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Local electronic and crystal structures of FeTe doped with cobalt

K. Żebrowska[1]*, M. Bagińska[1], M. Wojdyła[1], E. Salas-Colera[2], P. Zajdel[1**]

[1]*Institute of Physics, University of Silesia, ul. Universytecka 4, 40-007 Katowice, Poland*
[2]*SpLine CRG, European Synchrotron Radiation Facility, CS40220, F-38043 Grenoble Cedex, France*

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*e-mail: kasia20075@onet.eu
**e-mail: pawel.zajdel@us.edu.pl

Due to inherent phase separation, it has been so far impossible to grow ideally stoichiometric (1:1) tetragonal (*P*4/*nmm*) iron telluride. The excess iron ions are located in the inter-planar positions and usually represented as a fraction x in a general formula $Fe_{1+x}Te$ [1], where x ranges from about 4% to 17%. The additional iron has been found to negatively correlate with the level of anion site doping and subsequently with hindering the superconductivity (SC), for example in the Fe(Te,Se,S) series [2], where SC can be induced by doping with selenium or small amounts of sulfur.

In our work, we attempted to create and investigate compounds electronically equivalent to variable iron stoichometry by substituting Fe with different transition metals [3]. Here we report our results for single crystals of FeTe doped with cobalt.

Samples several millimeter in size were grown by solidification from melt method in the substitution range x=0.01 to 0.1. The incorporation of dopant into host was confirmed by WDS-SEM and observed trends in lattice parameters obtained from single crystal diffraction. However, it is not clear if Co is located in in-plane (IP) or out-of-plane (OOP) positions See Fig. 1 due to low level of doping and weak X-ray contrast between Co and Fe.

In order to gain new insight into the problem we have performed Fe K, Co K and Te L edge XAFS studies on ESRF CRG SpLine [4] and MAXLAB-II I811 [5] beamlines.

Our preliminary results shall be presented which indicate that the cobalt and iron positions cannot be described by only two (IP or OOP) possible locations, which is in agreement with earlier Mossbauer studies [6].

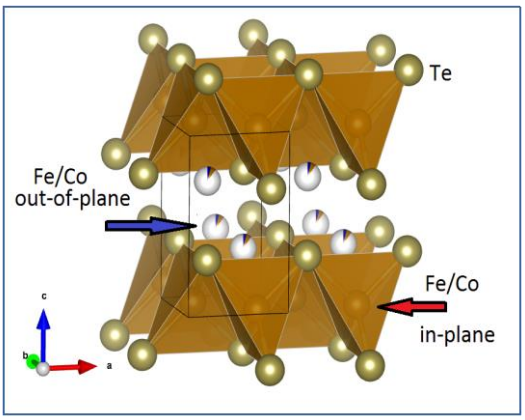

Figure 1. Possible locations of additional cobalt ions (a) in-plane, (b) out-of-plane.

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