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K+ vacancy correlated disorder and spin structure in KLi2Cr6O12 high-pressure oxide.

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Topics

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Abstract

Low-dimensional solids show interesting properties. For instance, the mixed-valent hollandites $K_2M_8O_{16}$ (M = V or Cr), obtained via high-pressure and high-temperature synthesis (HPHT), show respectively a spin-singlet-metal-insulator and ferromagnetic-half-metal-insulator transitions at low temperatures, both accompanied by a structural transition within a ?2 x ?2 x 1 supercell. These hollandites are based on edge-shared double octahedral chains interconnected via vertex, thus defining a structure with two types of channels.[1-3]

We have prepared the new mixed-valent oxide $KLi_2Cr_6O_{12}$ at 12 GPa and 1100 °C using a Walker-type multi anvil apparatus. The average structure crystallizes with a $P6_3/m$ symmetry and a = 9.0096(3) Å and c = 2.86312(5) Å. Similar to the hollandites, the structure shows double octahedral chains interconnected by corners forming hexagonal and trigonal channels running along the c direction (Figure 1a). Potassium resides in the hexagonal channels with some degree of positional disorder, while the triangular channels accommodate lithium ions.

Transmission electron microscopy along with EDX expose K+ vacancy correlated disorder, resulting in diffuse scattering streaks (cuts to diffuse sheets) perpendicular to the c^* direction and at ±¼ of the main reflections (Figure 1b). These imply a 4c K+ vacancy long-range order but with little or no transverse correlation from tunnel to tunnel. Magnetic susceptibility measurements reveal an antiferromagnetic ordering below T_N = 75 K. Neutron diffraction experiments show a magnetic structure with k1 = [1/3 1/3 ¼] and k2 = [0 0 ¼] which can be understood as a triple harmonic of k1 which may be related to the observed structural supercell.

[1] M. Isobe, S. Koishi, ett. J. Phys. Soc. Jpn. 2006, 75, 073801.

[2] K. Hasegawa, M. Isobe, etc. Phys. Rev. Lett. 2009, 103, 146403.

[3] M. L. Foo, T. He, etc. J. Solid State Chem. 2006, 179, 941.

Annexes

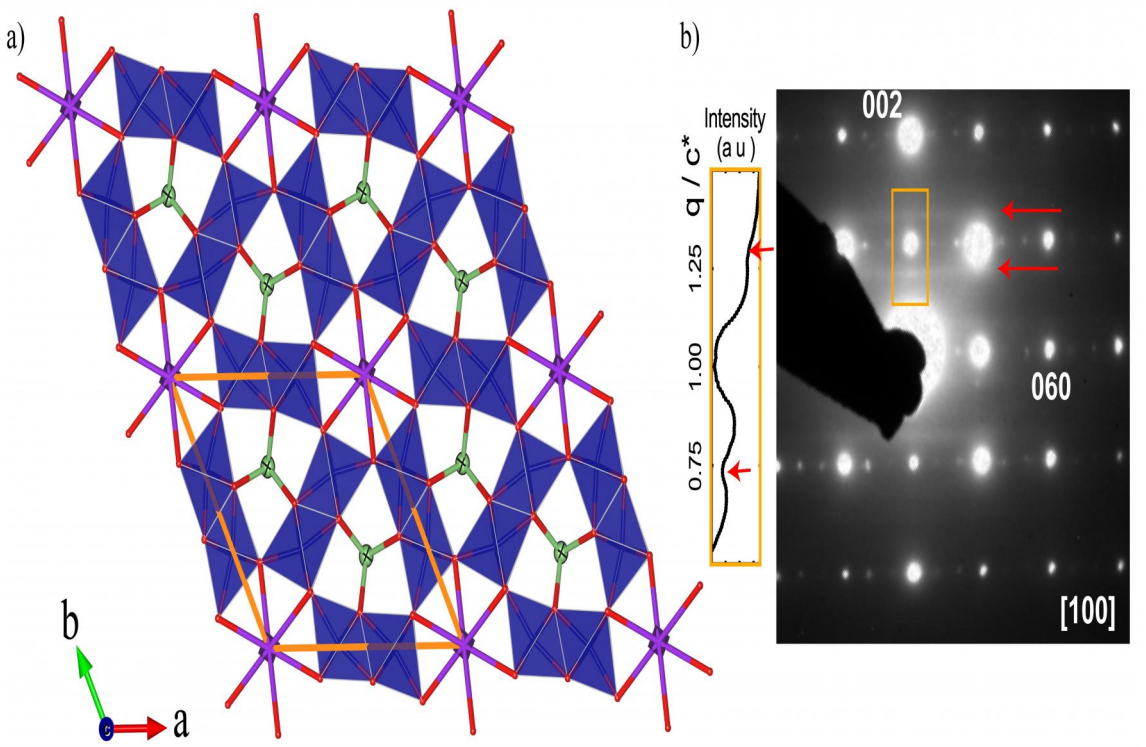

Figure 1: Figure 1. a) KLi2Cr6O12 crystal structure view along the c axis. Green, purple and red spheres represent Li, K and O respectively, Cr octahedra are in blue. b) [100] electron diffraction along with its corresponding intensity scan of the orange squa