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T-dependent matrix elements in x-ray magnetic circular dichroism YONGBIN LEE, BRUCE HARMON, ALAN GOLDMAN, Ames Laboratory - US DOE, JONATHAN LANG, Argonne National Laboratory — Dramatic changes in the Er L_2 and L_3 XMCD spectra in Er_2Fe_{17} as a function of temperature have been investigated with detailed experiments and first principles calculations. This study seeks to understand the fundamental mechanisms governing the spectral shape and magnitude of the L_2 and L_3 XMCD spectra as a step toward developing XMCD as a quantitative probe for rare earths similar to its effectiveness for transition metals via the use of sum rules (which do not work for rare earths). The calculations simulate the key thermal physics by evaluating the spin polarized band structures obtained with the 4f moment on the Er atom constrained to values of 0, 1, 2, and 3 Bohr magnetons. Both the theory and our experiments, performed at the Advanced Photon Source, show the XMCD L_2-edge spectrum changes sign as the temperature is lowered, and the L_3-edge spectrum also shows systematic and significant changes. We will discuss the effects of dipole matrix elements, spin-orbit coupling, hybridization between 5d-3d orbital, and magnetic anisotropy on the XMCD spectra. Quadrupole transitions and core hole effects will be also discussed.

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