Plasmon-Coupling Theory of the Electron Inelastic Mean Free Path, energy loss functional and the dielectric function for LEEMPEEM, for low energy electrons

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We review new self-consistent models of inelastic electron scattering in condensed matter systems for accurate calculations of low-energy electron inelastic mean free paths (IMFPs) for XAFS and low energy diffraction. *Our model implements plasmon coupling mechanisms for the first time, in addition to causally-constrained lifetime broadening and high-precision density functional theory, and enables dramatic improvements in the agreement with recent high profile IMFP measurements.*

The accuracy of theoretical determinations of the electron inelastic mean free path (IMFP) at low energies is one of the key limiting factors in current XAFS modeling and Monte Carlo transport. Recent breakthroughs in XAFS analysis show that there exist significant discrepancies between theoretical and experimental IMFP values [1], and that this can significantly impact upon extraction of other key structural parameters from both XANES and XAFS. Resolution of these discrepancies is required to validate experimental studies of material structures, and is particularly relevant to the characterization of small molecules and organometallic systems for which tabulated electron scattering data is often sparse or highly uncertain.

We present a theoretical approach for IMFP determination linking the optical dielectric function and energy loss spectrum of a material with its electron scattering properties and characteristic plasmon excitations. We review models inclusive of plasmon coupling, allowing us to move beyond the longstanding statistical approximation and explicitly demonstrate the effects of band structure on the detailed behavior of bulk electron excitations in a solid or small molecule [2]. This interrogates the optical response of the material, which we obtain using density functional theory [3].

We find that our developments dramatically improve agreement with experimental electron scattering results in the low-energy region (<~100 eV) where plasmon excitations are dominant. Corresponding improvements are therefore made in theoretical XAFS spectra and detector modelling.

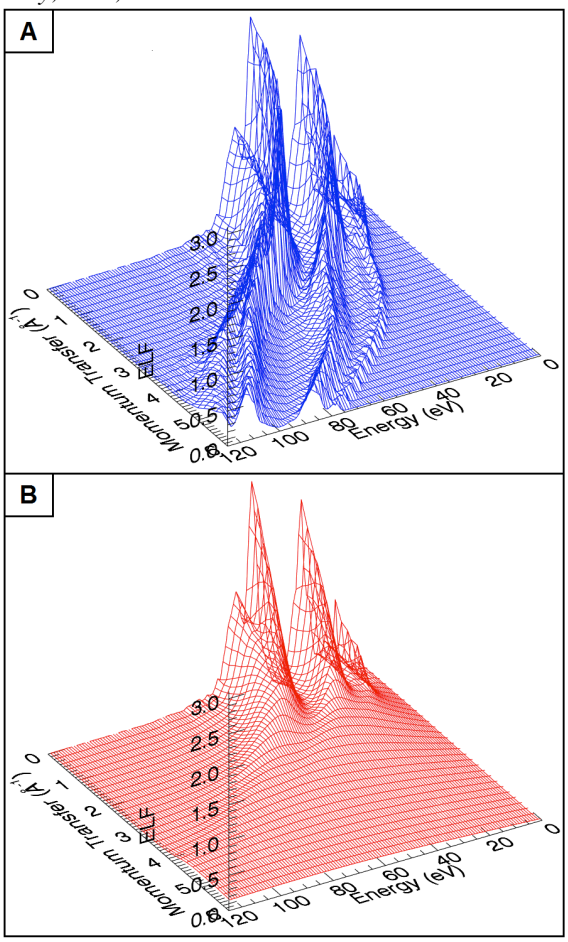

Figure 1: The electron energy loss function (ELF) of Mo. (A) is calculated using a lossless Lindhard type model, while (B) utilises a self-consistent coupled-plasmon model.

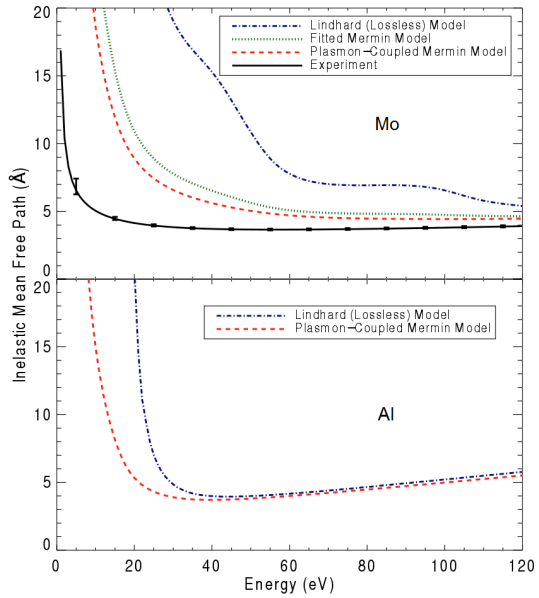

Figure 2: Theoretical and experimental determinations of the electron IMFP for molybdenum and aluminium

References

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