Chapter 15
Appendix F: The Mermin Theory and the Generalized Oscillator Strength Method

Dielectric formalism is the most used method for investigating the interaction of swift electrons with solid targets. In this chapter the Mermin energy loss function-generalized oscillator strength method (MELF-GOS method) is briefly described within the framework of dielectric formalism [1–4].

15.1 The Mermin Theory

The Mermin dielectric function [1] is given by:

$$\varepsilon_M(\mathbf{q},\omega) = 1 + \frac{(1+i/\omega\tau)[\varepsilon^0(\mathbf{q},\omega+i/\tau)-1]}{1+(i/\omega\tau)[\varepsilon^0(\mathbf{q},\omega+i/\tau)-1]/[\varepsilon^0(\mathbf{q},0)-1]}\,, \tag{15.1}$$

where $\mathbf{q}$ is the momentum, ω the frequency, τ the relaxation time, and $\varepsilon^0(\mathbf{q},\omega)$ the Lindhard dielectric constant [5]

$$\varepsilon^0(\mathbf{q},\omega) = 1 + \frac{4\pi^2 q^2}{e^2} B(\mathbf{q},\omega)\,, \tag{15.2}$$

$$B(\mathbf{q},\omega) = \int \frac{d\mathbf{p}}{4\pi^3} \frac{f_{\mathbf{p}+\mathbf{q}/2} - f_{\mathbf{p}-\mathbf{q}/2}}{\omega - (\varepsilon_{\mathbf{p}+\mathbf{q}/2} - \varepsilon_{\mathbf{p}-\mathbf{q}/2})/\hbar}\,. \tag{15.3}$$

In these equations e is the electron charge, $f_{\mathbf{p}}$ is the Fermi-Dirac distribution, and $\varepsilon_{\mathbf{p}}$ the free electron energy.

Note that the Lindhard dielectric function [5] can be numerically calculated by using Eqs. (15.2) and (15.3). The integration can also be carried out in closed form. The result of the integration is the following [2, 3, 6]:

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$$\varepsilon^0(q,\omega) \;=\; 1+\frac{\chi^2}{z^2}[f_1(u,z)\;+\;i\;f_2(u,z)]\,, \tag{15.4}$$

where $u=\omega/(qv_F)$, $z=q/(2q_F)$, and $\chi^2=e^2/(\pi\,\hbar\,v_F)$ is a measure of the electron density [6]. In this equation, v_F is the Fermi velocity of the valence electrons of the target and $q_F=mv_F/\hbar$. The functions $f_1(u,z)$ and $f_2(u,z)$ are given by

$$f_1(u,z) \;=\; \frac{1}{2}\;+\;\frac{1}{8z}\,[g(z-u)\;+\;g(z+u)]\,, \tag{15.5}$$

$$f_2(u,z)=\begin{cases}\frac{\pi}{2}u, & z+u<1\\ \frac{\pi}{8z}[1-(z-u)^2], & |z-u|<1<z+u\\ 0, & |z-u|>1\,,\end{cases} \tag{15.6}$$

where

$$g(x) \;=\; (1-x^2)\,\ln\left|\frac{1+x}{1-x}\right|\,. \tag{15.7}$$

15.2 The Mermin Energy Loss Function-Generalized Oscillator Strength Method (MELF-GOS)

Let us now consider a superposition of free and bound oscillators. For any oscillator, the energy loss function is given by the opposite of the imaginary part of the inverse of the Mermin dielectric function:

$$\mathrm{Im}\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i\,;q,\omega)}\right] \;=\; \frac{\varepsilon_{M_2}}{\varepsilon_{M_1}^2+\varepsilon_{M_2}^2}\,, \tag{15.8}$$

where

$$\varepsilon_M \;=\; \varepsilon_{M_1}+i\varepsilon_{M_2} \tag{15.9}$$

and ω_i and γ_i are, respectively, the frequency and the damping constant associated to each specific oscillator. A linear combination of Mermin-type energy loss functions, one per oscillator, allows to calculate the energy loss function (ELF) for $q\;=\;0$, for any specific material [2–4]:

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(q\,=\,0,\omega)}\right] \;=\; \sum_i A_i\,\mathrm{Im}\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i\,;q\,=\,0,\omega)}\right]\,. \tag{15.10}$$

In this equation, A_i, ω_i, and γ_i are determined by looking for the best fit of the available experimental optical ELF. Actually, as both Mermin and Drude-Lorentz oscillators converge on the same values in the optical limit (i.e. for $q = 0$) [7]

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(q=0,\omega)}\right] = \sum_i A_i \mathrm{Im}\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i\,;q=0,\omega)}\right] = \sum_i A_i \mathrm{Im}\left[\frac{-1}{\varepsilon_D(\omega_i,\gamma_i\,;q=0,\omega)}\right], \tag{15.11}$$

where the Drude-Lorentz functions $\mathrm{Im}\left[\frac{-1}{\varepsilon_D(\omega_i,\gamma_i\,;\mathbf{q}=0,\omega)}\right]$ are given by [8]

$$\mathrm{Im}\left[\frac{-1}{\varepsilon_D(\omega_i,\gamma_i\,;\mathbf{q}=0,\omega)}\right] = \frac{\gamma_i\omega}{(\omega_i^2-\omega^2)^2+(\gamma_i\omega)^2}, \tag{15.12}$$

the best fit can also be obtained using a linear combination of Drude-Lorentz functions, instead of Mermin functions. Once the values of the best fit parameters have been established (see, for example, Refs. [4, 9, 10]), the extension beyond the optical domain ($\mathbf{q} \neq 0$) can be obtained by [2–4]

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(\mathbf{q},\omega)}\right] = \sum_i A_i \mathrm{Im}\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i\,;\mathbf{q},\omega)}\right]. \tag{15.13}$$

Planes et al. [2], Abril et al. [3], and de Vera et al. [4] construct the ELF in the optical limit including the contribution of the electrons from the outermost atomic inner shells as follows:

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(q=0,\omega)}\right] = \begin{cases} \sum_i A_i \mathrm{Im}\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i\,;q=0,\omega)}\right] & \omega < \omega_{i,edge} \\ \sum_{i,sh} A_{i,sh} \mathrm{Im}\left[\frac{-1}{\varepsilon_M(\omega_{i,sh},\gamma_{i,sh}\,;q=0,\omega)}\right] & \omega \geq \omega_{i,edge} \end{cases} \tag{15.14}$$

where the first term represents the contribution of the outer electrons while the second one includes the electrons of the outermost atomic inner shells.

15.3 Summary

In this chapter, after a brief discussion about the Mermin theory [1], the Mermin energy loss function-generalized oscillator strength method (MELF-GOS method), in the framework of the dielectric formalism, was shortly described [2–4].

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