Structural Studies of Ag_2SO_4 and TlX (X = Cl, Br, I) by *In-Situ* ED-XRD to 6GPa and 550°C	X17B1

Q. Chen and R. A. Secco, (U. West. Ont.), E.A. Secco, (St. Francis Xavier U.), J. Chen, M.T. Vaughan, G. Chen, J.Z. Zhang, and D.J. Weidner (CHiPR, SUNY, Stony Brook)

High pressure (P) electrical conductivity measurements on TlX (X = Cl, Br, I) and Ag_2SO_4 show distinct conductivity jumps with increasing temperature (T). For Ag_2SO_4, this is associated with a transformation from low T orthorhombic (β-phase) to high T hexagonal (α-phase) structure. The α-β phase boundary reaches a maximum at 1.6 GPa (observed only by differential thermal analysis (Pistorius, 1965, J. Chem. Phys. 46, 2167)) and is accompanied by anomalous decreasing activation energy of conduction with P in this region. *In-situ* XRD experiments were therefore carried out to check for possible structural cause(s) of this anomalous behaviour. In the TlX system, structural studies were also carried out to investigate the nature of the conductivity increases. Energy dispersive XRD experiments were carried out at X17B1 using SAM85 with NaCl as the internal pressure calibrant.

Ag_2SO_4: The ortho-hex structural transformation is confirmed in the XRD patterns at low P but there are marked differences at T > 450°C between P < 1.6 GPa and P > 1.6 GPa as shown in the figure below suggesting a possible new phase in the high P, T region. The similarity of patterns at 22°C and 1 atm. before and after high P,T exposure indicate lack of reaction between sample and boron nitride container.

TlX (X = Cl, Br, I): Both TlCl and TlBr do not show any evidence of P- or T-induced modification of their 22°C and 1 atm cubic (CsCl) structure at P up to 6GPa and T up to 550°C. In comparison, changes observed in TlI patterns are more complex as shown in the figure below.

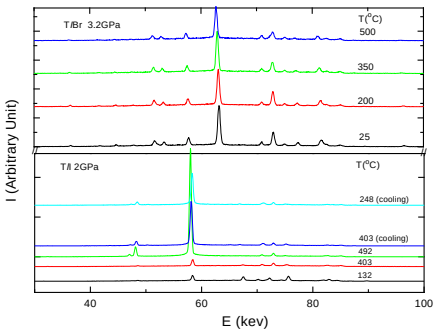

Figure 1.

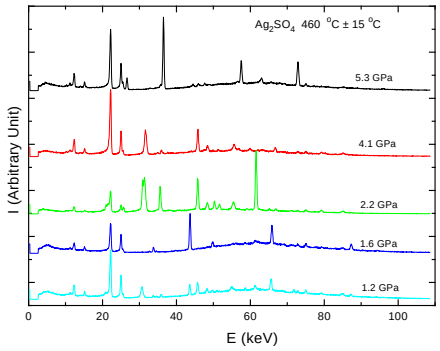

Figure 2.