



Elastic behaviour and high-pressure phase transition of the $P2_1/n$ $\text{LiAlGe}_2\text{O}_6$ pyroxene

Andreas Artac (1), Ronald Miletich-Pawliczek (1), Fabrizio Nestola (2), Günther J. Redhammer (3), and Luciano Secco (2)

(1) Institut für Mineralogie und Kristallographie, Universität Wien, Vienna, Austria (andreas.artac@univie.ac.at), (2) Dipartimento di Geoscienze, Università di Padova, Padua, Italy (fabrizio.nestola@unipd.it), (3) Department of Materials Engineering and Physics, Division of Mineralogy, University of Salzburg, Salzburg, Austria (guenther.redhammer@sbg.ac.at)

In a recent work by Redhammer et al. (2012), investigating a synthetic pyroxene sample with composition $\text{LiAlGe}_2\text{O}_6$, a new space group for the big family of pyroxenes has been surprisingly discovered renewing the interest for Li-bearing pyroxene compounds. Actually, the authors of that work intended to investigate the effect of the Si-Ge substitution on the high-pressure behaviour and possibly on the phase transition with respect to spodumene, $\text{LiAlSi}_2\text{O}_6$, investigated by Arlt and Angel in 2000. Spodumene in fact, not only shows a strong first order phase transition at 3.19 GPa from $C2/c$ to $P2_1/c$ but the low symmetry $C2/c$ shows the greatest bulk modulus never found in pyroxenes (i.e. 144.2 GPa with the first pressure derivative fixed to 4). Redhammer et al. (2012) discovered that substituting Si for Ge in the spodumene structure the effect is dramatic in terms of symmetry change at room conditions with the Ge-spodumene showing a $P2_1/n$ space group, first discovery of such symmetry in the big family of pyroxene.

In this work we loaded one crystal of $\text{LiAlGe}_2\text{O}_6$ in a diamond-anvil cell and investigated the elastic behaviour and its possible high-pressure phase transition by single-crystal X-ray diffraction. In detail, we measured the unit-cell parameters using a Huber four-circle diffractometer equipped with a point detector up to about 9 GPa. The crystal structure was measured at different pressures loading simultaneously two fragments of the same crystal with a different orientation in the same diamond-anvil cell in order to cover a wider portion of the reciprocal space. The intensity data were measured on a STADI IV four-circle diffractometer equipped with a CCD using a diamond-backing plate cell, which gives better structural results with respect to a beryllium backing plate one (i.e. Periotto et al. 2011).

The first important result of our work is that we found at about 5.2 GPa a very strong first-order phase transformation from $P2_1/n$ to $P2_1/c$ and this is the first discovery of such a transition in pyroxenes. The volume discontinuity at the transition is marked by a big volume decrease reaching a variation of about 3.6% between 5.207 and 5.249 GPa. The entire volume decrease up to 9 GPa is of nearly 10%. The equation of states of the two symmetries $P2_1/n$ and $P2_1/c$ clearly show that the high pressure phase is slightly less compressible than the $P2_1/n$ and this is an anomalous behaviour in Li-bearing pyroxenes, which usually show the higher symmetry phase having a higher compressibility (i.e. Nestola et al. 2008).

Structural details and elasticity data will be discussed.

References

Arlt T., Angel R.J. (2000) Displacive phase transitions in C-centered clinopyroxenes: spodumene, $\text{LiScSi}_2\text{O}_6$ and ZnSiO_3 . *Physics and Chemistry of Minerals*, 27, 719-731.

Periotto B., Nestola F., Balic-Zunic T., Angel R.J., Miletich R., Olsen L.A. (2011) Comparison between beryllium and diamond-backing plates in diamond-anvil cells: Application to single-crystal x-ray diffraction high-pressure data. *Review of Scientific Instruments*, 82, Article Number: 055111.

Redhammer G.J., Nestola F., Miletich R. (2012) Synthetic $\text{LiAlGe}_2\text{O}_6$: the first pyroxene with $P2_1/n$ symmetry. *American Mineralogist*, 97, 1213-1218.

Nestola F., Boffa Ballaran T., Ohashi H. (2008) The high-pressure $C2/c$ – $P2_1/c$ phase transition along the $\text{LiAlSi}_2\text{O}_6$ - $\text{LiGaSi}_2\text{O}_6$ solid solution. *Physics and Chemistry of Minerals*, 35, 477-484.