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ABSTRACT BOOK

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High pressure softening of grossite ($CaAl_4O_7$)

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The elasticity of grossite ($CaAl_4O_7$) has been investigated by experimental (synchrotron radiation high-pressure single crystal X-ray diffraction, using an ETH-type Diamond Anvil Cell and and M.E.W. as pressure-transmitting fluid, at Xpress beamline at Elettra, Trieste, λ = 0.4957 Å) up to 8.6 GPa and first-principle methods (using a WC1LYP hybrid functional and Crystal program). On compressing, a displacive first order phase transition has been observed between 6.1 and 7 GPa by ca. a 3% change in lattice volume and the violation of *C*-centring extinction conditions. In fact, the symmetry changes by losing the centring of the lattice and the centre of symmetry, passing from *C*2/*c* to *Pc* space group. A dramatic change on the isothermal bulk modulus (K_0) of grossite accompanies the transition: by preliminary fitting of lattice parameters data using a BM2 EoS we obtain changes from 123(4) GPa in the low pressure regime to 35(8) GPa in the high-*P* phase, which shows a very soft and anisotropic behaviour (linear compressibility changes from 1.19:1.00:1.00 in *C*2/*c* to 1.74:5.74:1.00 in *Pc*). Intensity data was collected at 17 *P* values (data collected every 0.5-1.0 GPa up to 8.6 GPa). We have been able to solve the structure of the high-*P* phase from experimental data by group theory symmetry reduction and structure refinement of a symmetry relaxed model. The structure has two symmetrically independent AlO_4 tetrahedra in the *C*2/*c* phase, which become seven symmetrically independent AlO_4tetrahedra plus one AlO_5 pyramid (the *Al*(21) site) in *Pc* phase (= 1.884(1) Å, polyhedral volume 5.04 $Å^3$). The change in coordination of the Al atom at the *Al*(21) site is probably the driving force of the strong compressibility along [010] in high-*P* phase. First principles calculations agree very well with the experimental data. By fitting ab initio energy-volume data with a BM3 EoS in the range V/V_0 = 0.95 ¸ 1.04 we obtain K_0= 128.8(1) GPa and K'_0 = 4.0(1) for the *C*2/*c* phase. The calculated static value of K_0 is, in turn, perfectly consistent with aggregate bulk modulus obtained from static elastic constants by using a Voigt-Reuss-Hill average scheme (i.e. K_{VRH} = 129.2 GPa). Ab initio calculation of the full elastic tensor (with 13 independent components) permits to define the shear modulus (i.e. G_{VRH} = 52.1 GPa) and seismic anisotropy of this phase, for which no experimental data exist so far. Computed volume and axial compressibilities match the observed trends within 1%, except for c/c_0 which is slightly overestimated by WC1LYP calculations. Further ab initio calculations on both *C*2/*c* and *Pc* phases are currently in progress in order to characterize the thermodynamic features of the phase transition. The unattended behaviour of grossite implies drastic changes on the mechanical response of this phase that should be accounted for when modelling phase diagrams of the CAS ($CaO-Al_2O_3-SiO_2$) system and the mechanical response of high alumina cements (HAC).

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