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Surface excitation parameter for semiconducting III–V compounds

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Abstract

In the rapid development of mesoscopic science, the study of surface excitations in solids and overlayer systems plays a crucial role. The surface excitation parameter which describes the total probability of surface plasmon excitations by an electron traveling in vacuum before impinging on or after escaping from a semiconducting III–V compound has been calculated for 200–2000 eV electrons crossing the compound surface. These calculations were performed using the dielectric response theory with sum-rule-constrained extended Drude dielectric functions established by the fits of these functions to optical data. Surface excitation parameters calculated for InSb, InAs, GaP, GaSb or GaAs III–V compounds were found to follow to a simple formula, i.e. $P_s = aE^{-b}$, where P_s is the surface excitation parameter and E is the electron energy. These surface excitation parameters were then applied to determine the elastic reflection coefficient for electrons elastically backscattered from III–V compounds using the Monte Carlo simulations. Good agreement was found for the electron elastic reflection coefficient between calculated results and experimental data.

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1. Introduction

Quantitative information on electron inelastic interaction cross sections in solids is important in surface spectroscopies. A study of the inelastic

cross section requires the consideration of surface excitations. Such surface excitations are characterized by the so-called surface excitation parameter (SEP), defined as the average number of surface excitations by an electron crossing the solid surface [1]. Recent studies on the energy-loss spectra [2–4] for electrons reflected from solid surfaces have demonstrated that the contribution from surface excitations was important for electron

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energies from a few hundred eV to ~ 2 keV, especially with oblique incident or escaping electrons. The improvement in quantitative surface analysis was significant when surface excitations were considered.

In the present work, theoretical approaches to surface excitations were dealt with the dielectric response theory [3–6]. These excitations were modeled in terms of the surface energy loss function, $\text{Im}[-1/(\varepsilon(q, \omega) + 1)]$, where $\varepsilon(q, \omega)$ is the dielectric function with momentum transfer q and energy transfer ω . The SEPs for semiconducting III–V compounds were calculated for 200–2000 eV electron energies based on the dielectric functions by the fits of extended Drude functions to measured optical data. Due to the strong overlapping of oscillator strengths between electrons in the valence band and the outermost inner shells, such fits were performed to include the contribution from outermost inner shells. Measured optical data were taken from ellipsometric measurements [7] in the infrared spectral region and from energy loss measurements [8] in the ultraviolet spectral region. Such a combination of data provided detailed information on the interband transitions and the plasmon excitations. In all fits, the real- and imaginary-parts of the dielectric function and the bulk and surface energy-loss functions were in good agreement with experimental data. The SEPs for electrons incident into or escaping from the semiconducting III–V compounds were then calculated. These SEPs were applied to determine the elastic reflection coefficient of elastically backscattered electrons. A comparison was made between calculated results and measured data.

2. Theory

The SEP was calculated by an integration of the surface excitation probability over all electron distances outside the solid [1]. Such a probability was determined by evaluating the surface energy loss-function given in terms of the dielectric function. In the present work, the extended Drude dielectric function model was used. The dielectric function is given by [9]

$$\begin{aligned} \varepsilon(q, \omega) &= \varepsilon_1(q, \omega) + i\varepsilon_2(q, \omega) \\ &= \varepsilon_B + \sum_i \frac{A_i}{\omega^2 - \left(\omega_i + \frac{q^2}{2}\right)^2 + i\omega\gamma_i}, \end{aligned} \quad (1)$$

where A_i , γ_i and ω_i are, respectively, the oscillator strength, the damping coefficient and the resonant frequency, all associated with the i th group electrons in the valence band and outermost inner shells. The background dielectric function in Eq. (1), ε_B , is to account for the influence of polarizable ion cores [10]. All parameters are determined by the fit of $\varepsilon_1(0, \omega)$, $\varepsilon_2(0, \omega)$, $\text{Im}[-1/\varepsilon(0, \omega)]$ and $\text{Im}[-1/(\varepsilon(0, \omega) + 1)]$ to optical data of the semiconducting III–V compounds [7,8].

