4] Li Dongqi, Dowben P A and Onellion M 1991 *Magnetic Surfaces, Thin Films and Multilayers; Mater. Res. Soc. Symp. Proc.* **231** 107
- [5] Dowben P A, LaGraffe D, Li Dongqi, Dottl L, Hwang C, Ufuktepe Y and Onellion M 1990 *J. Phys.: Condens. Matter* **2** 8801
- [6] Cox P A 1974 *Structure and Bonding (Springer Tracts in Physics 24)* (Berlin: Springer) p 59
Lang J K, Baer Y and Cox P A 1981 *J. Phys. F: Met. Phys.* **11** 121
Cox P A, Lang J K and Baer Y 1981 *J. Phys. F: Met. Phys.* **11** 113
- [7] Dowben P A, LaGraffe D and Onellion M 1989 *J. Phys.: Condens. Matter* **1** 6751
- [8] LaGraffe D, Dowben P A and Onellion M 1989 *Phys. Rev. B* **40** 970
- [9] LaGraffe D, Dowben P A and Onellion M 1990 *Phys. Lett. A* **147** 240

- [10] LaGraffe D, Dowben P A and Onellion M 1991 *Mater. Res. Soc. Symp. Proc.* **187** 225
- [11] Dowben P A, LaGraffe D, Li Dongqi, Miller A, Zhang L, Dotti L and Onellion M 1991 *Phys. Rev. B* **43** 3171
- [12] Blyth R I R, Barrett S D, Dhese S S, Cosso R, Heritage N, Begley A M and Jordan R G 1991 *Phys. Rev. B* **44** 5423
- [13] Blyth R I R, Cosso R, Dhese S S, Newstead K, Bedley A M, Jordan R G and Barrett S D 1991 *Surf. Sci.* **251/252** 722
- [14] Barrett S D, Blyth R I R, Begley A M, Dhese S S and Jordan R G 1991 *Phys. Rev. B* **43** 4573
- [15] Dowben P A, Kime Y J, Varma S, Onellion M and Erskine J L 1987 *Phys. Rev. B* **36** 2519
Onellion M, Erskine J L, Kime Y J, Varma S and Dowben P A 1986 *Phys. Rev. B* **33** 8833
- [16] Sacchi M, Sakho O and Rossi G 1991 *Phys. Rev. B* **43** 1276
- [17] Dotti L, Onellion M and Dowben P A 1992 in preparation