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# Photoelectron spectroscopy study of Fe-diluted Au–Fe alloys

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## Abstract

The electronic structure of Fe-diluted Au–Fe alloys has been studied by taking core-level and valence-band spectra using x-ray photoemission spectroscopy and synchrotron radiation. From the core-level spectroscopy, we found that the Fe 2p spectrum is composed of  $d^6$  and  $d^7$  multiplets from Fe impurity atoms. This behaviour is qualitatively discussed within the context of electron–electron interaction. In order to explore the electron-correlation effects in the valence band, we obtained Fe 3d partial spectral weights by taking advantage of the Cooper-minimum phenomenon of an Au 5d photoionization cross section. It was found that the spin-down states have an appreciable amount of spectral weights throughout the host Au 5d band, contrary to previous one-electron calculations predicting two-peak structure of the Fe 3d states. We suggest that this discrepancy results from the correlation effect of the Fe 3d electrons.

## 1. Introduction

The Au–Fe alloy system is one of the prototypes of the Kondo effect when the Fe concentration is below 100 ppm, and is also a prototype exhibiting spin glass behaviour due to the RKKY (Ruderman–Kittel–Kasuya–Yosida) interaction which competes with the Kondo effect [1–3]. These phenomena are regarded as a result of the atomic nature of Fe 3d electrons which enables the impurity atoms to have local magnetic moments. For Fe concentrations larger than 25 at.%, Au–Fe alloys are ferromagnetic, but as the Fe concentration is lowered, the averaged magnetization is decreased. At around 12–15 at.% of Fe, a very complex behaviour sets in and this regime smoothly fits into the spin glass behaviour below 12 at.% [4, 5].

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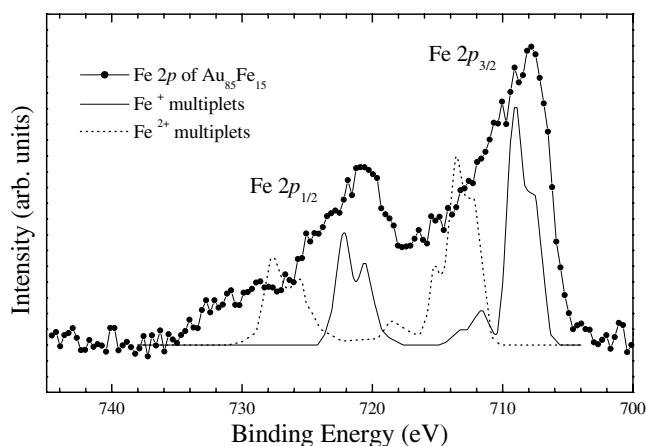
The electronic structure of Au–Fe alloys in the Fe-diluted regime has been studied theoretically to explain the local magnetic moments [6] and the frustrated magnetic moments in the spin glass state [5]. These calculations predicted that the Fe 3d states form two discernible peaks in density of states (DOS) with a small bandwidth of less than 0.05 Ryd. One of these peaks is near or at the top of the host Au 5d band composed of almost fully occupied spin-down states and the other at the Fermi level composed of spin-up states. This atomic nature of Fe 3d states has been widely accepted, but the Fe 3d partial spectral weights of Au<sub>90</sub>Fe<sub>10</sub> obtained from a photoemission (PE) spectroscopy experiment did not confirm it [7]. The detailed structure could not be determined due to low energy resolution, but the experimental result showed that the Fe 3d states have non-negligible weight at the bottom of the Au 5d band, suggesting some strong mixing between Fe 3d and Au 5d bonding states. This is even in contrast to the band calculation of the Fe<sub>1</sub>/Au<sub>1</sub> multilayered system, which is connected to the L1<sub>0</sub> ordered structure [8]. Therefore it can be said that the energy distribution of the Fe partial spectral weights in Fe-diluted Au–Fe alloys is not yet fully understood.

