

[o.m4.p5] The Single Crystal X-Ray Diffraction Study of KPb_2Cl_5 . L.I. Isaenko, A.A. Merkulov, V.M. Pashkov, *D&T Institute of Monocrystals SB RAS, 43 Russkaya Str., 630058 Novosibirsk, Russia*; A.V.Virovets, *Institute of Inorganic Chemistry, SB RAS & D.Y.Naumov, Institute of Solid State Chemistry, SB RAS.*

Keywords: twinning.

The KPb_2Cl_5 crystals are considered as a promising media for solid state lasers operating in the mid-IR due to low-energy phonon spectrum ($\nu < 250 \text{ cm}^{-1}$). The single crystal X-ray analysis of KPb_2Cl_5 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 $\text{P}2_1/c$, $a = 8.854(2)$, $b = 7.927(2)$, $c = 12.485(3) \text{ \AA}$, $\beta = 90.05(3)^\circ$, $V = 876.3(4) \text{ \AA}^3$, $Z = 4$. Such twinning is possible because of monoclinic angle is about 90° . Refinement of twin structure was performed using SHELXL97 program² 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 $F \geq 4\sigma(F)$, $R1 = 0.0903$, $wR2 = 0.2130$ for all 5275 unique reflections with $R_{\text{int}} = 0.0972$.

The title compound appeared to be isostructural with ammonium salt $\text{NH}_4\text{Pb}_2\text{Cl}_5$. Potassium cation was placed in NH_4^+ position. Two models suggested for $\text{NH}_4\text{Pb}_2\text{Cl}_5$ by Keller³ and Ras⁴ correspond to major and minor twin components in KPb_2Cl_5 respectively. The mechanisms of twin formation in KPb_2Cl_5 are discussed.

[o.m4.p6] Structures of SrGeO_3 - CaGeO_3 solid solutions. F. Nishi¹ and Y. Matsumoto². *1 Saitama Institute of Technology, Saitama, JAPAN. 2 Tohoku University, Sendai, JAPAN.*

Keywords: germanates, wollastonite, XRD.

SrGeO_3 - CaGeO_3 solid solutions have at least three different phases. The first phase having pure SrGeO_3 chemical components showed a monoclinic symmetry. The space group is $\text{C}2/c$ and the lattice constants are: $a = 12.533(3) \text{ \AA}$, $b = 7.262(1) \text{ \AA}$, $c = 11.259(3) \text{ \AA}$, $\beta = 111.30(2)^\circ$. The structure can be summarized: (1) it includes the layers comprised by GeO_4 three-membered rings and the layers comprised by SrO_8 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 $(\text{Sr}_x\text{Ca}_{1-x})\text{GeO}_3$ ($0.3 < x < 0.9$) showed a triclinic symmetry and the lattice constants are: $a = 9.723(3) \text{ \AA}$, $b = 6.962(3) \text{ \AA}$, $c = 6.937(2) \text{ \AA}$, $\alpha = 103.04(3)$, $\beta = 83.60(3)$, $\gamma = 109.29(3)$. The structure is been studying now. The third one having $(\text{Sr}_x\text{Ca}_{1-x})\text{GeO}_3$ ($0.1 < x < 0.15$) showed a triclinic symmetry too. The lattice constants are: $a = 8.147(1) \text{ \AA}$, $b = 7.569(2) \text{ \AA}$, $c = 7.300(1) \text{ \AA}$, $\alpha = 90.18(1)^\circ$, $\beta = 94.26(1)^\circ$, $\gamma = 103.46(1)^\circ$ 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 (CaSiO_3) [2][3] which includes the single chains of SiO_4 tetrahedra. The third crystal, instead of silicon atoms, includes those of GeO_4 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.

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