Optical data are available for the extinction coefficient, k , in a limited energy transfer range $\omega_1 \leq \omega \leq \omega_2$ and for the refraction index, n , in $\omega_3 \leq \omega \leq \omega_4$. Due to the lack of information on k in $\omega < \omega_1$ and $\omega > \omega_2$, extrapolations are applied as

$$k(\omega) = \begin{cases} k(\omega_1) \frac{\omega}{\omega_1} & \text{for } \omega < \omega_1, \\ k(\omega_2) \left(\frac{\omega}{\omega_2}\right)^p & \text{for } \omega > \omega_2, \end{cases} \quad (2)$$

where the parameter p is determined from the f-sum rule

$$\int_0^\infty \omega k(\omega) d\omega = \frac{\pi}{4} \omega_p^2, \quad (3)$$

$\omega_p = (4\pi NZ)^{1/2}$ is the plasma energy, N is the molecular density and Z is the total number of electrons per molecule. Note that all quantities are expressed in atomic units (a.u.) unless otherwise specified. Further, the Kramers–Kronig dispersion relation is applied to obtain the refraction index at any ω in the range of $\omega < \omega_3$ and $\omega > \omega_4$. Finally, the validity of the inertial sum rule

$$\int_0^\infty [n(\omega) - 1] d\omega = 0 \quad (4)$$

is checked.

With the available dielectric functions, the SEP may be calculated using formulas given elsewhere [1]. Also, the elastic reflection coefficient of elastically backscattered electrons may be calculated following equations derived in the previous works [11,12].

3. Results and discussion

Eq. (1) was fitted to measured optical data for several semiconducting III–V compounds. A comparison on $\varepsilon_1(0, \omega)$, $\varepsilon_2(0, \omega)$, $\text{Im}[-1/\varepsilon(0, \omega)]$ and $\text{Im}[-1/(\varepsilon(0, \omega) + 1)]$ for InSb is shown in Fig. 1 among present fittings (solid curves), previous fittings of Kwei and Tung [13] (dotted curves), and experimental data [7,8] (dashed curves). It reveals that the present fittings are in better agreement than the previous ones as compared to optical data for all dielectric functions plotted. The better agreement is due to the considerations of the polarizable ion cores and partial 4d inner shell electrons in the dielectric functions. Without such considerations, the previous fittings produce poor agreement with optical data on ε_1 and ε_2 at small ω and on bulk and surface energy-loss functions at large ω . Further, the positions and the heights

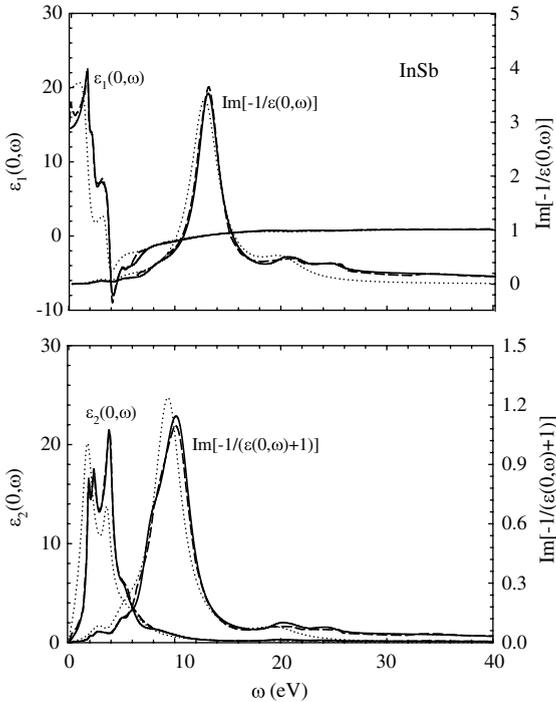


Fig. 1. A plot of the dielectric functions, $\varepsilon_1(0, \omega)$, $\varepsilon_2(0, \omega)$, $\text{Im}[-1/\varepsilon(0, \omega)]$ and $\text{Im}[-1/(\varepsilon(0, \omega) + 1)]$, for InSb. Solid curves are the results of the present work. Other calculated results [13] (dotted curves) and experimental data [7,8] (dashed curves) are also plotted for comparison.

