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Low-Energy Electron Inelastic Mean Free Path

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We present calculations of low-energy electron inelastic mean free paths (IMFPs) within the dielectric formalism, using the energy-loss function (ELF) from *ab initio* calculations. The ELF is obtained from the time-dependent density functional theory in the adiabatic local density approximation (ALDA). We give an example of the ALDA-ELF and ALDA-IMFP for Fe. The obtained results agree well with other theoretical and experimental data.

Knowledge of IMFPs is necessary to study electron transport in matter. Within the dielectric formalism, the IMFP is given by (in Hartree atomic units, $\hbar = m_e = e = 1$)

$$\lambda_{in}^{-1} = \frac{1}{\pi E}\int_0^{E-E_F} d\omega \int_{k_-}^{k_+} \frac{1}{k}\,\mathrm{Im}\left[\frac{-1}{\varepsilon(k,\omega)}\right] dk \qquad (1)$$

where E is the electron energy, E_F is the Fermi energy, ω is the energy loss, k is the momentum transfer, $k_\pm = \sqrt{2E} \pm \sqrt{2(E-\omega)}$, $\varepsilon(k,\omega)$ and $\mathrm{Im}\left[-1/\varepsilon(k,\omega)\right]$ are the dielectric and energy-loss functions of the system, respectively. The problem here is to determine accurately the energy-loss function (ELF).

The ELF can be extrapolated from the optical data [1-8]. However, such an ELF is unsuitable for calculating IMFPs of low energies (typically less than 100 eV). Here we calculate the ELF with the time-dependent density functional theory (TDDFT) in the adiabatic local density approximation (ALDA). We then use the ALDA-ELF to determine the IMFP at energies below 100 eV.

The ELF calculations are performed with the EXCITING code [9]. First, ground state calculations are carried out with the Perdew-Burke-Ernzerhof exchange-correlation functional, using a $30\times30\times30$ $\boldsymbol{k}$ grid, a plane-wave cutoff $R_{MT}|\boldsymbol{G}+\boldsymbol{k}|_{max} = 9$, and a muffin-tin (MT) radius $R_{MT} = 2$ bohr. Then, the ELF is calculated with the TDDFT in the ALDA *with* and *without* local field effects (LFE). Finally, the IMFP is determined from the definition (1), using the ALDA-ELF.

We show in Figs. 1 and 2 an example of the ALDA-ELF and ALDA-IMFP for Fe, respectively. Figure 1 displays the ELF in the optical limit ($k = 0$). In the valence-electron energy range 0-50 eV, the ALDA-ELFs agree reasonably with the results [10] from density functional theory (DFT) calculations and reflection electron energy loss spectroscopy (REELS) measurements.

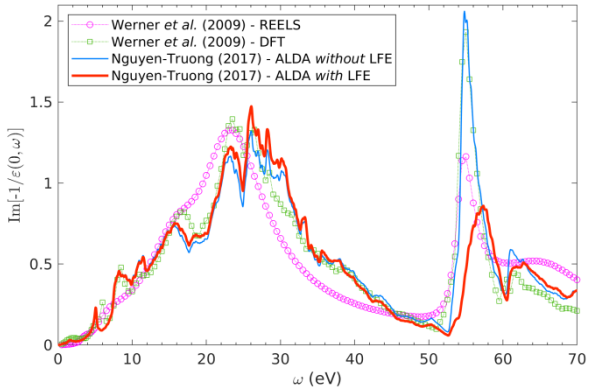

Fig. 1. The optical ELF for Fe [11].

The difference between the ALDA-ELF *with* and *without* LFE is significant at the inner-core excitation edge of 52.7 eV, which corresponds to the binding energy of 3*p* electrons [12]. This difference results in the strong discrepancy between the ALDA-IMFPs *with* and *without* LFE (Fig. 2). The reason is related to the electron configuration of Fe: [Ar] $4s^2$ $3d^6$. The most

outer-shell $3d^6$ remains unfilled and hence tends to attract external electrons to fill the shell. This leads to a strong inhomogeneity of the electron system. In such a system, the LFE play an important role.

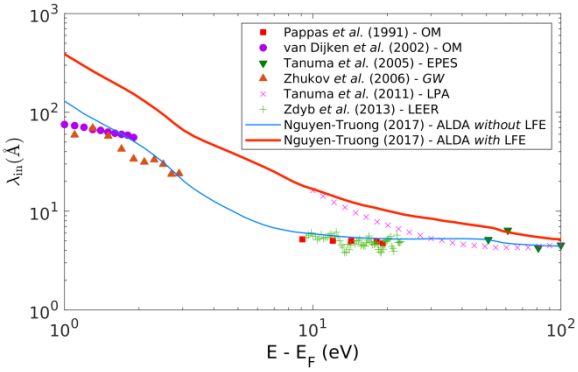

Fig. 2. The IMFP for Fe [11]. The Fermi energy $E_F = 8.9$ eV [13].

For comparison, we also include in Fig. 2 available data of IMFPs for Fe determined by overlayer method (OM) [14, 15], elastic-peak electron spectroscopy (EPES) [16], low-energy electron reflectivity (LEER) [17], and by *GW* calculations [18] and the Lindhard-Penn algorithm (LPA) [13]. Surprisingly, the IMFP *without* LFE agree better with theoretical and experimental data than the IMFP *with* LFE. The present results show that the IMFPs at low energies can be determined by using the ELF from the TDDFT calculations in the ALDA.

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