

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Spin glass and semiconducting behavior of the flux grown $\text{BaFe}_{2-\delta}\text{Se}_3$ crystals¹ BAYRAMMURAD SAPAROV, STUART CALDER, BALAZS SIPOS, HUIBO CAO, SONGXUE CHI, DAVID SINGH, ANDREW CHRISTIANSON, MARK LUMSDEN, ATHENA SEFAT, Oak Ridge National Laboratory — In this talk, physical properties and crystal and electronic structures of $\text{BaFe}_{2-\delta}\text{Se}_3$ crystals, synthesized using tellurium flux, will be discussed. This phase is an iron-deficient derivative of the ThCr_2Si_2 -type and its structure is made of double chains formed from edge-sharing FeSe_4 tetrahedra. The semiconducting $\text{BaFe}_{2-\delta}\text{Se}_3$ with $\delta \approx 0.2$ does not order magnetically, however, there is evidence for short-range magnetic correlations of spin glass type below 50 K in magnetization, heat capacity and neutron diffraction results. The semiconducting behavior of $\text{BaFe}_{2-\delta}\text{Se}_3$ is in line with the detrimental influence of iron deficiency to the superconductivity in $A_x\text{Fe}_{1.8}\text{Se}_2$ (A = alkali metal) superconductors. The electronic structure calculations suggest that this compound can be considered as a low-dimensional (1D) ladder structure with a weak interchain coupling. Based on the survey of available data on BaFe_2Se_3 so far, lower concentrations of iron vacancies may lead to a long range antiferromagnetic order, whereas higher concentrations of iron vacancies may suppress long range order and then lead to a spin glass behavior.

¹This work was supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division and Scientific User Facilities Division.

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Date submitted: 08 Nov 2011

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