

MS15-P15 Anomalous thermal expansion in α -titaniumBoris N. Kodess¹, Hakon Hope²

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The unit cell parameters of single crystals of Ti were determined in the range 10 to 295 K. For several samples of two single crystals, experiments were also carried out at room temperature in full Ewald sphere. Results showed homogeneity of the characteristics in different parts of the single crystals. A comparison of the lattice parameters of Ti determined on different diffractometers showed very good reproducibility when used for calculations in the high-angle region (the difference is not more 0.00002 nm). The values of the cell parameters correspond to high-purity powders of Ti in the JCPDS database [1]. For the sample with the best micro-structures were constructed temperature dependencies from of the axial ratios of the unit cell parameters, c/a , and the thermal expansion coefficient, TEC. At low temperatures we found negative value of TEC, attributed to c only. It is important that in the same range of temperatures from 10 to 50 K have been found anomalies in the elastic constants [2] and the temperature dependence of paramagnetic susceptibility [3]. We consider two complementary hypotheses. First - the anomalous TEC can be connected with an electronic topological phase transition. The possibility of this type phase transition for Ti is described in [4]. Second - in the low-temperature range occurs the possibility of appearance precursors of the low-temperature phase transition to the ω phase. Note that this ω phase for Ti occurs after low pressures at room temperature [5]. Extrapolation of the transition temperature of hcp - ω -phase, which depends on pressure and temperature [5, etc.], is the reason for suggesting that this ω phase may occur due to compression of the lattice when the temperature is lowered to the range 10-30 K, under normal pressure. It is an interesting fact that the ω phase of elemental Ti corresponds to structural type A1B2 (C32), which favors the appearance of the superconducting state. [1] JCPDS (Joint Committee on Powder Diffraction Standards), No. 44-1294, [2] Fisher, E. S., Renken, C. J. Phys. Rev. (1964) 135, Issue 2A, pp. 482-494 [3] Collings E.W. & Ho, J. C. (1971) Phy. Rev. B, 4(2), 349 [4] Souvatzis P., Eriksson O., Kaznelson M.I. Phys. Rev. Lett. (2007), v.99, 015901 [5] Zhang J., Zhao Y., Hixson RS, Gray III GT, Wang L, Utsumi, W. Hiroyaki S., Takanori H. Phys. Rev. (2008), B78, p. 054119

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MS15-P16 Structure and multiferroic properties of a new Sr-based pyroxene familyPierre Bordet¹, Lei Ding¹, Claire V. Colin¹, Céline Darie¹

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Compounds belonging to the Pyroxene family are well known as rock-forming minerals, and have thus drawn substantial interest by mineralogists. In this family of general chemical formula $AM(Si, Ge)_2O_6$, A is usually an alkali metal monovalent cation or a divalent alkaline earth cation, and B may be a trivalent or divalent transition metal cation. Among pyroxene compounds, the monoclinic clinopyroxenes are characterized by isolated one-dimensional chains of MO_6 octahedra linked by edge-sharing. Due to this specific arrangement, clinopyroxene compounds where M is a magnetic transition metal cation have attracted considerable attention in recent years. Investigations revealed that these compounds present a rich diversity of intriguing low-dimensional magnetic properties. The existence and possible interplay of low dimensionality and magnetic frustration may result in multiferroic and/or magneto-electric (ME) properties.

We have undertaken the study of pyroxene compounds where A and M are divalent cations. Among these, Sr-based pyroxenes were not reported up to now. Here we present the synthesis of the new compounds $SrCoGe_2O_6$ and $SrMnGe_2O_6$ which both display the high clinopyroxene structure with space group $C2/c$. We will show their structure determination using single crystal and powder x-ray diffraction and neutron powder diffraction (NPD, D1B-ILL) and compare their structures to those of their Ca-based analogues. The magneto-electric properties of both compounds were investigated by polarization measurements vs applied magnetic field and NPD. $SrMnGe_2O_6$ displays multiferroic properties with a cycloid-type incommensurate spin structure, while $SrCoGe_2O_6$ is an antiferromagnet with a similar magnetic structure as the $CaCoGe_2O_6$ compound. These results will be detailed at the conference.

Keywords: Multiferroics, Pyroxene, magnetic structure