HIGH-PRESSURE COMPRESSION BEHAVIOUR OF ORTHORHOMBIC $LiScGe_2O_6$

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Pyroxene-type phases are subject to systematic investigations of the thermomechanical behaviour and related structure-property relationships for various reasons (e.g., HOFER et al., 2015). Therefore, several stable orthorhombic and monoclinic pyroxene polymorphs at various temperature and pressure were identified. Regardless of whether silicon or germanium based phases, the relative sizes and the interplay of the ions at T, M1 and M2 positions in the $M2M1T_2O_6$ compounds appear to control the structural stabilities and transformations. To support the understanding of phase transition driving parameters, the high-pressure behaviour of germanium compounds is in the current focus of systematic compressibility studies.
In this study we investigate the structural compression of an orthorhombic lithium-scandium-germanate end-member (with M2 = Li, M1 = Sc and T = Ge) and determine the equation of state (EoS) using a STOE AED2 four-circle X-ray diffractometer and Mo-$K_{alpha1,2}$-radiation. For each pressure point about 15 unique diffraction peaks were used for each LSG and quartz (pressure standard, e.g., SCHEIDL et al., 2016) in order to refine high-precise lattice parameters. Then, EoSFIT7-GUI (e.g., GONZALEZ-PLATAS et al., 2016) was used to fit a third order Birch-Murnaghan EoS onto the derived unit cell volume (Fig. 1) clearly indicating a structural phase transition near 9 GPa.

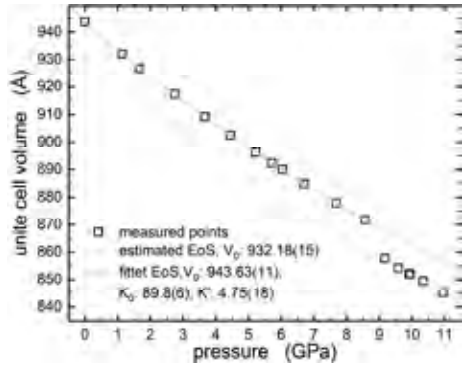

Figure 1. Unite cell volume determined by single-crystal X-ray diffraction experiments on a synthetic $LiScGe_2O_6$ crystal within a diamond-anvil cell. A probable first order phase transition is clearly visible around 9 GPa.

HOFER, G., KUZEL, J., SCHEIDL, K.S., REDHAMMER, G., MILETICH, R. (2015): J. Solid State Chem., 229, 188-196.
SCHEIDL, K.S., KURNOSOV, A., TROTS, D.M., BOFFA BALLARAN, T., ANGEL, R.J., MILETICH, R. (2016): J. Appl. Cryst., 49, 2129-2137.
GONZALEZ-PLATAS, J., ALVARO, M., NESTOLA, F., ANGEL, R.J. (2016): J. Appl. Cryst., 49, 1377-1382.