

**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 XRES 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 XRES 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  $90^\circ$ . The asymmetry ratio reverses sign on crossing  $90^\circ$  (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  $\sim 5$  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  $\sim 4$  eV and feature B at  $\sim -3$  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

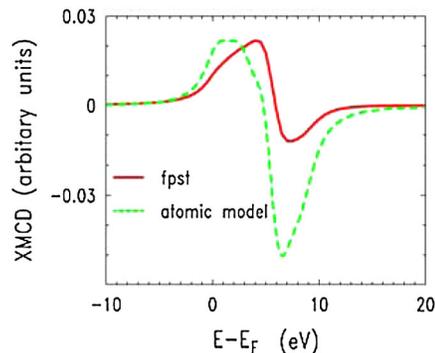


FIG. 1 (color online). The  $E1$  contribution to the XMCD spectrum for Gd metal calculated from first principles scattering theory (FPST) including matrix elements (solid line) and directly from spin and orbital polarized densities of states using a simple atomic model, neglecting matrix elements (dashed line).

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

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[2] S. D. Brown *et al.*, Phys. Rev. Lett. **99**, 247401 (2007).