

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**Invar effect and non-collinear magnetism in CuFe alloys** MARKUS EISENBACH, G. MALCOLM STOCKS, Oak Ridge National Laboratory, Oak Ridge, TN — The Invar effect has been observed in many Fe rich alloys, most famously Ni Invar. Generally the Invar behavior is associated with the strong coupling between the lattice and magnetic degrees of freedom, and therefore depends on the magnetic ordering in these alloys. Recent experimental works observed an Invar effect in fcc-FeCu solid solutions. [Gorria et al., PRB 69, 214421 (2004)] We investigate the magnetic states of fcc-FeCu solid solutions in the Invar regime and compare it with the order in low Fe concentration alloys, to establish the connection between the Invar effect and the magnetic order. To study this we employ the locally selfconsistent multiple scattering (LSMS) real space method for solving the LDA Kohn-Sham equation as well as its extension to fully relativistic calculations to investigate all effects leading to anisotropies and non collinear ordering of magnetic moments. We find that the magnetic order in the iron rich alloys (44%-65% Fe) is non-collinear and disordered. We will present the dependence of the magnetic disorder on iron concentration and lattice constant in both the Invar and non-Invar regimes to establish the validity of the standard magnetic disorder explanation of the Invar effect for FeCu solid solutions. Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

Markus Eisenbach  
Oak Ridge National Laboratory, Oak Ridge, TN

Date submitted: 27 Nov 2007

Electronic form version 1.4