Citation for published version


DOI

https://doi.org/10.1103/PhysRevLett.102.129702

Link to record in KAR

http://kar.kent.ac.uk/31279/

Document Version

Publisher pdf

Copyright & reuse

Content in the Kent Academic Repository is made available for research purposes. Unless otherwise stated all content is protected by copyright and in the absence of an open licence (eg Creative Commons), permissions for further reuse of content should be sought from the publisher, author or other copyright holder.

Versions of research

The version in the Kent Academic Repository may differ from the final published version. Users are advised to check http://kar.kent.ac.uk for the status of the paper. Users should always cite the published version of record.

Enquiries

For any further enquiries regarding the licence status of this document, please contact: researchsupport@kent.ac.uk

If you believe this document infringes copyright then please contact the KAR admin team with the take-down information provided at http://kar.kent.ac.uk/contact.html
Brown et al. Reply: The Comment of Goldman et al. [1] makes a number of claims regarding our recent Letter [2]. First, they claim that we did not include matrix element effects in our calculation of the dipolar (E1) contribution to the XRIS spectra of the heavy rare earth metals. Data were modeled using both an atomic-like model and a fully relativistic first principles scattering theory (FPST), where the former related the measured spectra to the calculated spin and orbital polarized densities of states without including matrix elements. However, Refs. [17] and [18] in our Letter [2] clearly show that the FPST did indeed include matrix elements. They further claim that we found it necessary to invert the calculated XRIS spectra for Tm, with respect to the experimental spectra. In fact, we inverted the model, the FPST, and the experimental spectra. As stated in the caption of Fig. 1 in [2], the scattering angle for Tm, and only Tm, was less than 90°. The asymmetry ratio reverses sign on crossing 90° (Eq. (3) in [2]) and our only motivation for inverting the Tm spectra was to allow direct comparison with the other heavy rare earths. We also point out that the origin of the energy scale used in Fig. 1 of [1] differs from ours by ∼5 eV, and we note that the vertical dashed lines do not coincide with features A and B of [2]. On Goldman et al.’s energy scale, feature A of [2] would be at −4 eV and feature B at −3 eV.

Goldman et al. state that differences in the dipole matrix elements between spin-up and spin-down radial wave functions and the 2p state can lead to inversion of experimental features compared to calculation using only the density of states. We note that they refer to the empty 5d states as “more strongly localized.” In our calculation, the 5d electrons are itinerant, in agreement with the conventional wisdom where the 5d electrons move through the solid and mediate the indirect exchange. Also, they refer to an effect observed in absorption, whereas our work related to scattering, which involves additional matrix elements. Figure 1 shows the results obtained using the FPST to calculate E1 XMCD from the imaginary part of the forward scattering amplitude for Gd, as opposed to Tm. Gd was chosen, as for Tm the spin and orbital 5d moments are comparable and it is not clear to us to what extent the spin dependence of matrix elements influence the spectra independently of orbital effects. We have repeated this calculation for Fe and thus confirmed the correct polarity of our calculation. For comparison, we also show the XMCD calculated directly from the spin and orbital polarized densities of states using a simple atomic model. Two things are clear from this figure. First, there is no inversion between the FPST result and the atomic result. Second, the mostly negative result obtained from the atomic model is transformed into a mostly positive result with the inclusion of matrix elements. We note that there are considerable differences between our results and those of Goldman et al. Comparison between the two calculations is not straightforward because we present a 2nd order calculation of scattering whereas their work refers to a 1st order calculation of absorption. Furthermore, the fully relativistic basis of our method is different from the method of Goldman et al. and this may also contribute to the difference between our results. We are continuing to investigate this sign discrepancy and intend to present our findings in a future publication.

S. D. Brown,1,8 P. Strange,2 L. Bouchenoire,1,8 B. Zarychta,3 P. B. J. Thompson,1,8 D. Mannix,1,8 S. J. Stockton,3 M. Horne,3 E. Arola,3,4 H. Ebert,5 Z. Szotek,6 W. M. Temmerman,6 and D. Fort7 1XMaS, European Synchrotron Radiation Facility, B.P. 220, 38043 Grenoble Cedex, France 2School of Physical Sciences, University of Kent, Canterbury, Kent, CT2 7NH, United Kingdom 3Keele University, Keele, Staffordshire ST5 5BG, United Kingdom 4Optoelectronics Research Centre, Tampere University of Technology, P.O. Box 692, FIN-33101, Tampere Finland 5Department Chemie/Physikalische Chemie, Universitat Munchen, butenandstrasse 5-13, D-81377, Munich, Germany 6Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, United Kingdom 7The University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom 8Liverpool University, Liverpool L69 3BX, United Kingdom

Received 9 February 2009; published 27 March 2009
DOI: 10.1103/PhysRevLett.102.129702
PACS numbers: 78.70.Ck, 61.05.cc, 78.70.En