SYNTHESIS, CHARACTERISATION AND THERMOELECTRIC PERFORMANCE OF THE NEW METAL-RICH TELLURIDES MGeTe (M = Co, Rh)

Vaqueiro P.[1], Sobany G. G.[1], Guinet F.[1], Leyva-Bailen P.[1]

1- Department of Chemistry, Heriot-Watt University, Edinburgh EH14 4AS, UK

During the course of our investigations on ordered ternary skutterudites of the type $MGe_{1.5}Q_{1.5}$ (M = Co, Rh, Ir; Q = S, Se, Te),[1] we have found a new family of metal-rich tellurides, with general formula MGeTe. Following the initial identification of these phases by powder X-ray diffraction, chemical vapour transport was used for the growth of single crystals, suitable for crystal structure determination. This enabled us to establish that these materials crystallize in the orthorhombic space group *Pbca* (a =6.1930(4) Å, b = 6.2326(4) Å, c = 11.1289(7) Å for M = Co). The MGeTe phases adopt an ordered $NiAs_2$-type structure, in which the transition metals are octahedrally coordinated by three germanium and three tellurium atoms, which are ordered in a facial configuration. Whilst the ordered skutterudite structure of $MGe_{1.5}Q_{1.5}$ contains corner-linked MGe_3Q_3 octahedra, in the new MGeTe materials, the MGe_3Te_3 octahedra are linked through both corner- and edge-sharing. This structural type, which is relatively uncommon, can be considered to be intermediate between the pyrite and the marcasite structures. Measurements of resistivity, Seebeck coefficient and thermal conductivity have been carried out. The electrical transport properties of these materials are consistent with semiconducting behaviour, and the sign of the Seebeck coefficient indicates that the majority of the charge carriers are electrons. The thermoelectric performance of these new materials will be compared with that of related phases.

1. P. Vaqueiro, G. G. Sobany, A. V. Powell and K. S. Knight, *J. Solid State Chem.*, **179**, 2047 (2006); P. Vaqueiro, G. G. Sobany and M. Stindl, *J. Solid State Chem.*, in press (doi: 10.1016/j.jssc.2008.01.025).

E-mail Presenting Author : P.Vaqueiro-Rodríguez@hw.ac.uk