o.m13.p24.la Structural and Anisotropic Thermal Expansion Correlation of Li_2ZrO_3 at Different Temperatures. Z. Heiba, K. El-Sayed. *Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt, E-mail: Karima@FRCU.EUN.EG*
Keywords: structure, thermal expansion, anisotropy.

The crystal structure of Li_2ZrO_3 have been studied at three different tempratures (room, 573K and liquid nitrogen temperatures) using the X-ray powder diffraction & the Rietveld refinement methods.

Li_2ZrO_3 is considered to be one of the oxide materials, which has many practical applications. It crystallizes in the monoclinic space group C2/c, the cell constant & atomic coordinates refined from the data recorded at room temperatures in this work are in good agreement with that previously reported at the same temperature using the single crystal & neutron refinement methods. The lattice parameters are: a=5.42403(10), b=9.02625(17), c=5.41965(10) & β=112.70119(7).

The result revealed anisotropic changes in the cell lattice parameters & in the co ordinates of Li & O atoms at higher & lower temperatures. The anisotropy in thermal expansion was found to be large, this could be indicated by the relative changes in the cell parameters in the temperature range (room-573K) in the following: $\Delta a/a$ = 0.0083, $\Delta b/b$ =0.0031, $\Delta c/c$ =0.0052.

As can be seen the relative changes in a is nearly twice that of c, although the two lattices are almost the same in magnitudes as previously shown from the analysis at room temperature.

Correlation between structure, thermal expansion in different directions & thermal vibrations are being discussed in full details.

o.m13.p25.la Novel Ta-bronzes. The crystal structure and conductivity of $K_6Ta_{6.5}O_{15+x}F_{6+y}$ with partialy reduced Ta ions. A.V. Arakcheeva, V.V. Grinevitch, V.A. Mitin, V.F. Shamray. *Baikov Institute of Metallurgy RAS; Leninskii pr. 49, Moscow 117334, Russia.*
Keywords: bronze, crystal structure, T-dependence of conductivity.

Three new Ta-bronzes were obtained on cathode by the molten salts' electrolysis of the system K_2TaOF_5-$(KF+NaF+LiF)_{eut}$. They are: (I) $K_6Ta_{6.5}O_{15+x}F_{6+y}$ - sp.gr. P6/m, a = 13.118, c = 3.862 A - hexagonal bronze; (II) $K_{6-x}Ta_{10+y}(O,F)_{30}$ - sp.gr. P4/mbm, a = 12.50, c = 3.98 A - tetragonal bronze; (III) $K_{1-x}Ta(O,F)_3$ - sp. gr. Pm3m, a = 4.00 A - cubic bronze (perovskite structure type).

Every one of them has metal-like appearance, and it is characterized by the chemical composition and crystal structure closed to those for the well known transparent crystals: (Ia) $K_6Ta_{6.5}O_{14.5}F_{9.5}$[1] - sp.gr. P-6, a=13.11, c=3.88 A; (IIa) $K_6Ta_{10.8}O_{30}$[2] - sp.gr. P4/mbm, a=12.569, c=3.978 A; (IIIa) $KTaO_3$[3] - sp.gr. Pm3m, $\boldsymbol{a}$ = 3.988 A.

The main differences of the related compounds are due to the various oxidation state of Ta, being 5+ in the transparent crystals and lower then 5+ in the bronzes.

The crystal structure and the temperature dependence of conductivity for I and Ia has been studied. The conductivity of the bronze I ($\rho = 4 \times 10^{-3}$ Om.sm) is found independent from the temperature in the range 4 - 300 K, while the transparent crystals Ia are isolator.

The structure both I and Ia characterizes by the same main framework $[K_6Ta_6O_{15}F_6]$ which is formed by $[TaO_6F]$ octahedrons shared common O-corners. F-corners form the width (~8 A diameter) hexagonal tunnel elongated in the [001] direction. K ions are in the walls of the tunnel. This framework is neutral in Ia and it has negative charge in I. Addition 0.5Ta ions are in the center of the tunnel. They statistically occupy two positions in 6-fold axis in the structure Ia and they are essentially delocalized along this axis in the structure I. These addition Ta ions are surrounded by the (O,F) anions in the ordering manner in the structure Ia and more less amount of such anions are delocalized in the tunnel of the structure I.

Temperature independence of conductivity for the crystals of the bronze I was considered in the frame of the minimal metallic conductivity conception[4].

The study is supported by the Russian Foundation for Basic Research, project no. 98-04-32804.

[1] Vlasse M., Boukhari A., Chaminada J.P., Pouchard M. «Crystal structure of potassium tantalum oxyfluoride $K_6Ta_{6.5}O_{14.5}F_{9.5}$» Materials Research Bulletin (1979), 14, 101-108.
[2] Awadalla A.A., Gatehouse B.M. «Crystal structure of some niobium and tantalum oxides» J. of Solid State Chemistry (1978), 23, 349-355.
[3] Zhurova E.A., Zavodnik V.E., Ivanov S.A., Syrnikov P.P., Tsirelson V.G. «Electron density and anharmonic thermal motion of atoms in perovskites $K_{1-x}Li_xTaO_3$ (x=0, 0.05, 0.15)» Zhurnal Neorganicheskoi Khimii (1992), 37, 2406-2412.
[4] Mott N., Devis E. «Electronic processes in noncrystalline substances» 1982, Moscow «Mir», (transl. from Eng. into Russ.)