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X-ray Absorption Near Edge Theory

P.I. John J. Rehr, Dept. of Physics, Univ. of Washington, Seattle, WA 98195-1560

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I. Overview

This is the final report of 3 year DOE grant, "X-ray Absorption Near Edge Theory," DE-FG06-90ER45415 which extends from Sep 15, 1993 to Sep 14, 1996. One of our long term research goals has been to attain a quantitative theory of deep core x-ray spectroscopies. These spectroscopies include x-ray absorption fine structure (XAFS),¹ x-ray absorption near edge structure (XANES),¹ x-ray magnetic circular dichroism (XMCD),² diffraction anomalous fine structure (DAFS),³ photoelectron diffraction (PD),⁴ and others. All are used extensively at modern synchrotron radiation facilities. Since they share in common the same excited state electronic structure, these spectroscopies have similar theoretical underpinings: they all can be described in terms of a curved wave multiple scattering (MS) formalism. These spectroscopies are important probes of local atomic structure, especially in non-crystalline materials where conventional diffraction techniques are inapplicable. However their interpretation usually requires accurate theoretical models⁵⁻¹¹ or experimental reference standards. With the development of our fast XAFS codes FEFF,⁵⁻⁷ we have taken a giant step toward these goals. Indeed, we now regard the problem of EXAFS (i.e., extended XAFS) as well understood. For example, the EXAFS spectra calculated with FEFF for close-packed metals^{6,7} converge to full-MS band-structure calculations,¹² and also agree with experiment to high accuracy.¹³⁻¹⁶ The name FEFF refers to the effective curved-wave scattering amplitude f_{eff} for each scattering path in the fast Rehr-Albers MS theory.¹⁷ Our MS codes are generally equivalent or better than experimental standards, and have been recognized as the best of those available.¹³ Indeed they are used by scientists throughout the world and have revolutionized the field. The summary presentation at the 1994 International XAFS Conference in Berlin¹⁸ mentions FEFF prominently and concludes that EXAFS analysis is no longer limited to first neighbors. We have been invited to review these advances in Reviews of Modern Physics. Our project is important

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to the DOE mission for several reasons: scientific interest in the theory and applications; the increasing use of synchrotron radiation facilities by physicists, chemists and other scientists; and the significant technology transfer provided by our work. Our project had an overall rating of "outstanding" (9.0) by the DOE Assessment Office, which is within the highest priority category for continued funding.

II. RECENT WORK

Our work during the first two grant years led to many important developments including XANES calculations of many materials using our XAFS/XANES code FEFF6, the observation of AXAFS, i.e., fine structure in the XAFS background, and the first calculation of XCMD [see the attached publication list in Sec. IV.].

In remainder of this report we review what we proposed and summarize our accomplishments during the past year Nov 15, 1995 – Sep 14, 1996, i.e., the final year of the grant. One graduate student, Alexey Ankudinov, was supported for 10 calendar months during this period.

A. Improved Photoelectron Self-energy

1. We proposed to improve the electron-self energy approximation for near edge calculations. Our project has followed our original proposal, namely the replacement of Hedin-Lundqvist (HL) self-energy with an improved, partly non-local model. The work is part of the Ph. D. dissertation of our student, A. Ankudinov. The first account will be reported at the 1996 March APS Meeting: [Bull. Am. Phys. Soc., 41 in press, (1996)] and we plan other publications:

Partly nonlocal self-energy models for x-ray absorption calculations

Alexei Ankudinov and J. J. Rehr

Ab initio calculations of X-ray absorption spectra (XAS) and its fine structure (XAFS) are sensitive to the many-body exchange and correlation interaction between the photoelectron and other states. Non-local Hartree-Fock exchange provides a better description of exchange with core electrons, while the local density approximation (LDA) is usually better for the interaction with valence electrons. The GW approximation for the photoelectron self-energy Σ provides a systematic way of joining HF and LDA, using the natural separation of Σ into core and valence parts.¹ This hybrid exchange model is implemented in a new Dirac-Fock based generalization of the FEFF6 code² for XAS calculations. Significant improvements are found compared with LDA based codes. These include more accurate excitation energies, and better XAFS phase shifts, amplitudes, and mean-free

paths. These lead to improved peak positions and magnitudes in near edge region and improved distance and coordination number determinations from XAFS analysis.

