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Low-T magnetic anomaly in Ca2Fe2O5 studied by single-crystal neutron diffraction

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Ca2Fe2O5, which belongs to the Brownmillerite family of promising solid-oxide fuel cell membrane materials, is an antiferromagnet (AFM) below TN = 720 K. A small ferromagnetic (FM) canting perpendicular to the AFM easy axis has previously been established by physical properties measurements, but never observed crystallographically. More intriguingly, it has been known for some time to display an anomalous elevation in magnetic susceptibility for 60 K < T < 140 K. [1] Based on measurements performed with small oriented single crystals, Zhou et al. [2] proposed that this anomaly was due to a reorientation of the spins from the crystallographic a axis to the c axis below 40 K, with a region of minimal magnetocrystalline anisotropy in the anomalous temperature interval. In order to test this, we grew a very large (~1 cm3) single crystal by the floating-zone method and collected neutron Laue diffraction data, against which we refined both the atomic and magnetic structures of Ca2Fe2O5 between 10 K and 300 K. We designed and built an ad hoc sample mount to apply a small (~35 Oe) magnetic field to the sample, ensuring perfect consistency with the magnetic susceptibility data, which were collected in a comparably small field. Our refinements against both zero-field and in-field diffraction data reproduce the G-type AFM structure of Ca2Fe2O5 excellently at room temperature, including the FM canting which we have refined to statistical significance for the first time. We can also show that in the intermediate temperature interval (T = 100 K), the spins are slightly less well-ordered due to competing sublattice interactions. However, careful examination of the data reveals that the material is still best described by the room-temperature magnetic structure at all measured temperatures – i.e., the spin-reorientation hypothesis is incorrect.

[1] *A. Maljuk, J. Strempfer, C.T. Lin, J. Cryst. Growth, 2003, 258, 435-440.,* ***[2]*** *H.D. Zhou, J.B. Goodenough, Solid State Sciences, 2005, 7, 656-659.*

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