

superconductor at high pressure due to the high density of states at the Fermi level. Matsuoka *et al* [2] followed Feng's work and indeed found  $\text{CaLi}_2$  become a superconductor at 11 GPa. However, the crystal structure of  $\text{CaLi}_2$  under pressure is still not well established. In this work, the crystallography of  $\text{CaLi}_2$  at high pressure has been extensively investigated by the evolutionary algorithm USPEX. We explored several new phases of  $\text{CaLi}_2$  at pressures in range 50 – 250 GPa. The chemical bonding and the electronic structures of the high pressure phases  $\text{CaLi}_2$  are studied in detail. The high-pressure structures of  $\text{CaLi}_2$  and the physical mechanisms of phase transitions will be discussed.

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Keywords: *ab-initio* structure determination, high pressure, electronic structure

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### Effect of pressure on the crystal structure of $\alpha'$ - $\text{Ca}_{1.5}\text{Sr}_{0.5}\text{SiO}_4$

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One of the high-temperature polymorph of  $\text{Ca}_2\text{SiO}_4$ ,  $\alpha'$  phase, which is stable above 973 K [1] is known to become quenchable to room temperature with incorporation of Sr [2]. It is reported that the phase transition between  $\alpha'_L$  and  $\alpha'_H$  is displacive and  $\alpha'_L$  is a hettotype of  $\alpha'_H$  which is isostructural with  $\beta$ - $\text{K}_2\text{SO}_4$ . In order to estimate the structural distortion of the  $\alpha'_L$  phase from the  $\alpha'_H$  phase, the tolerance factor (*t*) for the  $\beta$ - $\text{K}_2\text{SO}_4$  type structure was defined in this study. For the purpose of studying the effect of pressure on *t*, the crystal structure of  $\text{Ca}_{1.5}\text{Sr}_{0.5}\text{SiO}_4$  was analyzed at 2.9 GPa and 4.6 GPa. A synthesized single crystal of  $60 \times 60 \times 30 \mu\text{m}$  was placed in a modified Merrill-Bassett type diamond anvil pressure cell [3]. The pressure medium was a 4:1 mixture of methanol and ethanol and a stainless steel (SUS301) plate was the gasket. Pressure was calibrated by the ruby fluorescence method [4]. X-ray intensity measurements were performed using the BL-10A beam line at the Photon Factory (High Energy Accelerator Research Organization, Tsukuba, Japan). Judging from the observed bond compressibilities, *t* decreases with pressure and the structural distortion of  $\text{Ca}_{1.5}\text{Sr}_{0.5}\text{SiO}_4$  increases with pressure.

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Keywords: high pressure, single crystals, X-ray diffraction

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### Rietveld refinement of natural fluorapatite from ultrahigh pressure eclogite

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Fluorapatite (FAP), found within eclogite from ultrahigh pressure orogen of China, is attracted for their structural response to pressure. Zhang et al. (2005) estimated the formation conditions of the ultrahigh pressure eclogite as  $>940^\circ\text{C}$  and  $>4.5\text{GPa}$ . Additional stress on FAP was kept away from crashing eclogite with hammer and grinding with agate mortar during the course of sample preparation. Powder X-ray diffraction method was used since the FAP aggregates containing amount of exsolutions on a scale of micrometer. The Rietveld method was performed for structure refinement. Polynomial background and the Pseudo-Voigt function were used for simulating measured profile. K-alpha 2 component was stripped and no smoothing was made. The final structure of the FAP is derived under the agreement index GOF=1.19. The space group of FAP is P63/m, and the refined cell parameters are  $c=6.8849(7)$  and  $a=9.3842(2)\text{\AA}$ . That leads to a cell volume  $V=525.08\text{\AA}^3$ . Metaprisim twist angle  $\phi$ , defined as the (001) projected angle of O1-Ca1-O2, is measured as  $23.91^\circ$  from the refined structural model. The  $X^-$  ionic radius is measured as  $1.313\text{\AA}$  from tunnel Ca-F minus  $\text{Ca}^{+2}$  radius. This  $X^-$  ionic radius is less than  $1.33\text{\AA}$  an expected dimension of closest packing model when  $c/a=0.734$ . The formula of the FAP is, on averaged, derived as:  $(\text{Ca}_{3.98}\text{Sr}_{0.01})_{3.99}(\text{Ca}_{5.96}\text{Na}_{0.01}\text{Sr}_{0.02})_{5.99}(\text{P}_{5.98}\text{S}_{0.02})_6\text{O}_{24}\text{F}_{1.99}$ . As compression on flexible one-dimension tunnel in apatite leads to structurally adjustment through an increase in angle  $\phi$ , it follows that higher pressure correlates with higher angle  $\phi$ . The structure of the FAP from ultrahigh pressure eclogite of China possesses a small cell volume and a large twist angle and demonstrates a good record for the ultrahigh pressure processes underwent.

Keywords: apatite, Rietveld refinement, ultrahigh pressure

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### Pressure-induced structural change of Ca and Mg aluminosilicate melts

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Viscosity and density are important physical properties to control the transportation of magma in the Earth's interior, which are strongly correlated to microscopic structure of magma. Magmas have been considered to be densified by changing its structure with increasing pressure. We have studied the static structure of the  $\text{Ca}_3\text{Al}_2\text{Si}_6\text{O}_{18}$  and  $\text{Mg}_3\text{Al}_2\text{Si}_6\text{O}_{18}$  melts up to 5 GPa by X-ray diffraction analysis, in order to clarify pressure-induced structural change in topology and aluminium coordination environment. We have found the degenerated T-O peaks splitting into two peaks up to 5 GPa, indicating the coordination change of aluminium with pressure. This observation is consistent with the results of NMR studies on the  $\text{Ca}_3\text{Al}_2\text{Si}_6\text{O}_{18}$  glasses quenched from high-*P* melts, showing the increase of population of highly coordinated aluminium