The presence of electron–electron interaction usually causes complex behaviour of excitation spectra when both the initial and final states in the PE process are represented by more than one electronic configuration. The configuration interaction results in unexpected features both in core- and valence-band PE spectra. In the case of transition metal compounds, these phenomena can be explained by introducing charge transfer from ligands to transition metal ions [9] and this explanation can in principle be applied to the transition metal impurity within a pure metal host when the effective electron–electron interaction strength is relatively large. Since the Fe 3d magnetic moment of Au<sub>90</sub>Fe<sub>10</sub> determined by a magnetic susceptibility measurement was 3.68  $\mu_B$  [10], it is expected that due to the atomic nature of Fe 3d states, one may observe  $2p^53d^6$  as well as  $2p^53d^7$  multiplet structures in Fe 2p core-level photoelectron spectra, and as a result, the electron-correlation driven satellite structures in the valence band.

In this paper, we performed x-ray, ultraviolet and soft x-ray photoemission spectroscopies (XPSs) to deduce the Fe 3d partial spectral weights. From the core-level XPS on Au<sub>95</sub>Fe<sub>05</sub> and Au<sub>85</sub>Fe<sub>15</sub>, we found that the Fe 2p core-level spectra have complex lineshapes, which can be decomposed into at least two different electronic configurations,  $2p^53d^7$  and  $2p^53d^6$  multiplets. Then we determined the Fe 3d partial spectral weights of Au<sub>85</sub>Fe<sub>15</sub> from PE spectra with synchrotron radiation with the use of Cooper minimum phenomenon of Au 5d states. It was found that the Fe 3d states have an appreciable amount of spectral weights within the host Au 5d band, and the most plausible explanation for this discrepancy between our result and the one-electron calculations is the electron-correlation effect of Fe 3d states.

## 2. Experimental details

Disordered Au<sub>95</sub>Fe<sub>05</sub> and Au<sub>85</sub>Fe<sub>15</sub> alloys were made by arc melting of 99.99% Au and 99.9% Fe in an atmosphere of argon gas on a water-cooled copper hearth. Both metal wires were melted separately before mixing and then melted together several times to ensure homogeneity. The face-centred-cubic structure was checked with x-ray diffraction and no other phase could be detected within experimental error. Although the miscibility of Fe-diluted alloy is low, it was reported that the metastable solid solutions, as quenched, are quite stable even at an Fe concentration as high as 35 at.% [11]. However, there was a report on the TEM image of Au<sub>85</sub>Fe<sub>15</sub> which revealed formation of precipitate responsible for its magnetic behaviour [12], and we checked the Fe 2p spectrum to see whether there is any contribution from Fe clusters. It is expected that the binding energy of Fe 2p electrons in clusters is very close to that of bulk Fe, but after fitting the data, it was found that the number of Fe atoms attributable to precipitates is at most 3% of total Fe atoms, if any.



**Figure 1.** Fe 2p PE spectrum of  $\text{Au}_{85}\text{Fe}_{15}$  after scraping. The inelastic background of the PE spectrum was removed. Full and dashed curves represent atomic calculations for the  $\text{Fe}^+$  and  $\text{Fe}^{2+}$  multiplets, respectively.

For the core-level XPS experiments, we used unmonochromatized Al  $K\alpha$  lines ( $h\nu = 1486.6$  eV). The photoelectrons were counted by a VSW hemispherical analyser HA150, and the total resolution was 1.0 eV in full width at half maximum (FWHM). The base pressure was  $5 \times 10^{-10}$  Torr.

We also measured the valence-band PE spectra of pure Au and Fe metals and disordered Au–Fe alloys using synchrotron radiation in the photon energy range 60–160 eV. The spectra at this soft-x-ray regime were taken at the beamline 2B1 in a Pohang Light Source (PLS). The total resolution at the Fermi level was less than 0.3 eV FWHM. The spectra were measured with a VG CLAM2 analyser with three channeltron detectors. All measurements were performed under a pressure of low  $10^{-10}$  Torr.

To remove contaminations, sample surfaces were either scraped using a diamond file or sputtered with  $\text{Ar}^+$  ions at 1.5 keV for about 20 min. We observed a preferential sputtering effect which removes more Fe atoms from the surface, but the relative intensities between Fe 2p and Au 4f lines after 20 min sputtering and after scraping did not differ by more than 10%.

### 3. Data and results

#### 3.1. Fe 2p core-level spectrum of $\text{Au}_{85}\text{Fe}_{15}$

Figure 1 shows the Fe 2p PE spectrum of  $\text{Au}_{85}\text{Fe}_{15}$  after scraping. The inelastic background of the PE spectrum was removed by assuming step-function type electron energy loss. The lineshape was the same for both scraped and sputtered samples, and the difference was the relative intensity of the Fe 2p PE line to Au 4f.

