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X-RAY ABSORPTION FINE STRUCTURE ABOVE THE Ti L-EDGE*

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ABSTRACT

We report the first measurement of an EXAFS signal from an L-edge in the intermediate energy range 200-1000 eV, obtained using synchrotron radiation and by the use of a specially-designed multi-element detector system. Observations of the near-edge absorption fine structure show the hole-state spin-orbit splitting and give clear evidence that the Ti L-edge exhibits a "white line". In addition, pronounced oscillations were observed in the absorption spectrum, extending at least 350 eV above the edge. Three peaks were observed in the Fourier transform signal, corresponding to first, second, and fourth neighbor distances. Derived phase shifts were consistent with a predominant (~80%) d-wave character in the continuum final state.

I. INTRODUCTION

Recent applications of extended x-ray absorption fine structure (EXAFS) spectroscopy to a wide variety of structural problems have proved it a technique capable of providing unique structural information. The availability of an intense, highly-collimated, variable-energy x-ray photon source at the Stanford Synchrotron Radiation Laboratory (SSRL) has played a major role in the recent revival of interest in EXAFS. Until now, however, EXAFS studies by absorption have been largely restricted to photon energies above 3-4 keV; thus to elements with $Z \geq 20$. Because this excludes the (chemically most interesting) first- and second-row elements, it is important to extend the EXAFS method to lower energies. In this paper we report an absorption study on the $L_{II,III}$ edge of metallic titanium foil. To our knowledge this is the first instance in which EXAFS has been observed by photon absorption and analyzed in detail in this energy range.

Absorption measurements in the soft x-ray region between the carbon K-edge (~ 280 eV) and about 1500 eV pose several problems, and only very few absorption investigations have been reported for this energy range.¹⁻⁶ The main experimental difficulties arise from contamination of the optical elements (mirrors and grating) resulting in low photon fluxes and a high scattered light background.⁴ Another factor which is particularly important for EXAFS studies is the close proximity of absorption edges (carbon at 284 eV, nitrogen at 399 eV, and

oxygen at 532 eV) in the soft x-ray range. The short x-ray absorption lengths⁷ in this region furthermore require that such experiments be carried out in vacuum and necessitate thin film ($\sim 2000\text{\AA}$) samples.

In contrast to absorption from K-edges, there are actually three L excitations, which can leave a $2s_{1/2}$, $2p_{1/2}$, or $2p_{3/2}$ hole. These are usually labeled the L_I , L_{II} , and L_{III} -edges, respectively. This multiplicity can cause serious interference unless one of the following three criteria is satisfied:

- 1) the spin-orbit splitting is small compared to the period of the EXAFS oscillations;
- 2) the energy separation between edges is larger than the energy range needed to interpret EXAFS (several hundred eV); or
- 3) the successive edges are too weak to interfere.

For high Z elements ($Z \geq 50$)⁸ the second criterion is fulfilled, and L-edge spectra for the high Z elements Au,⁹ Pt,¹⁰ W and Ta¹¹ have been reported and analyzed. Assuming a value of 10 eV for a typical EXAFS oscillation period the first criterion can be satisfied for $Z \leq 25$ (Mn).⁸ Measurements on such low-Z-element L-edges have been performed mainly by the DESY group.¹² Unfortunately these experiments only extend to about 100 eV above the $L_{II,III}$ -edge and are therefore not well suited for an analysis of the EXAFS structure.¹³ Titanium ($Z = 22$) is an intermediate Z element with a L_{III} - L_{II} spin-orbit splitting of 6 eV

and a L_{III} - L_I separation of 109 eV.⁸ While the spin-orbit splitting appears small enough not to disturb the EXAFS oscillations, the L_I edge is a priori more problematical. From the systematics of L-edge jump ratios⁷ and L-edge spectra of the light metals Na, Mg, and Al¹² the L_I -edge jump is expected to be less than 20% of the L_{III} jump. We will show below that the L_I jump in Ti is indeed a weak, broad structure which can be removed by a suitable background subtraction procedure.

