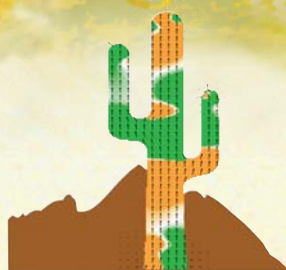# 56TH ANNUAL CONFERENCE ON MAGNETISM AND MAGNETIC MATERIALS

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ABSTRACTS

MMM 2011
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Session AR
STRONGLY CORRELATED SYSTEMS I
(POSTER SESSION)
Michael Loewenhaupt, Chair

CONTRIBUTED PAPERS

**AR-01. Temperature dependent magnetic structure of lithium delithiated Li_xFeSO_4F (x=0, 1) by Mössbauer spectroscopy.** *J. Lee*[1], S. Hyun[1], T. Kouh[1], I. Shim[1] and C. Kim[1] *1. Department of Physics, Kookmin University, Seoul, Korea, Republic of*

Recently, $LiFeSO_4F$ compound was found to be an attractive positive electrode material in lithium ion batteries [1]. In this paper, we have studied the crystal structure and temperature dependent magnetic structure of $LiFeSO_4F$ and it's fully delithiated $FeSO_4F$ compounds with x-ray diffractometer (XRD) and Mössbauer spectroscopy. Pristine $LiFeSO_4F$ polycrystalline powders were synthesized by the ionothermal process with reaction of $FeSO_4.H_2O$ and LiF in ionic liquid (EMI-TFSI). Fully delithiated $FeSO_4F$ samples obtained with chemical redox process using the $NOBF_4$ as an oxidation agent in acetonitrile solution. From the refined XRD pattern, the $LiFeSO_4F$ crystallized as a triclinic structure (space group: *P*-1) with the lattice parameter a_0=5.180, b_0=5.495, c_0=7.219 Å, α=106.594, β=107.171 and γ=97.745°. In case of $FeSO_4F$, the change in lattice parameter is caused by delithiation as a_0=5.084, b_0=5.098, c_0=7.349 Å, α=110.971, β=111.199 and γ=88.144°. The room temperature Mössbauer spectrum of the $LiFeSO_4F$ composed of two doublets which are indicating the existence of two Fe^{2+} sites with the values of δ_A=1.19 and δ_B=1.15 mm/s. The fitted spectrum for fully delithiated $FeSO_4F$ shows the one Fe^{3+} (δ=0.36 mm/s) doublet due to the valence transition by lithium ion delithiation. Mössbauer spectra of $LiFeSO_4F/FeSO_4F$ at 4.2 K showed a two set of eight/six line lorentzian with the measured value of $H_{hf,A}$= 286 kOe, $\Delta E_{Q,A}$= 3.30 mm/s, δ_A= 1.52 mm/s; $H_{hf,B}$= 292 kOe, $\Delta E_{Q,B}$= 2.65 mm/s, δ_B= 1.54 mm/s for $LiFeSO_4F$ and $H_{hf,A}$= 532 kOe, $\Delta E_{Q,A}$= 0.12 mm/s, δ_A= 0.43 mm/s; $H_{hf,B}$= 543 kOe, $\Delta E_{Q,B}$= 0.14 mm/s, δ_B= 0.45 mm/s for $FeSO_4F$, respectively. The magnetic Nèel temperatures of the $LiFeSO_4F$ and $FeSO_4F$ were determined to be 20K and 99K from the temperature dependent Mössbauer spectra. From these results, we can be explain the magnetic phase change in Li_xFeSO_4F by crystalline and $Fe^{2+/3+}$ valence transition which is coming from lithium delithiation.

[1] N. Recham, J-N. Chotard, L. Dupont, C. Delacourt, W. Walker, M. Armand and J-M. Tarascon, Nature Mater. 9, 68 (2010)

AR-02. The strong one-dimensional antiferromagnetism in a charge-transfer insulator: AgSO4. X. Zhang[1], T. Jia[1], T. Liu[1], Z. Zeng[1] and *H. Lin*[2] *1. Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Acadamy of Sciences, Hefei, China; 2. Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Hong Kong, China*

The strong one dimensional antiferromagnetism and the electronic structure of AgSO4 are investigated by performing the first-principles density functional calculations. The results show that the strong one dimensional antiferromagnetic coupling in AgSO4 is along the diagonal of the unit cell, and the obtained intra-chain exchange constant is in good agreement with experimentally observed results. In the planar rectangular cystal field, the Ag2+ 4d9 x2-y2 orbital is higher in energy (see Figure 1), therefore, the superexchange interaction between the x2-y2 orbitals gives rise to an unexpected strong one-dimensional antiferromagnetic behavior. We also found that AgSO4 is a charge-transfer insulator.
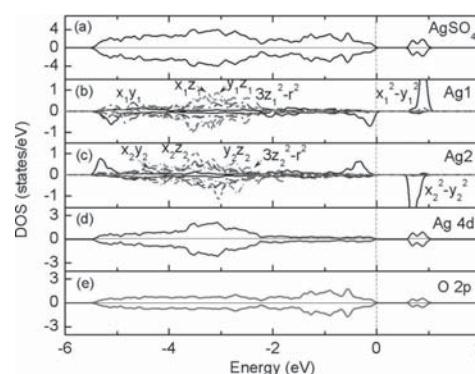
Figure 1. The total (a) and partial (b-e) DOS of AgSO4. (b-c) The partial DOS of 4d orbitals of neighboring Ag atoms Ag1 and Ag2. (d-e) The partial DOS of Ag 4d and O 2p in a unit cell.

AR-03. First-principles investigation of magnetic and elastic properties of Fe-Si. *W. Yun*[1], J. Lee[1], I. Kim[1], S. Hong[2] and J. Lee[3] *1. Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang 790-784, Korea, Republic of; 2. Department of Physics and Energy Harvest-Storage Research Center, University of Ulsan, Ulsan 680-749, Korea, Republic of; 3. Department of Physics, Inha University, Incheon 402-751, Korea, Republic of*

Silicon steels, especially with 3 wt% Si, are widely used as an energy converting material, e.g., transformers, motors, etc. Silicon steel with 6.5 wt% Si may be a promising future electrical steel, due to its zero magnetostriction, reduced magnetocrystalline anisotropy, higher permeability, and lower coercivity [1, 2]. However, the compounds with Si content higher than 4 wt% become significantly brittle and consequently its rolling process is very difficult to be achieved. Therefore, there is a need for a systematic first-principles study on its magneto-mechanical properties with different concentration of Si. In this study, we investigated fundamental magnetic and elastic properties of ferrites with the various Si concentrations (Fe100-xSix, x = 3.7, 6.25, and 12.5 at%) and its D03 structure using the highly precise all-electron full-potential linealized augmented plane wave (FLAPW) [3] method within the generalized gradient approximation (GGA) [4]. The lattice constant shrinks as the concentration of Si increases. In all the considered systems, the ferromagnetic state is more stable than the nonmagnetic one by big energy difference of about 473, 453, 394, and 351 meV/Fe-atom for x = 3.7, 6.25, and 12.5 at%, and the D03 structure, respectively. The magnetic moments of the Fe atoms nearest neighboring to the Si atoms decreases monotonically from 2.092 μB for x = 3.7 at% to 1.312 μB for the D03 structure. This feature is considered as the result of the stronger p-d hybridization for higher Si concentration. The mechanical properties of Fe100-xSix were also investigated in terms of elastic moduli, i.e., C11, C12, and C44, which are crucial for determining ductile-brittle criterion [5] as well as magnetostriction [6]. As