The highest binding peak of Fe  $2p_{1/2}$  at around 730 eV is  $2p^53d^6$  ( $\text{Fe}^{2+}$ ) multiplets, the detailed structure of which cannot be seen, probably due to a shorter lifetime than  $2p^53d^7$  ( $\text{Fe}^+$ ) multiplets at  $E_B = 720.5$  eV. The  $2p^53d^6$  multiplets of  $2p_{3/2}$  states appear only as a shoulder of the PE line, whose main peak at 708 eV is composed of  $2p^53d^7$  multiplets.

The calculated  $\text{Fe}^+$  and  $\text{Fe}^{2+}$  multiplets are also shown schematically in figure 1 [13]. The relative positions of  $\text{Fe}^+$  and  $\text{Fe}^{2+}$  multiplets are determined to give good agreement with the experimental spectrum when the multiplets are broadened. The position of the  $\text{Fe}^{2+}$

multiplets of  $2p_{1/2}$  states does not agree with the spectra because the  $2p_{1/2}$  photoelectrons are usually affected by the strong interference effect between the threshold Coster–Kronig decay and the valence electron rearrangement after the  $2p$  core hole creation [14]. Within the context of the charge-transfer model [9], the reason  $\text{Fe}^{2+}$  multiplets have higher binding energy than  $\text{Fe}^+$  multiplets by more than 4 eV, is essentially the screened on-site Coulomb interaction, which is related to the  $d$ – $d$  correlation energy [15]. We did not perform parameter-fitting of the Fe  $2p$  core-level spectra of alloys with the charge-transfer model, but the agreement of the rough structure has generally been found in many cases, including metal overlayers [16, 17].

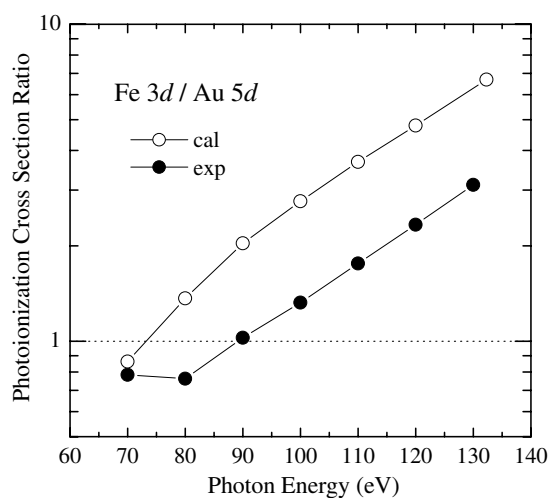
Finally, it should be mentioned that the lineshape is quite different from Fe oxides. The binding energy of Fe  $2p$  peaks of  $\text{Fe}_2\text{O}_3$  is almost 2 eV higher than the presented spectrum, and the Fe  $2p$  PE line of FeO does not have asymmetric lineshape [18]. The tail on the higher binding energy side of a peak is characteristic of a metallic phase [19], even when the atoms under consideration are impurity, and the Fe  $2p$  peaks in the spectrum are definitely from the metallic phase.

