Exceptionally Large Magnetovolume Effect In Mnte Driven by A Novel Magnetostructural Coupling Mechanism

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MnTe is an antiferromagnetic semiconductor known for its outstanding thermoelectric performance, which is driven largely by short-range magnetic correlations present in the system through a mechanism known as paramagnon drag. Less well studied is the effect of these magnetic correlations on the crystal structure through magnetostructural coupling; in fact, very little is known in general about magnetostructural effects driven by short-range magnetic order, regardless of the specific material system. To shed light on this topic, we present a combined x-ray and neutron total scattering study of MnTe as a function of temperature. We find that MnTe exhibits the largest known spontaneous magnetovolume effect for an antiferromagnet, with a magnetically driven volume contraction of nearly 1%.

Through combined atomic and magnetic pair distribution function (PDF) analysis, we demonstrate that this structural response couples linearly to the local magnetic order parameter, starting with short-range correlations above the Neel temperature and continuing into the long-range ordered state. This linear coupling is notable because it contrasts sharply with the typical quadratic coupling to the long-range ordered magnetic moment, pointing to a novel mechanism of spontaneous magnetostructural coupling in MnTe. We propose an explanation of this behavior and discuss its significance for other families of magnetostructurally active antiferromagnets. In addition to providing unique insight into magnetostructural effects driven by short-range magnetism, this study also highlights the power of combined atomic and magnetic PDF analysis for magnetic materials.