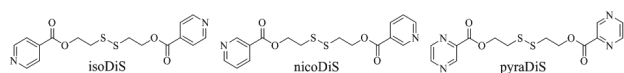


MS51-P3 Disulfide complexes: their interaction with silver(I) and copper(II)Massimo Varisco¹, Aurelien Crochet¹, Katharina M. Fromm¹

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Bisisonicotinate disulphide (isoDiS, Figure 1) was widely used in our research group for Au(111) surface pre-treatment in combination with antibacterial complexes[1, 2]. In order to increase our knowledge of the interactions taking place on the surface, crystallographic studies were performed using the metal ions that were coated on the surface during the above-mentioned studies. These ions are silver(I) nitrate and copper(II) nitrate, both have interesting antibacterial properties, but can interact with the sulphur atoms taking the place of the gold surface. Two similar ligands were also taken into account in order to look for a better alternative, thus improving the quality of the developed materials.

**Figure 1.** the three different ligands.**Keywords:** coordination chemistry, biomaterials**MS51-P4** Chemical composition range and flux crystal growth of $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutionsVladimir A. Ivanov¹, Mikhail O. Marychev¹, Pavel V. Andreev¹, Vladimir A. Lykov¹, Mikhail A. Faddeev¹, Iovka Koseva², Velin Nikolov¹

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The present studies included: solid state synthesis of $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ where $2x$ varied from 0 to 2; crystal growth from different solutions with Ca_2GeO_4 concentration in the range from 8 to 40 wt. %; X-ray phase analysis for determining the primary crystallizing phase and its cell parameters; elemental analysis of the obtained crystals.

A series of $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutions with $0 < 2x < 2$, were synthesized by the classical solid state method. X-ray analysis revealed that for $0 < 2x < 0.6$ only $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutions of Ca_2GeO_4 structure crystallized. The cell parameters of this phase linearly decreased upon increasing the lithium concentration, which means that the solutions are in accordance with the Vegard's law. For $2x > 0.6$ the specimens contained two phases: (i) $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ with maximum lithium concentration approximately equal to that for $2x = 0.6$ and minimum values of the cell parameters and (ii) $\text{Li}_2\text{CaGeO}_4$.

Both $\text{Li}_2\text{CaGeO}_4$ and Ca_2GeO_4 doped with chromium are promising laser materials with Cr^{4+} emission in the 1.1 – 1.6 μm range. From this point of view it was important to find suitable conditions for the crystal growth from $\text{Li}_2\text{CaGeO}_4$ and from $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutions in order to obtain good-quality crystals with the required dimensions.

High temperature solutions were used for $\text{Li}_2\text{CaGeO}_4$ and $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ crystal growth by spontaneous crystallization. $\text{Li}_2\text{CaGeO}_4$ crystals were grown in the concentration range 8-26 wt. % Ca_2GeO_4 in the temperature range 830-980 °C. Crystals with chemical compositions different from those of the $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutions were grown in the concentration range 26-40 wt % Ca_2GeO_4 in the temperature range 980-1090 °C.

The cell volumes calculated on the basis of the XRD measurements and the lithium concentrations obtained by ICP-OES analysis for some crystals were plotted on the linear dependence between the cell volumes and the lithium concentrations of the $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutions obtained after solid state synthesis (Fig. 4). As can be seen, all crystal specimens grown from the high temperature system are $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutions with cell volumes and lithium concentrations similar to those obtained by solid state synthesis.

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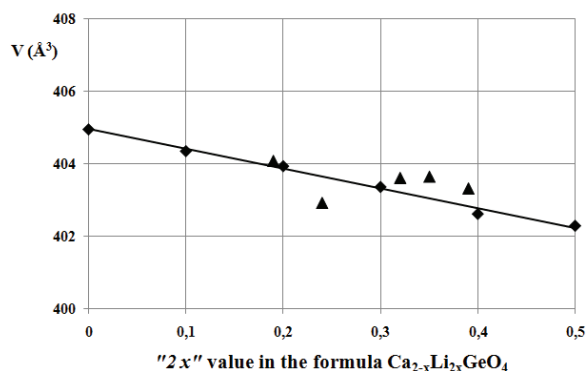


Figure 1. Dependence between the cell volume calculated from X-ray data and Li concentration in $\text{Ca}_{2-x}\text{Li}_{2x}\text{GeO}_4$ solid solutions (square) – solid state synthesis. \blacktriangle (triangle) – single crystals grown from high-temperature Li_2MoO_4 - Ca_2GeO_4 solutions.

Keywords: oxide materials, solid state reactions, crystal growth, X-ray diffraction

MS51-P5 Growth crystals KDP from water solutions with KMnO_4

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Crystals of potassium dihydrogen phosphate are widely applied in science and techniques, medicine and industry. In this work we grew up crystals of potassium dihydrogen phosphate with potassium permanganate up by the temperature differential method with concentration convection condition in thermostat with constant degree of supercooling 3.5-4 °C. It was established KMnO_4 influence on the growth of KDP. The grown crystals have prismatic habit without pinching. Crystals got brown coloring, and it was visible that in sector of growth of a side of a prism concentration of manganese more than in sector of growth of a bipyramid. The structure of this crystal was defined by single crystal X-ray diffraction. X-ray diffraction data for this sample were obtained with Oxford Diffraction (Gemini S) diffractometer on graphite monochromatic Mo-K_α radiation ($\lambda=0.71073 \text{ \AA}$) and with CCD Sapphire III detector in the ω -scan mode at a room temperature. The crystal structure was solved by direct methods (Shelx97) and refined by full matrix method (Shelx97). The reflection data were processed by using an analytical absorption correction algorithm. The crystal structure was solved by direct methods and refined by full matrix method. All non-hydrogen atoms were refined with anisotropic correction. Hydrogen atoms were located from difference Fourier synthesis and refined isotropically. Potassium permanganate (KMnO_4) addition to the KDP (KH_2PO_4) solution increases the growth rate of the $\{100\}$ faces and decreases that of the $\{101\}$ ones. The complex ion MnHPO_4^{4+} is an impurity affecting $\{101\}$ face growth rate. The manganese-ion Mn^{3+} replaces the K^+ ion in the KDP structure and causes the change of hydrogen positions. The increase of the $\{100\}$ face growth rate is connected with the capture of MnO_2 particles. The doping of KDP crystals by manganese decreases the effective quadratic nonlinear sensitivity of crystals [D.A. Vorontsov, A.E. Egorova, E.L. Kim, M.O. Marychev, A.A. Petrova, V.N. Portnov, N.V. Somov. Vestnik of Lobachevsky State University of Nizhni Novgorod, 2010, №5(2), p. 210–213.]. The analysis of element structure of crystals was carried out on a Wavelength Dispersive X-Ray Fluorescence Spectrometer of Shimadzu Lab Center XRF-1800 on intensity K_α -line of characteristic x-ray radiation (HRI) of potassium and manganese. So concentration of atoms Mn was measured by Optical Emission Spectrometer Varian ICP-OES.

Keywords: growth crystal, KDP (KH_2PO_4), X-ray