Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles study of magnetic interactions in 3d transition metal-doped phase-change materials TETSUYA FUKUSHIMA, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University, HITOSHI FUJII, Japan Synchrotron Radiation Research Institute, SPring-8, ELIAS RABEL, RUDOLF ZELLER, PETER DEDERICHS, Peter Gruenberg Institut and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, WEI ZHANG, RICCARDO MAZZARELLO, Institute for Theoretical Solid State Physics and JARA-Fundamentals of Future Information Technology, RWTH Aachen University — We investigate the electronic structure and the magnetic properties of the prototypical phase-change material $Ge_2Sb_2Te_5$ (GST) doped with V, Cr, Mn and Fe by density functional calculations. Both the supercell method and the coherent potential approximation (CPA) are employed to describe this complex substitutionally disordered system. As regards the first approach, we consider a large unit cell containing 1000 sites to model the random distribution of the cations and of the impurities in doped cubic GST. Such a large-scale electronic structure calculation is performed using the program KKRnano, where the full potential screened Korringa-Kohn-Rostoker Green's function method is optimized by a massively parallel linear scaling all electron algorithm. We find that ferromagnetic states are favorable in the cases of V and Cr doping, due to the double exchange mechanism. The ferromagnetic interaction is particularly strong in the case of Cr. As a result, high Curie temperatures close to room temperatures are obtained for large Cr concentration.

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Date submitted: 13 Nov 2014 Electronic form version 1.4