II. EXPERIMENTAL

The experiments were performed on the 4° port of Beam Line I at the Stanford Synchrotron Radiation Laboratory (SSRL). The grazing incidence "grasshopper" monochromator has been described elsewhere.¹⁴ Before the present measurements were made, new optical elements were installed to minimize the carbon build-up on the optical surfaces, which occurs on exposure to high fluxes of synchrotron radiation.¹⁵ Measurements of the monochromator transmission indicated the presence of monochromatic radiation up to a least 1400 eV. At the time of these measurements the bandpass of the monochromator was $\sim 0.2\text{\AA}$, corresponding to ~ 3 eV resolution of the Ti L-edge (455 eV).

The experimental apparatus used for our measurements is shown schematically in Fig. 1. A collimator served to reduce any background signal arising from stray light. Provisions were also made to insert a filter which was needed in some cases to suppress higher-order radiation, although the measurements reported here were performed without a filter. To avoid errors

caused by long-term beam intensity fluctuations as well as by any possible irreproducibility in the monochromator setting, measurements on the sample were alternated with measurements on a reference blank. The experimental procedure consisted of setting the monochromator, counting for 4 seconds with the sample in place, counting for 4 seconds on the blank, re-setting the monochromator, etc. A motor and cam raised and lowered the sample on the command of a microprocessor which also directed the monochromator settings. The raw sample and blank spectra were thus recorded, and a normalized spectrum (sample/blank) was calculated as the run progressed.

A somewhat novel multicathode detection system was employed for this work.¹⁶ A series of plates of different materials, including gold and an evaporated film of ZnS, were arranged so that any plate could intercept the transmitted beam. Each plate could thus be selected to serve as the cathode of a high current "channeltron" electron multiplier which amplified (at $\sim 10^6$ gain) the photoelectric yield from the respective cathode. In addition to yielding highly satisfactory signal levels, this arrangement allowed a ready choice of a cathode material that had a high sensitivity in a given energy range, and that would strongly discriminate against second-order light. For example, because the photoyield is known to mimic the absorption coefficient,¹⁷ one can estimate on the basis of cross-section calculations⁷ that a gold photoyield cathode is roughly three times more sensitive to the primary beam at the titanium-edge energy than to second-order light.

III. RESULTS AND DISCUSSION

The experimental transmission intensity through a free-standing $75 \mu\text{g}(\text{cm})^{-2}$ thick Ti metal foil is shown in Fig. 2. The spectrum was collected in one hour using a Au cathode detector. We have plotted $\mu x = \ln(I_0/I)$, where I_0 is the incident and I the transmitted intensity, as a function of photon energy in the range 435-800 eV. The absorption coefficients exhibit a pronounced peak just above the threshold, which at closer inspection is split into a doublet. The inflection point of the edge falls at 454 ± 1 eV while the two peaks lie at 457 ± 1 eV and 461 ± 1 eV. Above the threshold peak, pronounced fine structure oscillations are apparent which appear to extend beyond the 800 eV cutoff of the present measurements. No obvious sharp structure is observed at the expected L_I threshold indicated by an arrow in Fig. 2. The following discussion deals successively with the $L_{II,III}$ threshold structure, the effect of the L_I edge, and then treats the EXAFS structure in detail.

There has been considerable discussion recently of the "white line" structure which is observed for many materials near threshold. This term is derived from the x-ray literature, in which a strong absorption immediately above an x-ray edge appeared as a white line in the photographic emulsion used as a detector. It has been studied in detail by Stern and co-workers for platinum¹⁰ and the anisotropic materials TaS_2 and WSe_2 .¹¹ Comparing the value of μx obtained for Ti immediately above threshold with calculated atomic cross sections⁷ shows that Ti does show

a "white line", contrary to previous measurements.¹⁸ The enhancement can be understood in terms of a high density of empty d-derived states immediately above the Fermi level.¹⁹

The splitting of the "white line" initial peak is readily attributed to spin-orbit splitting in the $2p_{3/2}$ - $2p_{1/2}$ hole states. Two observations support this interpretation. First, the splitting of $\sim 4 \pm 1$ eV agrees fairly well with the value of 6.1 ± 0.1 eV obtained from photoemission data.²⁰ Second, existing band-structure calculations give no indication of such a large splitting in the conduction-band density of states above the Fermi energy. The observed splitting, while not very well resolved, was reproducible and convincing. We note that this fair agreement of the observed energy splitting with the photoemission values is all that can be expected in such a comparison, because hole states near absorption edges are strongly perturbed by the conduction electrons. Thus we believe that interaction with the conduction band distorts, but does not create, the splitting of the "white line" peak.

