SOFT X-RAY PHOTOABSORPTION AND PHOTOELECTRON SPECTROSCOPY OF DO_3 -TYPE $(Fe_{1-X}V_X)_3$ Al ALLOYS

We have investigated electronic structures and magnetic properties of a series of $D0_3$ -type pseudobinary alloys $(Fe_{1-x}M_x)_3Al$, where *M* stands for another 3*d* transition-metal element. High-resolution soft X-ray photoelectron spectroscopy (XPS) and soft X-ray photoabsorption spectroscopy (XAS) were conducted using highly-monochromatic, circularly-polarized light from beamline **BL25SU** [1]. In these pseudobinary alloys, the partial substitution of *M* (a metal to the left of Fe in the periodic table) for Fe in the $D0_3$-ordered ferromagnet Fe_3Al results in anomalous negative temperature dependence of their electrical resistivity and a remarkable reduction in Curie temperature and average magnetic moment [2,3].

In particular, the alloy with *M* = V and *x* = 1/3, (the Heusler-type intermetallic compound Fe_2VAl), exhibits semiconductor-like behavior , with a resistivity reaching 30 μΩ m at 2 K, disappearance of magnetic ordering, and the enhancement of the effective electron mass. These physical properties have strong similarities to the behavior observed in the heavy fermion compounds. In order to clarify the mechanism of these anomalous properties, their electronic structures were elucidated by synchrotron radiation photoelectron spectroscopy with high total energy resolution at the bulk-sensitive high-excitation photon energy $\hbar\omega$. Furthermore, magnetic circular dichroism (MCD) at the $L_{2,3}$ photoabsorption edges of the constituent transition-metal elements provides a site-specific and independent determination of the orbital and spin components of the magnetic moment [4], which may also give some insight into the

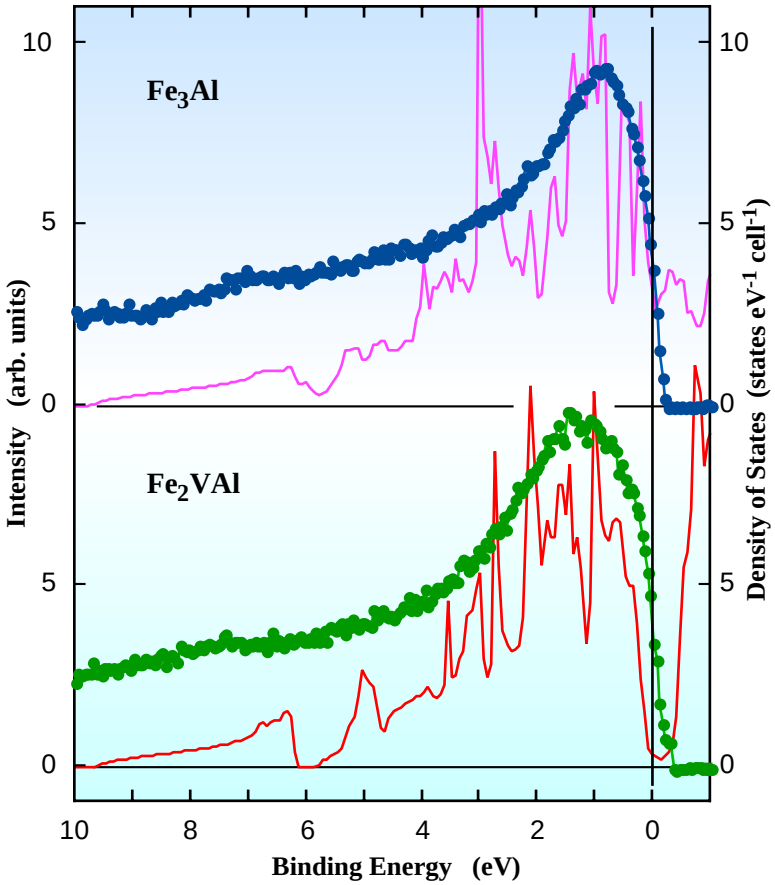

Fig. 1. Photoelectron energy distribution curves (closed circles) measured with the excitation photon energy of 700 eV in comparison with total density of states (thick curves) calculated by Botton et al. [5] for Fe_3Al and Fe_2VAl.

electronic structure. Here, we report our recent experimental results for $(Fe_{1-x}V_x)_3Al$ alloys.

Specimens used in this study were polycrystalline $(Fe_{1-x}V_x)_3Al$ alloys prepared in the $D0_3$ structure. Their surfaces were cleaned *in situ* with a diamond file in preparation for XPS measurement. The XAS spectra were obtained by measuring total photoelectric yields. All the XPS and XAS spectra were taken at the temperature of 20 K.

Figure 1 shows typical XPS spectra measured with $\hbar\omega$ = 700 eV for Fe_3Al and Fe_2VAl in comparison with their calculated total density of states (DOS) [5]. According to the theoretical results, Fe_2VAl is a semimetal with a pronounced pseudogap right at the Fermi level E_F. However, significanly high intensities are observed around E_F for both compounds, as seen in the low photoexcitation [2]. Except for the pseudogap, the overall spectral features as well as the assignments deduced from the photon energy dependence [1] are consistent with the band calculation. Although the unoccupied states have not yet been investigated, the pseudogap, if any truly exists, seems small compared to what was predicted or located on the higher energy side. In order to clarify the surface effect and the unoccupied DOS that is slightly higher than the E_F of Fe_2VAl, we are currently conducting a high-energy and higher-resolution (about 0.1 eV at $\hbar\omega$ = 900 eV) investigation of the dependence of these XPS spectra on the effective escape depth and spectra of $(Fe_{1-x}V_x)_3Al_{1-z}Si_z$ alloys.

