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Numerical simulation of valence losses in Si/SiO_2 films

J. Aizpurua*, A. Howie† and F.J. García de Abajo§

* Facultad de Químicas, UPV/EHU, Aptdo. 1072, 20080 San Sebastián, Spain
† Cavendish Laboratory, Madingley Road, Cambridge CB3 OHE, UK
§ Facultad de Informática, UPV/EHU, Aptdo. 649, 20080 San Sebastián, Spain

In the framework of local dielectric theory, valence losses in scanning transmission electron microscopy (STEM) can be conveniently understood as collective excitations produced in the material for specific modes defined by the geometry and composition of the sample. The normal modes of standard geometries such as the plane, sphere or cylinder can be obtained analytically and have successfully explained electron energy losses (EELS) in many practical situations. The presence of more complex structures in realistic experiments, such as a thin film containing an Si - SiO_2 normal interface as shown in the inset of figure 1, makes necessary the use of numerical simulations to obtain both the modes of the complete system and the weight of their interaction (for excitation and stopping) with the electron beam. In the non-relativistic case, the losses can be simulated by taking a distribution of surface and interface points, each associated with an interface charge. These charges interact self-consistently with each other as well as with the incident electron [1,2]. This method can be used to analyse the effect of the finite film effect on the Si-SiO_2 interface plasmon peak and provides quantitative criteria to establish the thickness d below which the planar interface approximation should be corrected.

1. The finite size effect: junction modes

In some practical situations in EELS (d exceeding 100 nm), the single planar approximation is sufficient to study the interface plasmon peak position [3] although relativistic effects (not considered here) may matter. In this case, the peak position at 8.6eV is given by the well known relation $\varepsilon_{Si} + \varepsilon_{SiO2} = 0$. The finite sample introduces new modes associated with the three media (Si-SiO_2-vacuum) junction at the interface edges which can also be excited by the electron beam. For thick samples, the main contribution to the losses comes from the planar interface peak but the junction modes are always present since they are a characteristic of the system. From numerical simulations, one can establish that the modes corresponding to the T junction Si-SiO_2-vacuum present at the edges of the interface in the thin film are given by the relation $\varepsilon_{Si} + \varepsilon_{SiO2} + 2 = 0$, which is obeyed for $\hbar\omega$=7.6 eV. For a case such as that shown in the inset of figure 1, and taking into account the position of all the modes, one can guess, for the energy range between 5 eV and 10 eV, a characteristic loss function of the form:

$$\frac{dP}{d\omega} = \frac{2e^2}{\pi\hbar v^2} L\left[A_1 \mathrm{Im}\left(\frac{-1}{0.5\varepsilon_{Si} + 0.5\varepsilon_{SiO_2}} \right) + A_2 \left(\frac{-1}{0.25\varepsilon_{Si} + 0.25\varepsilon_{SiO_2} + 0.5} \right) \right], \qquad (1)$$

where L=d is the path length travelled by the beam inside the SiO_2, and the coefficients A_j depend on the frequency ω and the impact parameter b. This characteristic energy loss function based on fixed positions for the interface and junction modes is valid for Si/SiO_2 films down to 5nm thick, since below this value the coupling of junctions and walls changes the mode positions significantly.

2. Interface plasmon peak shifts

The increasing importance of the junction mode in the spectrum of losses at smaller film thicknesses is clearly shown in figure 1. The presence of the extra boundaries corrects the spectra of losses in two ways: firstly, the introduction of new excitations at 7.6 eV associated with the junctions, and secondly, the correction to the weight of the extended interface plasmon peak at 8.6eV which is no longer proportional to the film thickness d. The proximity in value of both the interface mode and the junction mode, together with the broadening of the peaks means that the increasing excitation of the junction mode and the correction to the planar excitation appear as a shifting from 8.6 eV to 7.6 eV. From these simulations one can establish that the single interface approximation is sufficiently good for films thicker than ~50nm but otherwise, one should take into account the finite sample effect.

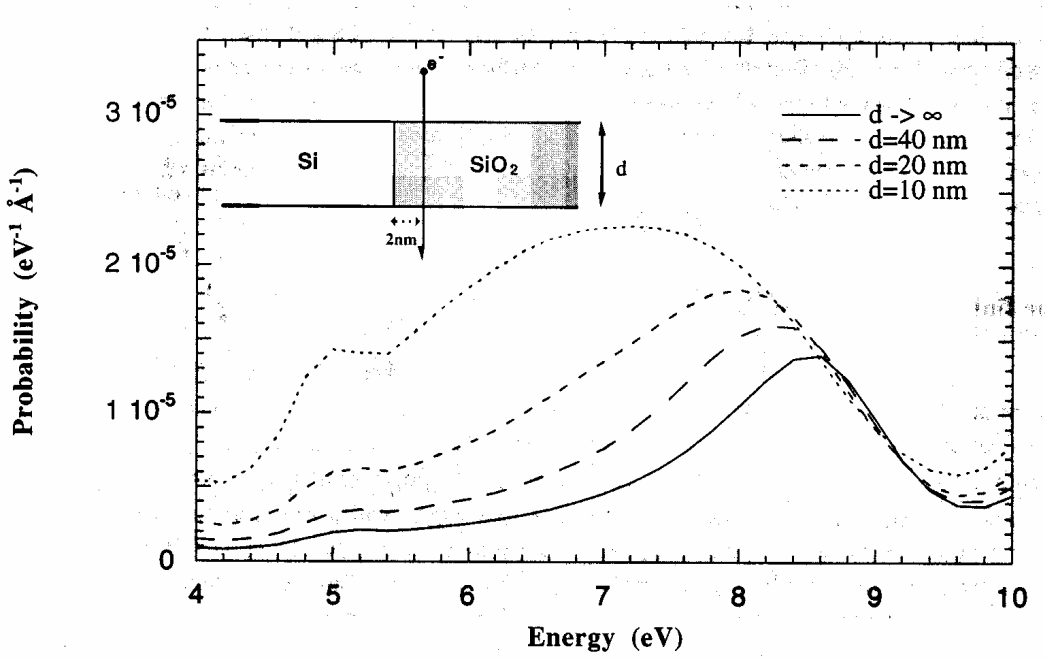

FIG. 1- Simulations for the energy loss probability per unit energy normalised to the film thickness for a 100 keV electron impinging on a Si/SiO_2 film as shown in the inset at 2nm from the interface inside the SiO_2. Spectra for different film thicknesses d are shown, and the case of the single Si/SiO_2 interface is denoted as d->∞.

References

1. Ouyang F. and Isaacson M., Phil. Mag. B, 60 (1989) 481.
2. García de Abajo F.J. and Aizpurua J., Phys. Rev. B, 56 (1997) 15873.
3. Moreau P., Brun N. Walsh C.A., Colliex C. and Howie A., Phys. Rev. B, 56 (1997) 6774.