Starting ~ 109 eV above the L_{III} edge an additional absorption, associated with a $2s_{1/2}$ core hole (the L_I edge), is expected. While no sharp onset is observed, there is a broad increase in the total absorption. This is consistent with observations on the L edges of the light metals Na, Mg, and Al.¹² The L_I contribution to the absorption served to complicate the background associated with the Ti EXAFS, but it was nonetheless satisfactorily accounted for by fitting the absorption tail to

a (low-order) polynomial spline function.

It is worth noting at this point that background subtraction in an EXAFS spectrum must be done carefully, and there appears to be no completely rigorous, unique way to do it. We were very hesitant at first to make a background correction and particularly to correct for the L_I -edge, for fear of biasing the results of our analysis. It turned out, however, that the main features in the results were insensitive to the details of this correction provided that a "stiff", or low-order polynomial, spline function was used. The final choice of background could be made by demanding that the spurious low frequency signal be minimized. This insensitivity is aided by the relatively low 2s photoelectric cross section.

The spectra well above the absorption edge, together with the smooth background for the $L_{II,III}$ -edge, plus the L_I edge structure, can be seen in Fig. 3 as the top and middle curves, respectively. In addition to the sharp initial peak and the gradual decrease in absorption strength, fine structure (EXAFS) oscillations are apparent that can be described by the formula⁹

$$\frac{\mu - \mu_0}{\mu_0} = \chi(k) = \frac{1}{k} \sum_j \frac{N_j}{R_j^2} |f(\pi)| \sin(2kR_j + \phi(k)) \exp(-2\sigma_j^2 k^2 - 2R_j/\lambda(k)) \quad (1)$$

where μ is the total absorption coefficient and μ_0 is that portion due to the slowly-varying background. The electron wave-vector is given by

$$k = 0.5123 (\hbar\omega - E_0 + E_i)^{1/2} \text{ \AA}^{-1}, \quad (2)$$

with energies expressed in eV, where E_0 is the onset of absorption and the inner potential E_i sets the zero of electron kinetic energy. We chose $E_i = 8$ eV here so that $k = 0$ coincides with the bottom of the valence band as determined by photoemission.²¹ The sum is taken over shells of j^{th} neighbor atoms consisting of N_j atoms at a distance R_j from a central atom. The backscattering strength is $|f(\pi)|$, and ϕ is the total energy-dependent phase shift that an electron experiences upon returning to the central site after backscattering. Thermal oscillations from the equilibrium lattice positions are described by σ , and λ is the mean electron attenuation length.

The remaining EXAFS signal, $\chi(E)$, is shown in Fig. 3c (lower curve), and the modulus of the Fourier transform of $k^2\chi(k)$ is given in Fig. 4. In real space the spectrum shows a sharp and symmetric peak at $R = 2.672\text{\AA}$, followed by much smaller peaks at approximately 3.9 and 4.8\AA. These secondary peaks were not easily separated from the background, however. The primary peak is readily assigned to the first shell of neighbors in the titanium hcp lattice. Because titanium departs from the ideal hcp structure ($c/a = 1.588$), the first shell is actually composed of a close doublet (unresolved in our data); six atoms lie in the hcp plane at $R_j = 2.95\text{\AA}$ and six out-of-plane neighbors lie at $R_j = 2.90\text{\AA}$ (Table I). Because the spectrum is clearly dominated by the first shell, the essential phase shift

information can be obtained from a fit of the spectrum to this shell. We estimated from the Debye formula²² $(\sigma^2)^{1/2} = 0.0534\text{\AA}$. Using a fit to the universal curve²³ for the electron mean free path,

$$\lambda(y) = 43.19 - 22.745y - 5.8044y^2 + 3.6208y^3 \quad (3)$$

where y is the $\log_{10}$ of the electron kinetic energy, measured from the Fermi level, and the form²⁴ for

$$|f(\pi)| = \frac{a}{1+(b(k-c))^2}, \quad (4)$$

we found $a = 0.866\text{\AA}$; $b = 0.696\text{\AA}$; $c = 5.701\text{\AA}^{-1}$; and $\phi = 12.843 - 0.484k$. In expanding $\phi(k)$ in powers of k , it was adequate to keep only the linear term. Keeping a quadratic term yielded only a negligible improvement in the fit to the data.