¹ L. Hedin, and S. Lundqvist, Solid State Physics, **23**, 1 (1969).

² S.I. Zabinsky et. al., Phys. Rev. B**52**, 2995 (1995).

2. The above work required the implementation of a relativistic, Dirac-Fock atom program, which we have turned into an automated subroutine that only requires the atomic number as input. The code has been submitted for publication in Computer Physics Communications (UW Preprint, February, 1996):

Single Configuration Dirac-Fock Atom Code
A. L. Ankudinov, S. I. Zabinsky and J. J. Rehr

A single configuration version of the multiconfigurational Dirac-Fock atomic code of Desclaux has been developed into an automated FORTRAN 77 subroutine, requiring only the atomic number as input. The output contains energies, wavefunctions, densities and other data comparable to that in standard atomic structure tables.

B. Intrinsic and Interference Effects

1. Our work in this topic has largely followed our original proposal. However, we have made a breakthrough in calculations of intrinsic and interference effects, working in collaboration with L. Hedin and W. Bardyszewski. A preliminary account was reported at the March 1995 APS Meeting. [Bull. Am. Phys. Soc. **40**, 852 (1995)]. Since that time, model calculations have been carried out which demonstrate the cancellation of extrinsic and intrinsic losses at low energies. More detailed calculations are in progress which we expect to be completed by summer 1996. In the future this treatment must be carried over to real materials, and is a topic of our renewal proposal.

C. APPLICATIONS to EXAFS, NEXAFS and Other Spectroscopies

1. Improved Edge Calculations – We proposed to incorporate the findings of our studies into our FEFF codes to improve their utility. For example, we have collaborated with E. Hudson (LLNL) on XANES calculations in very heavy materials, e.g., U L₃ edges. This work demonstrated the need for an improved edge-shape, namely a Lorentzian broadened edge instead of arctan approximation for short core-hole lifetimes. This change has been implemented in recent versions of FEFF. Our paper is Phys. Rev. B**52**, 13815 (1995):

Multiple-scattering calculations of the uranium L3-edge XANES

E. A. Hudson, J. J. Rehr, and J. J. Bucher

A theoretical study of the uranium L₃-edge x-ray absorption near-edge structure (XANES) is presented for several uranium compounds, including oxides, intermetallics, uranyl fluoride, and α -uranium. Calculations were performed using FEFF6, an *ab initio* multiple-scattering (MS) code that includes the most important features of current theories. The results, which account for both the fine structure χ and the atomiclike background μ_0 of the absorption coefficient μ , are compared to new and previously measured experimental spectra, revealing very good agreement for most systems. For several compounds, a more detailed theoretical analysis determined the influence of cluster size and scattering order upon the calculated spectra. Results indicate that MS paths and scattering paths that include rather distant atoms make significant contributions for UO₂, whereas XANES for crystals with lower symmetry and density can be modeled using only shorter single-scattering paths. In most cases, assumption of a screened final state in the calculation gives better agreement with experiment than use of an unscreened final state. The successful modeling of spectra for a variety of different uranium compounds, with differing spectral features, indicates that the semirelativistic treatment of XANES used here is adequate even for heavy elements. The well-known resonance, observed experimentally for uranyl (UO₂²⁺) compounds, ≈ 15 eV above the white line, is successfully modeled here for the first time, using multiple-scattering paths within the O-U-O axial bonds. Overlapping muffin-tin spheres were required in the calculation, probably as a result of the short uranyl axial bonds.

2. Background Fine Structure – Our work on the atomic background absorption has generated some controversy. In particular one group has attributed background absorption structure to multi-electron transitions, whereas our paper showed cases where the background structure was dominated by embedded atomic effects. Our Reply will be published in in Phys. Rev. B in press (1996):

Reply to “Comment on ‘X-ray-absorption fine structure in embedded atoms

J. J. Rehr, C.H. Booth, F. Bridges and S. I. Zabinsky

We respond to the previous Comment concerning evidence for weak oscillatory structure in the atomic background cross section in x-ray absorption fine structure (XAFS). We show that improved background calculations which suppress muffin-tin discontinuities still exhibit fine structure comparable to that observed.