Table 1
Fitted values of parameters a and b in Eq. (5)

	Escaping electrons		Incident electrons	
	a	b	a	b
GaP	1.322	0.4300	1.294	0.4282
GaAs	1.427	0.4344	1.385	0.4318
GaSb	1.522	0.4381	1.469	0.4351
InAs	1.450	0.4374	1.406	0.4354
InSb	1.540	0.4390	1.496	0.4371

of the resonant plasmon peaks in the previous fittings are different from experimental data.

Based on the dielectric response theory, the SEPs for normally incident and escaping electrons of 200–2000 eV were calculated using the fitted dielectric functions. An analysis of the calculated results yields the approximate relation for the SEP

$$P_s(E) = aE^{-b} \quad (5)$$

applicable to both incident and escaping electrons, where a and b are adjustable parameters. With E in eV in Eq. (5), the best fitted values of a and b are listed in Table 1 for the semiconducting III–V compounds.

Calculations were made for the elastic reflection coefficient of electrons elastically backscattered from semiconducting III–V compounds using the SEPs and the Monte Carlo simulations

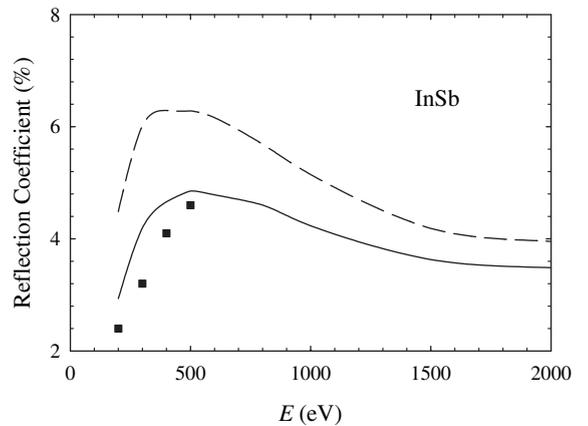


Fig. 2. A plot of the elastic reflection coefficient of electrons elastically backscattered from InSb. Solid and dashed curves are the results calculated with and without the SEP, respectively. Experimental data [15] (squares) are included for comparison.

[11,12,14]. Fig. 2 shows a plot of the calculated results (solid curve) as a function of electron energy for InSb. In the simulations, input data on electron inelastic mean free path were calculated using the present model for valence and partial 4d electrons and the local plasma approximation [15] for other inner shell electrons. For a comparison, measured data [16] (squares) and calculated results without the SEP (dashed curve) are also plotted. It is seen that the present results including the SEP agree better than those without the SEP as compared to experimental data.

4. Conclusions

Surface excitations are the important mechanism responsible for the energy loss of electrons in electron spectroscopies. The description of surface excitations was based on the extended Drude model which characterized the dielectric response functions. Experimental data taken from the optical ellipsometry for small energy transfers (<6 eV) and the energy-loss measurement for large energy transfers were used to obtain parameters in the model dielectric functions for GaP, GaAs, GaSb, InAs and InSb. Care was taken in the fittings of these dielectric functions against errors in ε_1 near energy transfers corresponding to $\varepsilon_1 = -1$, where any small difference in ε_1 could generate a large deviation in the surface loss-function. Using these model dielectric functions, the calculated SEPs for

the III–V semiconducting compounds were fitted very well to a simple formula. For other crossing angles, one should multiply Eq. (5) by $(\cos \alpha)^{-1}$ [1], where α is the angle between electron velocity and surface normal.

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