Because of the finite energy cutoff of the EXAFS data, the (Fourier transform) radial distribution function for the first shell contained significant sidebands which interfered with the signal arising from next-neighbor, etc., shells. To extract information about more distant shells, a new technique of successive filtering was employed. Using the single empirical spatial frequency of $2.672\text{\AA}$, a fit of the same form as Eq. (1) was made to $\chi(k)$ to obtain a spectrum of the fundamental $\chi_1(k)$, the EXAFS signal due only to the nearest neighbors. This was then removed from the spectrum and the filtered signal $\chi' = \chi - \chi_1$ was Fourier-transformed (Fig. 5). The result shows two strong peaks at $3.90\text{\AA}$ and $4.80\text{\AA}$. These peaks were found to be

quite insensitive to the choice cut-off point in the spectrum: a good indication that they are meaningful. A phase shift of $\frac{\alpha}{2} = .24$, the same amount required to bring the nearest neighbor Fourier transform peak into registry with the known Ti lattice spacings, will place the two peaks at 4.14Å and 5.04Å. The former corresponds to the second neighbor shell to within 0.01Å, and the latter lies close to the doublet (5.08Å, 5.11Å) which constitutes the fourth shell. The third shell consists of only two atoms (Table I), and is expected to yield a signal much weaker than that arising from the first, second, and fourth shells, and probably not strong enough to be distinguishable from the background noise. The strength of the second and fourth shells, while low, is comparable to the intensity seen in the K-edge EXAFS measurements.²⁵

While the apparent constancy of the phase shift $\frac{\alpha}{2}$ implies that the same type of scattering occurs for all the observed shells, the exact partial-wave character of this scattering remains to be established. For L-edge EXAFS in polycrystalline materials the scattering occurs predominantly via s- and d-partial wave states, because the electronic dipole selection rules $\ell \rightarrow \ell \pm 1$ should be nearly exact for excitations from core levels in the solid. It is instructive to compare our derived phase shifts to theoretical values. The total EXAFS phase shift,

$$\phi_{\ell\ell'} = \delta_{\ell}^{\ell'} + \delta_{\ell'}^{\ell} + \theta - \pi ,$$

has components δ'_0 and δ'_2 , associated with the central absorber, arising respectively from the outgoing and backscattered photoelectron waves. The component θ is due to backscattering from neighboring atoms. Only the terms ϕ_{00} and ϕ_{22} will be considered in this analysis, because angle-averaging will eliminate any contributions from ϕ_{02} and ϕ_{20} . Such contributions would otherwise be allowed because the c/a ratio of 1.588 in titanium leads to a nonzero term of Y_{20} symmetry in the crystal-field potential. The above relation thus reduces to

$$\phi_{\ell\ell} = 2\delta'_\ell + \theta - \pi, \quad \ell = 0, 2.$$

While θ has been calculated previously,²⁶ neither δ'_0 nor δ'_2 was available over the necessary energy range, so theoretical estimates were obtained from a fixed-core Hartree-Fock routine developed earlier by Williams and Shirley.²⁷ The phase shifts were calculated for an isolated Ti^+ ion made by introducing a hole in the 2p shell of a Ti atom, retaining unrelaxed atomic wave functions.²⁸ The theoretical phase shifts are shown in Fig. 6 together with our empirical phase shifts. At this point we encountered a problem in our analysis. The empirical phase shifts and their slopes lay almost exactly halfway between the values calculated for s and d waves. Of course it is a priori possible to have a 50-50 admixture of s and d character in the final free-electron state, but this would lead to a much broader line in the Fourier transform than shown in Fig. 4, or more likely two partially-resolved lines of similar intensity,

as reported in the L-edge studies of heavy elements.⁹ We were thus faced with a discrepancy. The single narrow peak in the Fourier transform argued strongly for the final state being predominantly of a single ℓ -wave character.