3. XANES of Silicate Glasses – We have collaborated with Gordon Brown (Stanford-SSRL) and F. Farges (LURE) and to apply the FEFF6 codes complex crystalline solids and minerals. The work showed that many MS paths and overlapped muffin-tin potentials are needed for preedge and XANES calculations, and yielded three papers in *Geochimica et Cosmochimica Acta*, (accepted 1996):

Coordination chemistry of Ti(IV) in silicate glasses and melts. I. XAFS study of Ti coordination in oxide model compounds

Farges F., Brown G.E., Jr. et Rehr J.J.

Coordination chemistry of Ti(IV) in silicate glasses and melts. II. Glasses under ambient conditions.

Farges F., Brown G.E., Jr., Navrotsky A., Gan, H. et Rehr J.J.

Coordination chemistry of Ti(IV) in silicate glasses and melts. III. Glasses and melts between 293 and 1650 K.

Farges F., Brown G.E., Jr., Navrotsky A., Gan, H. et Rehr J.J.

4. Improved FEFF Code – A dividend of these developments is an improved version of FEFF (version 7.0) which will be released early in 1996. The code has the following new features: A variable grid has been added to the phase shift program to improve convergence. The many `feff.dat` files are now replaced by a much smaller binary file `feff.bin`. The original LDA atomic code is replaced by a better, Dirac-Fock atom code, and a fully relativistic version of the cross-section code is used with both ($l \rightarrow l \pm 1$) dipole transitions and polarization dependence. For XANES the arctan approximation of the edge shape is replaced by a convolution with lorentzian. New self energy models are available including a hybrid partly nonlocal model with Dirac-Fock exchange for the core electrons and LDA exchange-correlation for valence electrons. An approximate calculation of the many-body overlap factor S_0^2 is also available. A more complete description will be given in the Ph. D. dissertation our research assistant, A. Ankudinov and in subsequent papers.

5. Full-MS XANES Calculations – Problems encountered in calculating XANES in many materials has demonstrated the need for better ways to treat very high order MS in the near edge region. Thus we have begun the development of a full MS extension of FEFF. A preliminary account will be presented at the March 1996 APS meeting, [Bull. Am. Phys. Soc. 41, in press (1996)], and the subject is a main topic of our Renewal proposal.

Exact Multiple Scattering Calculations XANES

B. Ravel and J. J. Rehr

Ab initio calculations of X-ray absorption near-edge structure (XANES), are made by inverting the full multiple-scattering (MS) matrix $(1 - Gt)^{-1}G$. Our approach uses the fast, quickly convergent Rehr-Albers¹ separable representation of the free electron propagator G together with atomic scattering t -matrices from the FEFF6 code,² which are calculated within the muffin-tin approximation with overlapped atom potentials. With this technique, XANES spectra and its polarization dependence can be calculated in reasonable cpu time

on large clusters. Good agreement with the XANES spectra of several sample compounds is obtained. A similar strategy is used to determine the local densities of states $\rho(E, \vec{r})$ from the full MS matrix. From $\rho(E, \vec{r})$ we calculate the Fermi energies and estimate charge transfer for our sample clusters. The prospect of quantitative analysis of XANES spectra and its preedge features is discussed.

¹ J.J. Rehr and R.C. Albers, Phys. Rev. B, **41**, 8139, (1990).

² S. I. Zabinsky, et al., Phys. Rev. **B52**, 2995 (1995).

6. XMCD – We have carried out the first successful calculation of the fine structure in the XMCD of Gd. Our paper was recently published [Phys. Rev. **B52**, 10214 (1995)]. The calculation was found to be in good agreement with experiment and has already been cited prominently in a recent review by Schütz and Ahlers. Our calculation was based on an experimental version of our FEFF which calculates XAFS for both spin up and spin down populations. A more substantial development is a topic of the Renewal proposal.

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