X-ray Absorption Spectroscopy Study of $Fe_2VSi_{1-x}Al_x$

Wei-Cheng Wang (王偉丞)[1], Yu-Nan Chen (陳禹男)[1], Yi-Sheng Liu (劉亦昇)[1], Jeng-Lung Chen (陳政龍)[1], Yung-Kang Kuo (郭永綱)[2], Chin-Shan Lue (呂欽山)[3], and Henry C.-L. Chang (張經霖)[1]

[1]Department of Physics, Tamkang University, Taipei, Taiwan
[2]Department of Physics, National Dong Hwa University, Hualien, Taiwan
[3]Department of Physics, National Cheng Kung University, Tainan, Taiwan

We have performed x-ray absorption near edge structure (XANES) study on a series of Fe_2VSi based Heusler type compounds to study the correlations between electronic structure and the thermoelectric property. A series of $Fe_2VSi_{1-x}Al_x$ compounds with different Al concentrations (x form 0 to 0.25) were studied. The XANES results show that the unoccupied density of states above Fermi level increases with increasing Al concentration, which is positively correlated with the results of resistivity and the Seebeck coefficient measurements. On the other hand, increased Al concentration does not affect the hybridization between transition metals V and Fe.

A series of $Fe_2VSi_{1-x}Al_x$ measurements were performed at National Synchrotron Radiation Research Center (NSRRC) in Taiwan. The Fe $L_{2,3}$-edge spectra were measured at Dragon (BL-11A) in total election yield mode. The V $L_{2,3}$-edge spectra were measured at HSGM (BL-20A) in total election yield mode. Fe and V *K*-edge spectra were measured at Wiggler (BL-17C) in fluorescence mode. All measurements were performed at room temperature.

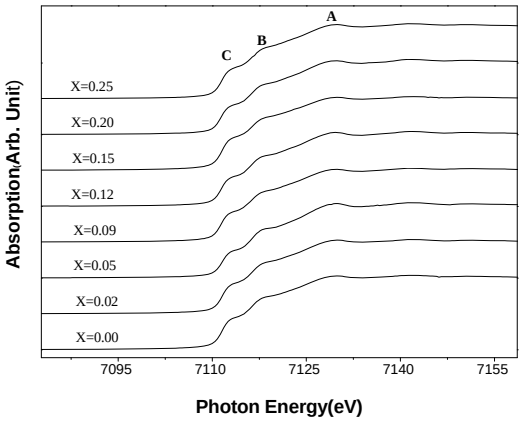

Figure 1. Fe *K*-edge XANES of $Fe_2VSi_{1-x}Al_x$ alloys. There are three main features (A, B and C) spectrum. The intensity of absorption varies with Al concentration. The feature-rich spectra are due to the transitions form the Fe 1s to 4*p*-derived unoccupied states, which consisted of strongly hybridized Fe 3*d* and Al 3*p*, and V 3*d* and Fe 4*p* orbitals [1,2].

[1] L. S. Hsu *et al*., Phys. Rev. B **66**, 205203 (2002).
[2] L. S. Hsu *et al*., Journal of Alloys and Compounds

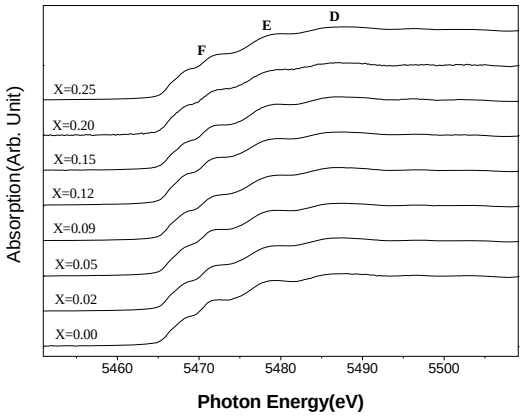

Figure 2. V *K*-edge XANES of $Fe_2VSi_{1-x}Al_x$ alloys.There are three main features (D, E and F) spectrum. The intensity of absorption varies with Al concentration. The feature-rich spectra are due to the transitions form the V 1*s* to 4*p*-derived unoccupied states, which consisted of strongly hybridized V 3*d* and Al 3*p, and* Fe 3*d* and V 4*p* orbitals [1,2].

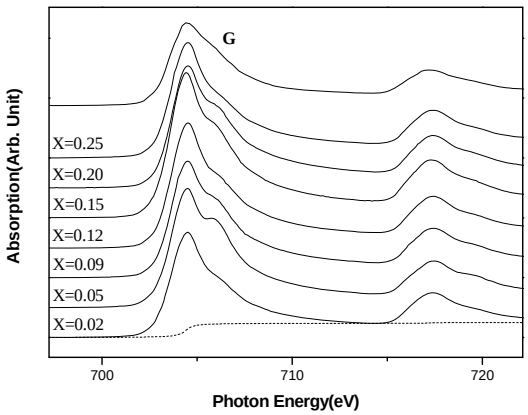

Figure 3. Fe $L_{2,3}$-edge XANES of $Fe_2VSi_{1-x}Al_x$ alloys and stander Fe. The intensity of absorption varies with Al concentration due to the variation of the *3d*-derived unoccupied states. The two prominent are the $2p_{3/2}$ (L_3) and $2p_{1/2}$ (L_2) peaks due to spin-orbit splitting. The satellite peak (G) after Fe L_3-edge is hybridized Fe 3*d* and Al 3*p* orbital [3,4].

[3] G. A. Botton *et al*., Phys. Rev. B **54**, 1682 (1996).
[4] K. Soda *et al*., Physica B **351,** 338–340 (2004).