To gain insight into the cause of this discrepancy, we have also plotted in Fig. 6 ϕ_{11} (calculated in the same manner as ϕ_{00} and ϕ_{22}) and one empirical p-wave EXAFS phase shift from the data of Lytle.²⁵ The theoretical ϕ_{11} is found to be very nearly the mean of ϕ_{22} and ϕ_{00} , in agreement with physical intuition, and the three phase shifts δ'_ℓ are in good agreement with previous low-energy calculations.²⁹ However, it is clear that the ϕ_{11} is lower than the empirically determined value by nearly $\pi/2$. If all the calculated phase shifts are translated up by an amount sufficient to bring ϕ_{11} into registry with the empirical values (Fig. 7), we find our L-edge empirical phase shift to be consistent with an interpretation in which there is mainly $\ell = 2$ final state scattering with perhaps a small admixture ($\sim 20\%$) of $\ell = 0$ scattering. This result is somewhat larger than the admixture found by Lytle, et al.⁹ in their analysis of Au L-edge EXAFS.

IV. CONCLUSIONS

In this paper we have reported the first clear-cut L-edge EXAFS measurement in absorption in the ultra-soft x-ray region. The $L_{II,III}$ splitting, while observable in the spectra, caused no substantial difficulties in interpreting the fine structure.

At the edge a "white line" was observed that can be ascribed to a high density of final states available above the Fermi level. Although the L_I -edge was observed, its effect could be separated from the EXAFS signal because it was weak and varied slowly with energy. The phase shift analysis is consistent with a model of scattering for which the partial wave contributions are in the proportions $\sim 80\%$ ($l = 2$) and $\sim 20\%$ ($l = 0$). When more reliable theoretical phase shifts become available, it should be feasible to use EXAFS spectra to study the partial wave character of the continuum final states in some detail.

Table I. Parameters for neighbor shells of atoms in titanium.

Neighbor	Occupancy of Shell	Quality Factor ^a	Distance (Å)	Experimental Distance (Å) ^b
1a	6	12.21	2.90	2.91
b	6		2.95	
2	6	3.06	4.13	4.14
3	2	0.79	4.68	—
4a	12	6.05	5.08	5.04
b	6		5.11	

a) $N_{\text{shell}} (R_1/R_{\text{shell}})^2$; $R_1 = 2.95\text{Å}$

b) Given by (observed spatial frequency) + 0.24Å .

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FIGURE CAPTIONS

- Figure 1. Diagram of the apparatus showing the collimator-filter pair, oscillating sample holder, and the multicathode detector.
- Figure 2. Ti L-edge absorption spectrum. The arrow indicates the L_I transition.
- Figure 3. Top curve: Ti L-edge extended fine structure. Middle curve: Background function including a broad L_I absorption feature. Bottom curve: The EXAFS oscillations following subtraction of the background function.
- Figure 4. Magnitude of the Fourier transform of $k^2\chi(k)$ (arbitrary units).
- Figure 5. Magnitude of the Fourier transform of the once-subtracted EXAFS signal $k^2\chi'$. The peaks at $3.90\text{\AA}$ and $4.80\text{\AA}$ are interpreted as real, and are quite insensitive to details of data handling. All the peaks at smaller R values are clearly artifacts because they are closer than the nearest neighbor distance. The peaks marked with arrows are at R values which are sums of two of the three distances $2.67\text{\AA}$, $3.90\text{\AA}$, and $4.80\text{\AA}$, and thus suspect as sum peaks.
- Figure 6. The calculated wavevector dependent phase shifts ϕ_{00} , ϕ_{11} , ϕ_{22} (dashed curves) and the empirical phase shifts ϕ_K and ϕ_L (solid curves). The curves

are all truncated at $3.0\text{\AA}^{-1}$, and grow more meaningful from left to right.

Figure 7. The curves have the same meaning as in Fig. 6, but the theoretical functions ϕ_{00} , ϕ_{11} , ϕ_{22} have all been translated upward together to bring ϕ_{11} and ϕ_K into registry. The thin line marked ϕ' is the linear combination $0.78 \phi_{22} + 0.22 \phi_{00}$.

XBL782-240

Figure 1

XBL 785-779

Figure 2

Figure 3

XBL 785-884

Figure 4

XBL 784 - 770A

Figure 5

XBL 784-769

Figure 6

XBL 786-9175

Figure 7

XBL 786-9176

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