
Keywords: twinning.

The KPb₂Cl₅ crystals are considered as a promising media for solid state lasers operating in the mid-IR due to low-energy phonon spectrum (ν<250 cm⁻¹) [1]. The single crystal X-ray analysis of KPb₂Cl₅ samples, grown by the Bridgeman techniques, showed that they can be satisfactorily described as pseudo-orthorhombic twins with the twinning matrix of (-1 0 0 / 0 1 0 / 0 0 1). Each of the components is monoclinic, space group P2₁/c, a = 8.854(2), b = 7.927(2), c = 12.485(3) Å, β=90.05(3)°, V=876.3(4) Å³, Z=4. Such twining is possible because of monoclinic angle is about 90°. Refinement of twin structure was performed using SHELXL97 program using TWIN instruction in anisotropic approximation, the relative weight of twin components being 0.664(3) and 0.336(3). Final residuals are: R₁=0.0702, wR₂=0.1908 for 4094 F ≥ 4σ(F), R₁=0.0903, wR₂=0.2130 for all 5275 unique reflections with R int =0.0972.

The title compound appeared to be isostructural with ammonium salt NH₄Pb₂Cl₅. Potassium cation was placed in NH₄⁺ position. Two models suggested for NH₄Pb₂Cl₅ by Keller [3] and Ras [4] correspond to major and minor twin components in KPb₂Cl₅ respectively. The mechanisms of twin formation in KPb₂Cl₅ are discussed.


---

Structures of SrGeO₃-CaGeO₃ solid solutions. F. Nishi¹ and Y. Matsumoto². 1 Saitama Institute of Technology, Saitama, JAPAN. 2 Tohoku University, Sendai, JAPAN.

Keywords: germanates, wollastonite, XRD.

SrGeO₃-CaGeO₃ solid solutions have at least three different phases. The first phase having pure SrGeO₃ chemical components showed a monoclinic symmetry. The space group is C2/c and the lattice constants are: a=12.533(3)Å, b=7.262(1)Å, c=11.259(3)Å, β=111.30(2)°. The structure can be summarized: (1) it includes the layers comprised by GeO₄ three-membered rings and the layers comprised by SrO₆ polyhedra. (2) they are piled up along c directions alternately and they are classified into the 6-layers structure in viewpoint of the polytypic considerations [1]. The second phase having (SrₓCa₁₋ₓ)GeO₃ (0.3<x<0.9) showed a triclinic symmetry and the lattice constants are: a = 9.723(3)Å, b = 6.962(3)Å, c = 6.937(2)Å, a=103.04(3), b = 83.60(3), β = 109.29(3). The structure is been studying now. The third one having (SrₓCa₁₋ₓ)GeO₃ (0.1<x<0.15) showed a triclinic symmetry too. The lattice constants are: a=8.147(1)Å, b=7.569(2)Å, c=7.300(1)Å, a=90.18(1)°, β=94.26(1)°, γ=103.46(1)° and the structure has a inversion center. A set of 2507 Bragg reflections were collected and the structure analysis was tried. As the result, we could succeed in solving the crystal structure and the last residual factor was about 5%. The basic structure is isostructure with the wollastonite (CaSiO₃) [2][3] which includes the single chains of SiO₄ tetrahedra. The third crystal, instead of silicon atoms, includes those of GeO₄ tetrahedra. It has the statistical distributions of calcium and strontium atoms in the three independent metal sites and this situation may affect the concept of “space-group twinning” and “structure twinning” what Ito (1950) suggested. We will report those details in our poster.