Study Ab Initio of the Effect of A-Site Substitution on the Fe1.12Te System

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Abstract In the present work, our aim is to verify the structural, electronic and magnetic properties of both systems $Fe_{1.12}Te$ and <RTX>(R = Fe, X = Te and T = Ni, Co) in the P4/nmm structure. For this task, we use the density functional theory (DFT) as a theoretical tool integrated into wien2k code (Blaha 2001). The solid $Fe_{1-x}M_xTe$ (M = Ni, Co) have been synthesised by Kazakov et al. (Chem. Met. Alloys 3, 155–160 2010). They have observed a systematic shift of the lattice parameters for both systems for M = Ni and Co till x = 0.1, then a secondary phase with the NiAs-type structure appeared when x passes 0.15. $Fe_{1-x}Ni_xTe$ retains its structure in a concentration between x = 0.1 and 0.15, and $Fe_{1-x}Co_xTe$ retains its structure when x is between 0.05 and 0.1 (Blaha 2001).

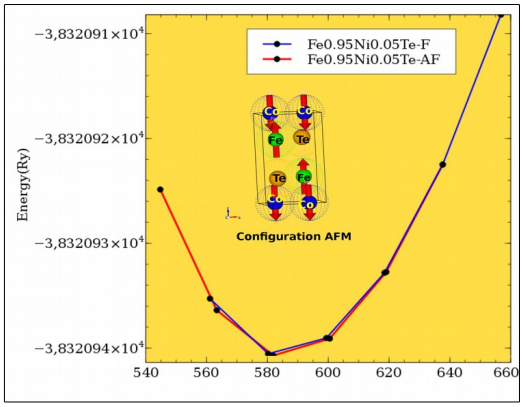

Figure1:The disappears AFM phase with dopant cantent for $Fe_{1.1-x}M_xTe$ (M = Ni, Co).

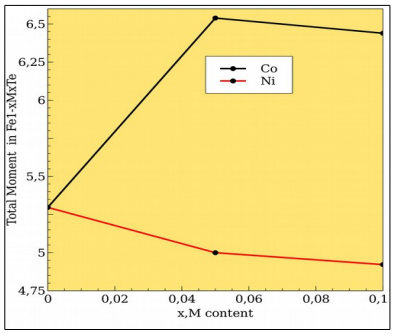

Figure2:Variation of the total moment as a function of the dopant content for $Fe_{1.1-x}M_xTe$ (M = Ni, Co).

[1] Blaha, P., Schwarz, K., Madsen, G.K.H., Kvasnicka, D., Luitz,J.: WIEN2K, An Augmented Plane Wave plus Local Orbitals Program for Calculating Crystal Properties. Vienna University of Technology, Austria (2001)