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Investigation of thickness dependence on electronic structures of iron and nickel thin films by L-edge X-ray absorption spectroscopy

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ABSTRACT

We have studied the effect of the film thickness on the electronic structure of pure nickel and iron thin films. Series of the thin films were evaporated by e-beam evaporation on SiN substrates. The electronic structure of the thin films was investigated using X-ray absorption near edge structure (XANES) spectroscopy. We have showed the thickness dependent variation of the experimental branching ratio (BR) and full-width at half-maximum (FWHM) at the L_3 and L_2 edges for both thin films. A strong thickness dependence of the $L_{2,3}$ BR and FWHM was found. We have also focused on the deviation of L_3 to L_2 ratio from its statistical value. The average L_3/L_2 white-line intensity ratio was calculated to be 3.4 and 3.0 from peak height and integrated area under each L_3 and L_2 peaks, respectively for iron. Additionally, a theoretical $L_{2,3}$ edge calculation for nickel was presented. The obtained results were consistent with the general view of the $L_{2,3}$ BR and FWHM of iron and nickel transition metals.

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1. Introduction

The X-ray absorption near edge structure (XANES) has proved to be a powerful technique to study thin film materials because of its chemical and elemental sensitivity and the possibility to derive ground state properties of a material. It corresponds to the electronic transition from a core level to an unoccupied or hybridized orbital and mainly reflects the unoccupied electronic states [1–3]. In an X-ray absorption process, a primary core level electron is stimulated by X-ray photon and moved into an excited state with a core hole leaving behind. The system can relax via filling of the core hole by an electron from an upper energy level. This process results in either the radiationless emission of an Auger electron or in the emission of a fluorescence photon.

For 3*d* transition metals (TM), $L_{2,3}$ edges of the XANES are characterized generally by two peaks, called as "white-lines". These absorption lines indicate from the excitations of 2*p* core electrons to unoccupied *d* states. Unique information can be obtained by exciting the 2*p* electrons into the unoccupied 3*d* valence orbitals or into the continuum. The intensity of the white-lines denotes the unoccupied 3*d* density of state (DOS) and the *d* states occupations of 3*d* transition metals which have been studied systematically in the literature [4–9]. Due to the dipole allowed transition (2*p*-3*d*), *L* edge absorption spectrum has several advantages compared to *K* edge spectrum of TM elements and compounds. L_2 and L_3 edges of 3*d* transition elements are dominated by the large Coulomb interaction between the 2*p* core hole and 3*d* electrons.

In the case of *K* edge of transition metals (1*s*-3*d*), the pre-edge peak is mainly due to dipole–forbidden transition from a core electron to 3*d* and leading to a weak signal in absorption spectrum [10]. In the last several years, renewed interest in X-ray absorption spectroscopy (XAS) has demanded a better understanding of the total electron yield (TEY) measurements of 3*d* transition metals [3,6,7,11,12]. Especially, thin film structures which contain iron and nickel layers have received particular attention owing to their technological importance, herein, it is crucial to determine their electronic structure depending on increasing the film thickness [13–15].

Branching ratio (BR) at the L_2 and L_3 edges is one of the important parameters for transition metals [16–22]. BR gives us useful information on the electronic structure of 3*d* metal that relates to chemical bonding and characteristics [23]. The BR is strongly influenced by electrostatic interaction (between *d* electron and valence hole) and spin-orbit splitting. In particular, the BR can be used as identification the spin state of 3d transition metals [17].

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But, experimentally obtained $L_{2,3}$ BR is normally not enough to give unambiguous information about the valence band spin-orbit splitting, the electrostatic interactions between core-hole and valence-electron, or the spin state. The BR is ranged from 0.63 to 0.70, with an average of 0.67 for low spin state and ranged from 0.71 to 0.76 with an average of 0.74 for high spin state [18]. Although many experiment has been performed to determine the $L_{2,3}$ branching ratio but, it is not completely trivial to obtain experimental values for this parameter [24–31]. Our aim in this work is to accurately determine thickness dependence of the iron and nickel $L_{2,3}$ branching ratio intensity and full-width at half-maximum (FWHM) change in L_2 and L_3 region. We hope that obtained results can be one of the key requirements for the development of TM based applications.

2. Experimental methods

The experiments were performed on beamlines 8.2 and 10.1 of the Stanford Synchrotron Radiation Lightsource (Menlo Park, CA-USA). The beamline 8.2 is a bending-magnet beamline dedicated to photoemission, photoabsorption spectroscopy, and XANES experiments within an energy range of 100–1300 eV. The beamline 10.1 is a wiggler-magnet beamline and primarily used for X-ray absorption and photoemission spectroscopies within an energy range of 250–1200 eV. The *L* edge spectra of iron and nickel thin films were measured in TEY mode. The TEY signal in 3*d* transition metals is generated by secondary electrons following X-ray photon absorption. The TEY spectra were collected at room temperature. The films were grown by e-beam evaporation on SiN coated Si wafers. The thicknesses of the nickel and iron layers were varied from 12 Å to 120 Å and from 3 Å to 112 Å respectively. The base pressure of the chamber was 1×10^{-10} Torr and below 1×10^{-9} Torr during the evaporation. The X-ray incidence angle was controlled by a rotatable manipulator with an accuracy of about 0.5°. The film thicknesses were determined by monitoring the growth rate with a quartz crystal thin film monitor (Inficon). The substrates were mounted on an aluminum sample holders through a thin copper wire connected. To eliminate the effect of the substrate from the absorption spectrum, we measured the photo-absorption of the clean SiN substrate itself immediately prior to the film deposition. In order to record the TEY spectra, the TEY signal was monitored by the sample drain current. This was simply done by measuring the current from a copper wire connected to the sample holder, which has been electrically isolated from the chamber. Simultaneously, the incident photon flux I_0 was determined by an 80% transmissive Au net. To avoid synchrotron dependent intensity, all TEY signals were normalized to I_0. The currents were recorded with a Keithley 427 current amplifier.

