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Anisotropy causes the Besnus transition in monoclinic 4C pyrrhotite

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Monoclinic 4C pyrrhotite (ideal formula Fe7S8) is the Fe-deficient end-member of the pyrrhotite omission series (Fe1-xS; $0 < x \leq 0.125$). The members of the pyrrhotite group have a hexagonal nickel-arsenide (NiAs) type substructure in common and in the 4C phase, the vancacy arrangement generates a monoclinic superstructure. In this phase, the vacancies are arranged in a stacking sequence of full and vacancy bearing Fe layers with a four-fold modulation with resepect to the NiAs substructure. The intralayer Fe2+ spins are ferromagnetically and spins of adjacent layers are antiferromagnetically coupled and this results in a relatively strong ferrimagnetism due to uncompensated sublattices. This ferrimagnetism is characterized by a peculiar anisotropy with easy axes in the c-plane and an extremely hard axis along the c-direction. 4C pyrrhotite shows an anomaly in magnetization at Tcrit $\approx$ 30 K (e.g., a decrease in SIRM) and in other physical quantities, such as heat capacity and resistivity known as Besnus transition. The link between physical and structural properties in 4C at the Besnus transition is a matter of debate and it is addressed in a combined structural and magnetic investigation using neutron diffraction, and magnetic torque analysis on a natural pyrrhotite crystal.

Rietveld refinement of the powder neutron diffraction patterns that provide structural and magnetic data reveal structural changes at an atomic level, but no crystallographic change [1]. The magnetic information shows a continuous out-of-plane Fe2+ spin rotation at T < 200 K down to the Besnus transition, and at lower temperature, the rotation remains nearly stable. The cease of the continuous rotation is associated with an adjustment in the Fe-Fe bond lengths and this leads to a modification of the spin-orbit coupling, i.e. the magnetic anisotropy. Magnetic torque measurements in the bc-plane shows that the Fe2+ spins form two components with different clockwise out-of-plane rotation behaviors that indicate different local anisotropies [2]. In the range of the Besnus transition, the two components show an opposite rotation behavior, i.e. one component rotates anti-clockwise and this in turn can explain the decrease in the SIRM.

In summary, the Besnus transition can be explained as a magnetic anomaly that stems from structural changes at an atomic level caused by the highly ordered vacancy arrangement of 4C pyrrhotite, and is a classical example for the close link between structural and magnetic properties in Earth materials.

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[2] D. Koulialias, M. Charilaou, C. Mensing, J. F. Löffler, and A. U. Gehring (2018). Torque analysis of incoherent spin rotation in the presence of ordered defects, Applied Physics Letters, 112(20), 202404