Typical XAS and MCD spectra are shown in Fig.2(a) and 2(b) for the Fe and V $L_{2,3}$ edges of $(Fe_{1-x}V_x)_3Al$ with x = 0.3, respectively. Here, curves with up and down triangles are XAS spectra measured with the applied magnetic field ***B*** antiparallel and parallel to the incident photon

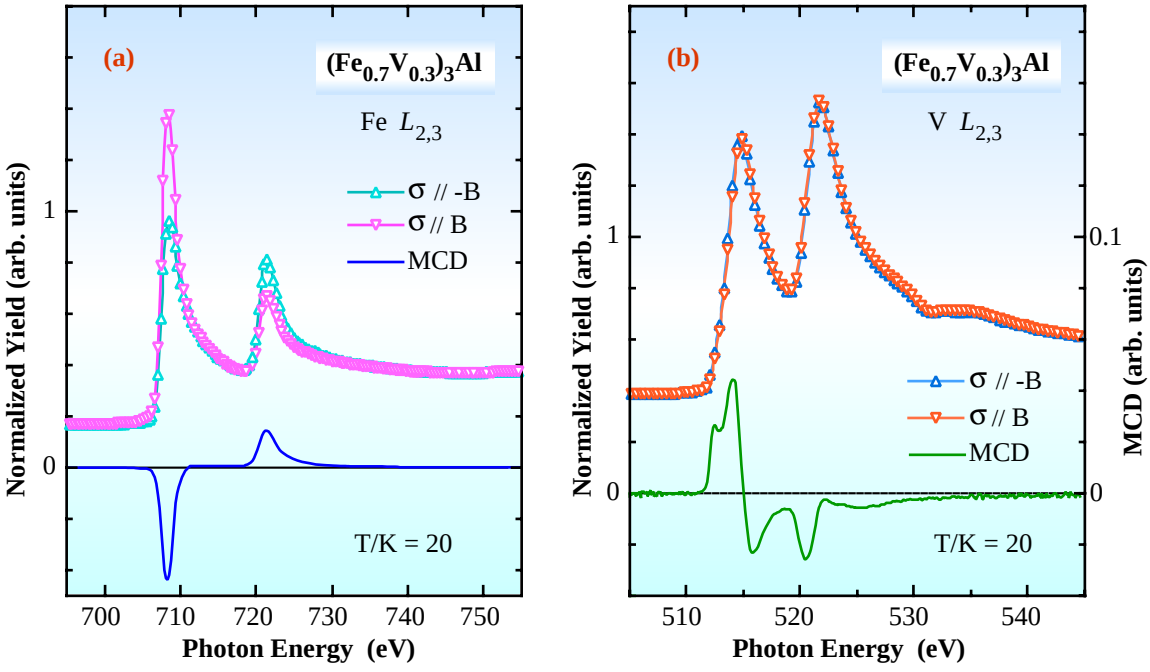

*Fig. 2. Photoabsorption spectra measured with the applied magnetic field **B** antiparallel and parallel to the incident photon spins (curves with up and down triangles), and magnetic circular dichroism spectra (curves without symbols) for **(a)** the Fe $L_{2,3}$ and **(b)** the V $L_{2,3}$ edges of $(Fe_{1-x}V_x)Al$ with x = 0.3.*

spin σ, respectively, and curves without symbols represent the difference between these XAS spectra (*i.e.* MCD spectra). In the figure, these XAS and MCD spectra are normalized so that the spectral increase at each L_3 edge is unity in the XAS spectrum averaged over the direction of ***B***. A large MCD signal is observed for the Fe$L_{2,3}$ edges, while the MCD spectrum for the V$L_{2,3}$ edges has small but complicated structures. It is also noticed that the magnetic moments of Fe and V are antiferromagnetically coupled. According to a crude analysis using the sum rules [4], the orbital part of the magnetic moments is almost quenched for both Fe and V in $(Fe_{1-x}V_x)_3Al$, and the spin component of the Fe moment decreases from 2.2 μ_B at $x = 0$ to 1.5 μ_B at $x = 0.33$. Although it is somewhat difficult to apply the spin sum rule to the V $L_{2,3}$ edges, the spin angular momentum for V is also reduced as the V substitution x is increased. Hence the estimated total magnetic moment decreases with x, as is typically observed in magnetization measurements. For Fe_2VAl, however, the magnetic moment remains fairly large – a third of the moment for Fe_3Al – which seems inconsistent with the magnetization measurement. This is partially a result of the present analysis, without any correction for the sum rule, and might be due to the magnetic cluster formed in the marginally magnetic Fe_2VAl compound.

In conclusion, these new methods have made it possible for us to collect new and complementary information about the electronic and magnetic properties of the fascinating transition-metal compounds such as Fe_2VAl.

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