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Local electronic and crystal structures of FeTe doped with nickel

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Keywords: XAFS, iron telluride, nickel

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Tetragonal (*P*4/*nmm*) iron telluride is known to possess natural non-stoichiometry, usually represented as a fraction x in a general formula $Fe_{1+x}Te$ [1]. The excess iron ions are located in the inter-planar positions and their content x ranges from about 4% to 17%. Due to inherent phase separation, it has been so far impossible to grow ideally stoichiometric (1:1) FeTe 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.

Here we report our results for single crystals of FeTe doped with nickel, which is follow up on our ealier work [3].

Single crystal 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, the SXRD study has not been decisive in location of nickel due to low level of doping and weak X-Ray contrast between Ni and Fe. There are two main locations of cations in the FeTe lattice. An in-plane (IP) position, which is in the centre of $FeTe_4$ tetrahedron and out-of-plane (OOP) site, which is located over the Te plane See Fig. 1.

In order to investigate a local environment around nickel we have Ni K XAFS studies on ESRF CRG SpLine [4] and MAXLAB-II I811 [5] beamlines. They were later accompanied by measurements of Fe K and Te L absorption.

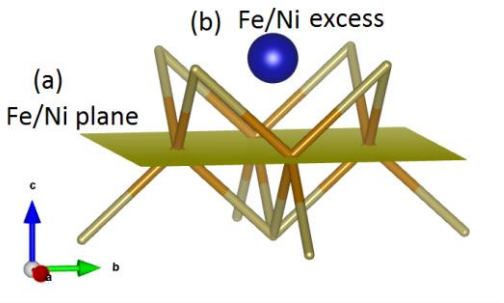

Figure 1. Possible locations of additional nickel ions (a) in-plane, (b) out-of-plane.

Our preliminary results shall be presented, which indicate that the local crystallographic postions of nickel cannot be described by only two (IP or OOP) components, which is in agreement with many sites suggested earlier by Mössbauer studies [6].

Acknowledgments: This work is supported by the Polish National Science Centre grant No 2011/01/B/ST3/00425.
The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) CALIPSO under grant agreement nº 312284
We would like to help N. Torapava for help during MAXLAB experiment.

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