Theoretical XANES amplitude for nickel $L_{2,3}$ edges was obtained by FEFF8 simulation. The FEFF8 program that is a self-consistent real space multiple-scattering code for simultaneous calculations of X-ray absorption spectra including polarization dependence, core hole effects and local field corrections was used to calculate L_3 and L_2 edges. Calculations are based on all electron real space relativistic Green's function formalism with no symmetry requirements [32].

3. Results and discussion

Fig. 1 demonstrates the evolution of the nickel $L_{2,3}$ absorption edges with varying thickness from 12 Å to 120 Å in TEY mode. In each spectrum, the TEY signal before the onset of the L_3 edge at 845 eV was set to zero, and the L_3 intensity of the thickest nickel film was normalized to one. The main features in the spectrum are two maxima at 852.6 eV and 870.2 eV corresponding to the edges of

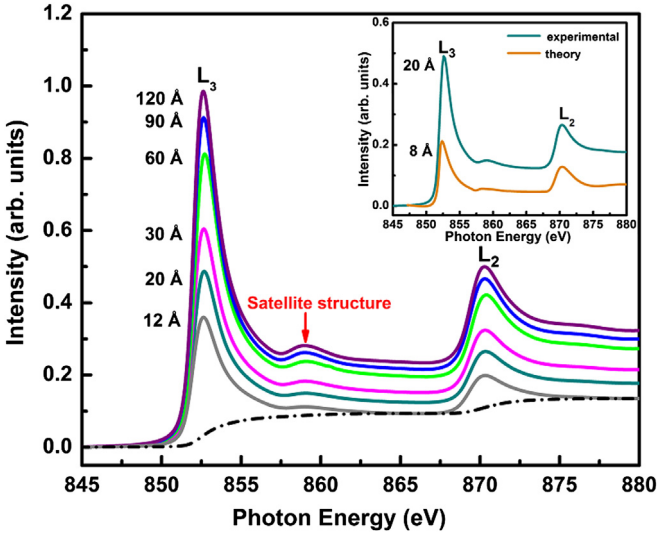

Fig. 1. Normalized total electron yield (TEY) spectra of nickel films with different film thicknesses. In each spectrum, the TEY signal before the onset of the L_3 edge at 845 eV was set to zero. The inset shows theoretical calculation for the nickel thin film with the thickness of 8 Å. The black dashed line demonstrates the two step-like functions for background subtraction of nickel film with 12 Å.

L_3 and L_2, respectively. The L_3 and L_2 lines correspond to transitions into nickel 3*d* states that produce $2p_{3/2}$ and $2p_{1/2}$ core holes. Thus, these two peaks can be explained by the electrostatic interaction between core-hole and valence electrons and the initial state spin-orbit splitting. The energy separation of the two peaks is 17.6 eV due to the spin-orbit interaction of the nickel 2*p* core level. We can also indicate that the each peak intensity is proportional the unoccupied states in *d* band.

From Fig. 1, we can determine the white-line intensity ratio (L_3/L_2) by measuring integrated areas under each corresponding peak. Generally, the L_3 and L_2 edges XANES spectra include excitations arising from the 2*p*-3*d* transitions with contribution from the 2*p* state to continuum states. To calculate L_3 to L_2 ratio from a precise estimation of the peak areas, it is necessary to subtract a background component from the excitation spectra to eliminate the transitions into continuum states. Two step-like functions aligned at the maxima of the L_3 and L_2 edges with relative heights of 2:1 (the expected intensity ratio for transitions into the L_3 and L_2 edges) was used for the background subtraction of the XANES spectra. Same method of background subtraction was used in the literature by Dhesi et al. [12] for nickel films on Co/Cu (001) and by Chen et al. [33] for Fe and Co thin films. The two step-like function used for the nickel thin film of 12 Å is shown in Fig. 1. The boundary between the integrated areas of the L_3 and L_2 sum spectra was at the just below the onset of the L_2 edge, namely 868 eV. Additionally, a theoretical calculation for the nickel film with the thickness of 8 Å is also shown in the inset of Fig. 1 for the purpose of comparison between experiment and theory. From the inset of Fig. 1, the intensity trend with increasing film thickness confirms our theoretical calculation to be in good agreement with the experimental spectra.

Fig. 2 represents the normalized and background subtracted TEY spectra of the nickel thin films with varying thicknesses. It is clear from Fig. 2 that the intensity originated from the $2p_{3/2}$ to 3*d* transition return to zero between the L_3 and L_2 edges. Therefore, there is a certainty in the choice of background which can effects the white-line intensity ratio. After the background subtraction, we calculated the white-line intensity ratio (L_3/L_2) for each nickel thin films. The obtained average value of L_3/L_2 ratio is 3.2 which is consistent with the literature [25,27]. In fact, our previous results of total yield

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