Poster Presentations

[MS19-P03] Synthesis, Structure and Properties of $A_4O_4TiSe_4$: a New Series of Oxychalcogenides

A. J. Tuxworth and J.S.O.

Evans, Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom.
E-mail: andrew.tuxworth@durham.ac.uk

Since the discovery of high temperature superconductivity in the layered oxypnictide systems there has been significant interest in mixed anions materials containing an oxide anion as well as another anion type involved in metal bonding [1]. Superconducting transition temperatures of up to 55 K have been reported for F- doped $LaOFeAs_{1-x}F_x$ systems [2]. Oxychalcogenide materials contain oxide anions along with heavier group 16 anions. While superconductivity has not been observed for oxychalcogenides, many materials with interesting electronic, magnetic and optical properties have been synthesised [3]. Due to the different sizes and coordination requirements preferred by the oxide and the heavier group 16 chalcogen anions, many oxychalcogenides tend to adopt layered structures to allow for anion segregation, but there are a growing number of materials where we can consider the structures to be built up from discrete blocks, of similar coordination to these layers. A number of these materials have been have been synthesised solely as single crystals [4]. A synthesis of bulk polycrystalline samples of one such series of materials will be presented. This series with $A_4O_4TiSe_4$ composition has been shown to be stable to a wide range of rare-earth cations (A^{3+}). The ability to synthesise bulk polycrystalline samples has allowed the investigation of the electronic and magnetic properties of these materials, which will be presented here, carried out via 4 probe conductivity measurements and SQUID magnetrometry. The structure has been described in terms of (OLa_4) and (OLa_3Ti) tetrahedra first linked by edge-sharing into blocks four units in length. These blocks are then linked together by octahedrally coordinated $TiSe_4O_2$, with similarity to the structure of $La_2O_2MnSe_2$ [5].

[1] Y. Kamihara, T. Watanabe, M. Hirano and H. Hosono, Journal of the American Chemical Society 2008, 130, 3296-3297.
[2] Z. A. Ren, W. Lu, J. Yang, W. Yi, X. L. Shen, Z. C. Li, G. C. Che, X. L. Dong, L. L. Sun, F. Zhou and Z. X. Zhao, Chinese Physics Letters 2008, 25, 2215-2216.
[3] S. J. Clarke, P. Adamson, S. J. C. Herkelrath, O. J. Rutt, D. R. Parker, M. J. Pitcher and C. F. Smura, Inorganic Chemistry 2008, 47, 8473-8486.
[4] A. Meerschaut, A. Lafond, V. Meignen and C. Deudon, Journal of Solid State Chemistry 2001, 162, 182-187.
[5] E. E. McCabe, D. G. Free, B. G. Mendis, J. S. Higgins and J. S. O. Evans, Chemistry of Materials 2010, 22, 6171-6182.

Keywords: Rietveld analysis, mixed anion, electronic structure and magnetism