

**s5.m15.p12** **Crystal structure of congruent lithium tantalate (CLT)**, Masato Okui,<sup>a</sup> Sei Fukushima,<sup>a</sup> Kenji Kitamura,<sup>b</sup> Nobuo Iyi<sup>b</sup> and Syunji Takekawa<sup>b</sup>, <sup>a</sup>*Spring-8 BL15XU, National Institute of Materials Science, Japan, and* <sup>b</sup>*Advanced Materials Laboratory, National Institute for Material Sciences, Japan. E-mail: okui@spring8.or.jp*

**Keywords: Lithium; Site defect; X-ray diffraction**

Lithium tantalate (LiTaO<sub>3</sub>) is a ferroelectric material, interested in the field of material sciences for its piezoelectric, electro-optical and linear properties. It had been practically impossible to elucidate the correlation between variation of the "non-stoichiometric" composition and that of structure, especially with respect to defect distribution, regardless of the knowledge that the non-stoichiometry is the key factor for the photo-induced refractive material. Quite recently, AML-NIMS<sup>c</sup>) succeeded in the composition control of growing crystal in the compositional range between stoichiometry and congruent composition by newly developing double crucible Czochralski method [1]. The present authors reported study of the crystal structure of a near stoichiometric lithium tantalate (NSLT) [2]. In the previous study, the authors suggested some possibilities about cation replacement of cation sites of NSLT. In the present study, the crystal structure of a congruent lithium tantalate (CLT) was determined based on X-ray single crystal diffraction data. The Li / Ta ratio of the present crystal was determined as 48.6 / 51.4. The chemical composition was estimated Li<sub>0.957</sub>Ta<sub>1.009</sub>O<sub>3</sub> from the given cation ratio. The single crystal diffraction data were measured by Mo K $\alpha$  radiation using a four-circle diffractometer, and 3966 reflections were collected in the 2 $\theta$  range from 5 to 120 degrees in all reciprocal lattice space. The measured crystal was formed a small sphere having a diameter of 0.06mm in order to reduce inference of absorption and extinction effects. The scale factor, occupancies of cations, atomic positions, and anisotropic temperature factors were refined by least squares method using 733 independent reflections, of which the each intensity obtained by averaging those of equivalent reflections. The total amount of lithium and tantalum ion was fixed above estimated chemical composition at the present occupancy refinement. The result of the refinement strongly suggests the vacancy is mainly existed in lithium site. The residual R and wR converged on 0.026 and 0.031, respectively.

- [1] Kitamura, K. et al. (1992) *J. Crystal Growth*, **116**, 327-332.  
 [2] Okui, M. et al. (2002) *Acta Cryst.*, **A58** (Supplement), C338,

**s5.m15.p13** **Structural features of Ca<sub>8</sub>Mg[SiO<sub>4</sub>]<sub>4</sub>Cl<sub>2</sub> - product of the people technical activity.** R.K. Rastsvetaeva<sup>a</sup>, A.V. Barinova<sup>a</sup>, A.A. Kashaev<sup>b</sup>, <sup>a</sup>*Institute of Crystallography RAS, Russia;* <sup>b</sup>*Irkutsk State University of Transport Communication, Russia. E-mail: rast@ns.crys.ras.ru*

**Keywords: Crystal structure; Technological activity**

A sample of compound Ca<sub>8</sub>Mg[SiO<sub>4</sub>]<sub>4</sub>Cl<sub>2</sub> was found by B.V. Chesnokov in the mine near Kopeisk (the Urals). The empirical formula on the base of electron-microprobe analysis: (Ca<sub>7.06</sub>Mg<sub>0.78</sub>Fe<sup>3+</sup><sub>0.08</sub>Al<sub>0.03</sub>)<sub>7.95</sub> [Si<sub>4.02</sub>O<sub>15.00</sub>] [Cl<sub>1.26</sub>OH<sub>0.36</sub>F<sub>0.32</sub>(SO<sub>4</sub>)<sub>0.06</sub>]<sub>2</sub>. Unit cell parameters of the cubic cell are:  $a=15.040(4)$  Å,  $V=3402.07$  Å<sup>3</sup>. X-ray single crystal data was collected using ENRAF-NONIUS diffractometer (Mo-radiation). Crystal structure was solved by direct methods and refined in the space group *Fd3* to  $R_{\text{aniso}} = 2.6\%$  (495 reflections).

The main fragment of the structure is cluster made of four Si-tetrahedra and one central Mg-tetrahedron linked through the vertex. Average distances Si-O=1.63 Å, Mg-O=1.866 Å. Si-tetrahedra in pairs are oriented in opposite directions. Ca atoms form two types of polyhedra - regular octahedron (Ca-O=2.358 Å) and 8-fold polyhedra (average Ca-O=2.619 Å). Cl is a common vertex of six Ca bipyramids. The mixed framework is built of Si and Mg tetrahedra and Ca octahedra while Ca bipyramids occupy the holes.

The compound under consideration is hightemperature product of the burned rocks as a result of people technological activity.

This study was supported by the Russian Foundation for Basic Research, project no. 02-05-64080.