

MS14-P21 | INVERSE CRYSTAL STRUCTURE BEHAVIOUR OF $\text{Ca}_3\text{Al}_4\text{ZnO}_{10}$ AT HIGH PRESSURE AND HIGH TEMPERATURE

Hejny, Clivia (Universität Innsbruck, Innsbruck, AUT); Kahlenberg, Volker (Universität Innsbruck, Innsbruck, AUT); Krüger, Hannes (Universität Innsbruck, Innsbruck, AUT)

$\text{Ca}_3\text{Al}_4\text{ZnO}_{10}$ was initially found in an investigation on the incorporation of ZnO into Portland cement clinker phases [1]. In contrast to a previous description of the structure in space group $Pbc2_1$ [2] $\text{Ca}_3\text{Al}_4\text{ZnO}_{10}$ was found to be isotypic with $\text{Ca}_3\text{Al}_4\text{MgO}_{10}$ [3]. $\text{Ca}_3\text{Al}_4\text{ZnO}_{10}$, $a = 5.1364(3)$, $b = 16.7403(9)$, $c = 10.7019(6)$ Å, $V = 920.20(8)$ Å³, $Z = 4$, crystallizes in $Pbcm$. Crystals were obtained in a crystal growth experiment and studied in-situ between ambient pressure and 6.8(1) GPa as well as 25(2)-797(2) °C. Lattice parameters change continuously in the examined P-T-range, thus allowing computation of a second-order Birch-Murnaghan equation-of-state. The structure represents a three-dimensional network of corner-sharing $[\text{AlO}_4]$ - and $[\text{ZnO}_4]$ -tetrahedra with Ca ions in six- and eightfold coordination. Analysis of the pressure- and temperature-induced response of the structure shows an inverse relationship of all observed mechanism contributing to overall structural changes. To give an example: The only Ca-O bond distance increasing with increasing pressure, i.e. Ca2-O3, is found to decrease with increasing temperature.

[1] H. Bolio-Arceo, F.P. Glasser; *Adv. Cem. Res.* **1998**, *10*, 25–32.

[2] V.D. Barbanyagre, T.I. Timoshenko, A.M. Ilyinets, V.M. Shamshurov; *Powder Diffr.*, **1997**, *12*, 22–26.

[3] V. Kahlenberg, R. Albrecht, D. Schmidmair, H. Krüger, B. Krüger, M. Tribus, A. Pauluhn; *J. Am. Ceram Soc.* **2019**, *102*, 2084-2093.