### 3.2. Determination of partial spectral weights

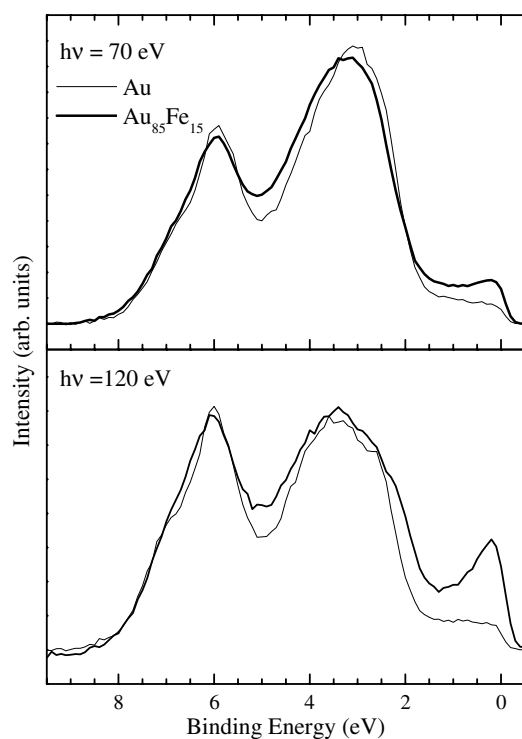
**3.2.1. Photoionization cross section.** In order to deduce the partial DOS of two constituents, we make use of the differences of alloy PES spectra due to the relative photoionization cross section change with photon energy. Therefore it is necessary to find the cross-section ratios between Fe  $3d$  and Au  $5d$  states accurately. The calculated atomic cross sections [20] are usually different from the values of bulk because of the solid-state effect, especially near the photon energies where the Cooper-minimum phenomena occur [21]. Hence we determined the cross-section ratios at  $h\nu = 70$ – $130$  eV experimentally. This was accomplished by using the intensity ratio of Fe  $3p$  and Au  $4f$  core-level peaks, which have comparable binding energies, as a reference. This is based on the fact that the intensity ratios of valence-band PE spectra taken at different photon energies are related to their cross-section ratios. To fix the proportionality constant, the intensity ratios of core levels and valence bands were measured under the same conditions. This procedure assumes that the calculated atomic cross-section values for core levels remain valid in solids, which can be justified since the core-level wavefunctions are not much changed in a solid from those in atoms.

The experimental result for the values of the cross-section ratios between Fe  $3d$  and Au  $5d$  states in the photon energy range of  $h\nu = 70$ – $130$  eV are shown in figure 2. The experimental values are lower than the atomic calculation as in the previous works on Cu–Au, Ni–Pt and Cu–Pt systems [22, 23]. The experimental values have monotonically increasing behaviour above 80 eV, and within the limit of good statistics and reasonable resolution, we chose to use low photon energy 70 eV and high photon energy of 120 eV to determine the partial spectral weights of  $\text{Au}_{85}\text{Fe}_{15}$  alloy.

**3.2.2. Partial spectral weights.** Figure 3 shows the spectra of pure Au and  $\text{Au}_{85}\text{Fe}_{15}$  at 70 and 120 eV. As can be expected from the values of the cross-section ratio, a peak at the Fermi level, which is composed of Fe  $3d$  spin-up states, is enhanced with  $h\nu = 120$  eV. The change of Au partial DOS can be seen in the spectra with 70 eV; the overall structure is smoothed and the broad feature at  $E_B = 2$ – $4$  eV is shifted to have higher binding energy. In the spectra with 120 eV, there is a structure at about 2 eV in addition to these features, and we can conclude that these photoelectrons are from Fe  $3d$  states. However, as mentioned before, this structure is too small to be interpreted as a peak composed of most of the Fe  $3d$  spin-down states, and it is necessary to extract the partial DOS from the spectra.

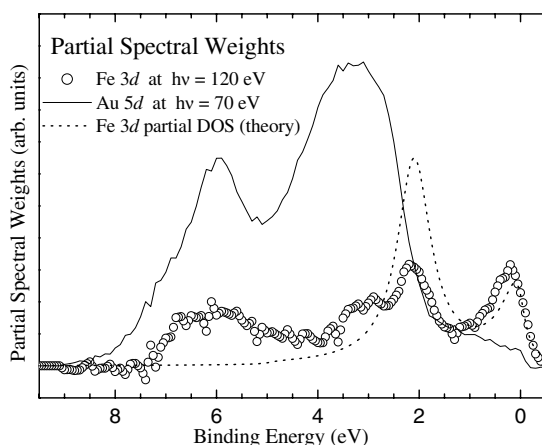


**Figure 2.** Photoionization cross-section ratios between Fe 3d and Au 5d states in the photon energy range of 70–130 eV. The values of the atomic calculation are from [20].



**Figure 3.** PE spectra of Au<sub>85</sub>Fe<sub>15</sub> and pure Au taken with  $h\nu = 70$  and 120 eV. Note the spectral increase at the Fermi level with  $h\nu = 120$  eV.

The procedure for extracting the partial spectral weights of binary alloy systems used in this work was discussed in detail in [24]. In this procedure, a PE spectrum is represented as the sum of contributions from different species of atomic sites weighted by their photoionization



**Figure 4.** Fe 3d and Au 5d partial spectral weights of  $\text{Au}_{85}\text{Fe}_{15}$ . A model Fe 3d partial DOS is also shown to emphasize the difference between the calculation in [6] and the excitation spectrum. The calculated peak position of the spin-down states is shifted to be aligned with the experimentally observed one.

matrix elements, which are dependent both on photon energy and binding energy. Because of the variation of matrix element with binding energy, the PE spectrum or the components from different species are not exactly equal to the total or the partial DOS of an alloy system. Therefore, for a comparison with calculated partial DOS, it is necessary to include the matrix elements correctly in extracting the partial spectral weights from the measured PE spectra. If we can determine the matrix elements of the constituents or at least the ratio of the matrix elements between different photon energies, then it is possible to extract the partial spectral weights. Here, we represent the change in matrix elements at two different photon energies as the ratio of the spectra of pure Au and Fe. It turned out that the Fe spectra at the two photon energies, 70 and 120 eV, do not differ much, and there was a negligible matrix element effect, at least between 70 and 120 eV. However, the Au spectra differ a lot, especially in their relative intensities between  $5d_{3/2}$  and  $5d_{5/2}$  states.

Since the experimental value of the cross-section ratio of the Fe 3d to the Au 5d state is 0.78 at  $h\nu = 70$  eV, we can regard the PE spectrum at that photon energy as the Au partial spectral weight, as a first approximation. The spectral ratio required for transforming the Au partial spectral weight at 70 eV into the one at 120 eV is the spectrum of pure Au at  $h\nu = 120$  eV divided by the spectrum at  $h\nu = 70$  eV. Using the measured cross-section ratio and the divided spectrum representing the change in the matrix elements of pure Au between different photon energies, the Fe partial spectral weight at  $h\nu = 120$  eV can be obtained. With this approximate Fe partial spectral weight, a better Au partial spectral weight at  $h\nu = 70$  eV can be determined by a similar method, and the process is iterated until we obtain self-consistent results. In this procedure, we neglect the possible wavevector  $k$  dependence of the matrix element.

The results of the analysis are shown in figure 4. The Au partial spectral weight is similar to the pure Au spectrum except that the  $5d_{5/2}$  structure shifts to the higher binding energy side. This can be understood as a result of band narrowing when the Au concentration is decreased. However, the Fe partial spectral weight is much different from the one-electron calculation results. They predict that most of the Fe 3d states have a binding energy of less than 2 eV, and that even spin-down states are not mixed strongly with the host 5d band. In figure 4, our result shows that the Fe partial spectral weight extends to the bottom of the Au 5d band. Possible

reasons for this discrepancy between one-electron calculations and our result are discussed in the following section.

#### 4. Discussions

The Fe 3d partial spectral weight we deduced is very different from the one-electron calculations [5, 6]. The calculation result of [6] is shown in figure 4 for comparison. We shifted the calculated peak position of spin-down states so as to align it with the experimentally observed peak, because the position of Au 5d band was not predicted correctly in [5] and [6]. In figure 4, only filled states are shown after broadening with the same width at the Fermi level as the spectra. All the calculated results of Fe 3d partial DOS, and both the impurity and the disordered-alloy case up to 25 at.% of Fe, predict a two-peak structure for the Fe 3d states, even when there is overlap between Fe 3d and Au 5d DOS. This nearly atomic DOS is predictable since Fe impurity atoms are embedded in a host Au metal whose inter-atomic distance of 2.88 Å is 16% larger than that of Fe atoms in bulk Fe. Although there must be lattice contraction around Fe atoms due to different atomic sizes, there have been no reports about a huge change in the partial DOS of impurity atoms whose atomic size is smaller than that of host atoms when lattice relaxation effect is taken into consideration.

Actually, there was a report showing strong mixing between Fe 3d spin-down states and Au 5d states [25]. The calculated DOS of Au<sub>75</sub>Fe<sub>25</sub> and that of Au<sub>90</sub>Fe<sub>10</sub> were reported to have almost the same structure, and only the results for Au<sub>75</sub>Fe<sub>25</sub> were shown. The calculated Fe 3d states of the paramagnetic phase had two well-separated peaks and the higher binding one is in resonance with the top of the Au 5d<sub>5/2</sub> states. For the ferromagnetic phase, calculation showed strong mixing of Fe 3d spin-down states with Au 5d. However, the position of the Fermi level is not in agreement with our result and we suspect the band structure of Au<sub>90</sub>Fe<sub>10</sub> is quite different from that of Au<sub>75</sub>Fe<sub>25</sub>, contrary to the authors' description.

The result in figure 4 is, of course, not an artifact. If it were, then a peak, or at least a big hump should have been observed in any of the spectra we took. As we have already compared the spectra with a model Fe 3d DOS, there cannot be such a big structure related to the spin-down Fe 3d states. Since we used experimentally determined values of the cross-section ratio, this may induce some error in analysis. If the cross section of Fe 3d states at  $h\nu = 120$  eV is overestimated, then the experimentally deduced Fe partial spectral weight will erroneously include part of the Au partial spectral weights, and as a result, the contribution of Fe 3d spin-down states to the partial spectral weights can be overestimated. In order to check this possibility, we compared the number of Fe 3d spin-down and spin-up electrons. We assumed that all the spectral weights with binding energy lower than 1.5 eV are those from spin-up Fe 3d electrons, and higher than 1.5 eV from spin-down states which is fully occupied. With this assumption, it was found that the spin-up states contribute 27% to the Fe 3d partial spectral weights. If we further assume that all magnetic moments are from spin moments, then this result corresponds to the magnetic moment value of  $3.2 \mu_B$ , which is lower than the experimental value of  $3.68 \mu_B$  [10] and the calculated value of  $3.4 \mu_B$  [6]. This implies that the number of spin-down states is rather underestimated in our analysis, and it can be concluded that the Fe partial spectral weights within the host d band is not an artifact.

The most probable explanation for this discrepancy between experiment and the one-electron theory seems to be the many-body effect. It is well known that when the magnitude of the on-site d–d Coulomb interaction is comparable to the width of the partial band, the incoherent part of the spectral weight can be observed as in pure Ni metal [26]. Since the one-electron theory predicts a linewidth of no more than 0.05 Ryd for the Fe 3d spin-down and spin-up states, the incoherent part may be present in PE spectra. For Au–Ni alloys, a study



using resonant photoemission spectroscopy (RESPES) confirmed the existence of the two-hole satellites within the Au host d band [27], which had been predicted on the grounds that the difference spectra between alloy and pure Au spectra has a peak which follows a similar photon energy dependence of the relative intensity [28].

Although two-hole satellites in transition metals left to Ni had not been expected much, a recent RESPES experiment on Cr and Fe reported the observation of a signal that is equivalent to the 6 eV satellite in Ni [29]. This structure should be more pronounced in Fe-diluted Au–Fe alloys due to its narrow Fe 3d partial band. A similar effect was observed in a surface alloy  $c(2 \times 2)$  CuMn/Cu(100) [30], in which distinct satellite structures both in the valence band and in the core level are clearly visible. This was interpreted as being a result of reduced dimensionality which decreases the partial bandwidth of Mn 3d states. Considering these previous reports, it is highly expected that a distinct satellite structure of Fe 3d states appears in PE spectra of Fe-diluted Au–Fe alloys, and broad Fe 3d partial spectral weights that we observed within the host band seem to be the electron-correlation driven satellite structure.

The best way to check the existence of a satellite structure is definitely a RESPES measurement, but due to the low partial intensity of Fe 3d states at lower photon energy and to the broad feature of the satellite structure, it was almost impossible to use Fe 3p resonance for this purpose.

## 5. Conclusion

In this work, we studied the electronic structure of Fe-diluted Au–Fe alloys by taking valence-band and core-level spectra using various PE spectroscopies. The Fe 2p spectrum was found to be composed of  $d^6$  and  $d^7$  multiplets from Fe atoms and the existence of the satellite is qualitatively discussed within the context of electron–electron interaction. In order to explore the electron-correlation effects in the valence band, we obtained Fe 3d partial spectral weights by taking advantage of the Cooper-minimum phenomenon of Au 5d photoionization cross section. It was found that the spin-down spectral weight has a very broad energy distribution throughout the host Au 5d band, contrary to the previous one-electron calculations predicting a two-peak structure of the Fe 3d states. We suggested that this discrepancy results from the correlation effect of the Fe 3d electrons.

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