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Surface excitation parameter for electrons crossing the AlN surface

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Abstract

Fast electrons crossing a solid surface induce surface excitations. The total probability of such excitations for electrons moving outside the solid, i.e. in vacuum, is characterized by the surface excitation parameter (SEP). In the present work, the SEP was calculated for either incident or escaping electrons with normal or glancing crossing angles over the surface of aluminum nitride (AlN), a wide-band-gap semiconductor. These calculations were performed based on the dielectric response theory using the sum-rule-constrained extended Drude dielectric function with parameters obtained from a fit of this function to experimental optical data and electron energy-loss data. Dependences of the SEP on electron energy and crossing angle were analyzed. A simple formula was proposed for the fitting of SEP as a function of electron energy and crossing angle.

Keywords: Electron; Surface excitation parameter; Dielectric function; AlN

1. Introduction

In the rapid development of mesoscopic science, the study of surface excitations is of growing interest in surface-sensitive electron spectroscopies. Recent investigations on the energy-loss spectra of electrons reflected from solid surfaces [1–3] have demonstrated that the contribution from surface excitations to the spectra was important for electrons in the energy range of a few hundred eV to ~2 keV. The improvement in the quantitative surface analysis was significant when surface excitations were considered. Such excitations were conveniently characterized by the so-called surface excitation parameter (SEP), which describes the total probability of surface excitations for electrons moving outside the solid, i.e. in vacuum, before impinging on or after escaping from the solid surface [4].

Theoretical approaches [4–11] have been proposed for the calculations of the SEP. Previously, Kwei et al. [4,11] developed a model to calculate the SEP for normally incident and escaping electrons. Recently, Li et al. [12] modified the model for an application to electrons with arbitrary crossing angles. In the present work, we used Li's model to calculate the SEP for obliquely incident and escaping electrons crossing the surface of aluminum nitride (AlN), a material which is of interest in the application of high-power, high-temperature electronics [13–17]. These calculations were performed based on the dielectric response theory using an extended Drude dielectric function with parameters obtained from a fit of this function to experimental optical data and electron energy-loss data [18,19]. Sum rules were employed to check the accuracy of these parameters. Dependences of the SEP on electron energy and crossing angle were analyzed.

2. Methods

When an electron moves inside a solid, surface and volume excitations are treated together by the use of a depth-independent inelastic mean free path (IMFP) owing to the approximate compensation of these excitations at any given depth [4,11]. Since only surface excitations are possible for an electron moving outside the solid, an SEP is defined as the total probability of surface excitations for the electron moving in vacuum. The SEP can be calculated as an integration of the inverse IMFP over electron path length in vacuum.

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Based on the dielectric response theory, electron inverse IMFP is derived by solving Poisson equations in the Fourier space of scalar potentials and applying boundary conditions. For obliquely escaping (from solid to vacuum: $s \to v$) and incident (from vacuum to solid: $v \to s$) electrons, the SEP may be given by [12]

$$P_s^{s\to v}(\alpha,E) = \frac{4\cos\alpha}{\pi^3}\int_{-\infty}^{0} dr \int_0^E d\omega \int_{q_-}^{q_+} dq \int_0^{\pi/2} d\theta \times \int_0^{2\pi} d\phi \left[2\cos\left(\frac{\tilde{\omega} r}{v}\right) - \exp(-|r|Q\cos\alpha)\right] \times \frac{q\sin^2\theta\exp(-|r|Q\cos\alpha)}{\tilde{\omega}^2 + Q^2 v_\perp^2} \times \mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)+1}\right], \quad (1)$$

and

$$P_s^{v\to s}(\alpha,E) = \frac{4\cos\alpha}{\pi^3}\int_{-\infty}^{0} dr \int_0^E d\omega \int_{q_-}^{q_+} dq \int_0^{\pi/2} d\theta \times \int_0^{2\pi} d\phi \frac{q\sin^2\theta\cos(q_z r\cos\alpha)}{\tilde{\omega}^2 + Q^2 v_\perp^2} \times \exp(-|r|Q\cos\alpha) \times \mathrm{Im}\left[\frac{-1}{\varepsilon(q,\omega)+1}\right], \quad (2)$$

where $Q = q\sin\theta$, $q_z = q\cos\theta$, $v_\perp = \sqrt{2E}\cos\alpha$, and $\tilde{\omega} = \omega - qv\sin\theta\cos\phi\sin\alpha$. Here $\varepsilon(q,\omega)$ is the dielectric function, q is the momentum transfer, ω is the energy transfer, E is the electron energy, and $q_\pm = \sqrt{2E} \pm \sqrt{2(E-\omega)}$ are derived from conservations of energy and momentum. The crossing angle, α, is the angle between the surface normal and electron velocity.

The response of electrons in the solid to an external electron may be described by a dielectric function. Assuming a linear superposition of oscillators for the valence band and outermost inner shells, the extended Drude dielectric function is given by [20]

$$\varepsilon(q,\omega) = \varepsilon_1(q,\omega) + i\varepsilon_2(q,\omega) = \varepsilon_B - \sum_i \frac{A_i}{\omega^2 - (\omega_i + (q^2/2))^2 + i\omega\gamma_i}, \quad (3)$$

where A_i, γ_i, and ω_i are, respectively, the oscillator strength, damping coefficient, and resonant frequency, all associated with the ith oscillator. The background dielectric function, ε_B, accounts for the influence of polarizable ion cores [21]. All parameters A_i, γ_i, ω_i, and ε_B in Eq. (3) are determined by the fits of $\varepsilon_1(0,\omega)$, $\varepsilon_2(0,\omega)$, $\mathrm{Im}\left[-1/\varepsilon(0,\omega)\right]$, and $\mathrm{Im}\left[-1/(\varepsilon(0,\omega)+1)\right]$ to experimental optical data and electron energy-loss data for AlN [18,19]. Sum rules [20] are used to check the accuracy of fitting parameters. Note that even though the fitting parameters are determined in the optical end at $q = 0$, they are also appropriate for $q \neq 0$ [22,23]. The deviation of this extension from the true dispersion relation makes only minor difference in the determination of SEPs.

3. Results and discussion

Eq. (3) was fitted to experimental data for AlN. A comparison between the present fittings (solid curves) and experimental data [18,19] (dotted curves) on the real part of the dielectric function, $\varepsilon_1(0,\omega)$, the imaginary part of the dielectric function, $\varepsilon_2(0,\omega)$, the energy loss function for volume excitations, $\mathrm{Im}\left[-1/\varepsilon(0,\omega)\right]$, and the energy loss function for surface excitations [24,25], $\mathrm{Im}\left[-1/(\varepsilon(0,\omega)+1)\right]$, for AlN is shown in Fig. 1. It reveals that the present fittings are in good agreement with the experimental data. The volume and surface excitations exhibit resonant plasmon peaks at around 23 and 19 eV, respectively. The large plasmon energies and the broad peaks indicate that a free-electron-gas model is not valid for AlN.

An analysis of the calculated results for the SEP using Eqs. (1) and (2) yields a simple formula as follows

$$P_s^{s\to v}(\alpha,E) \text{ or } P_s^{v\to s}(\alpha,E) = \frac{aE^{-b}}{\cos^c\alpha}, \quad (4)$$

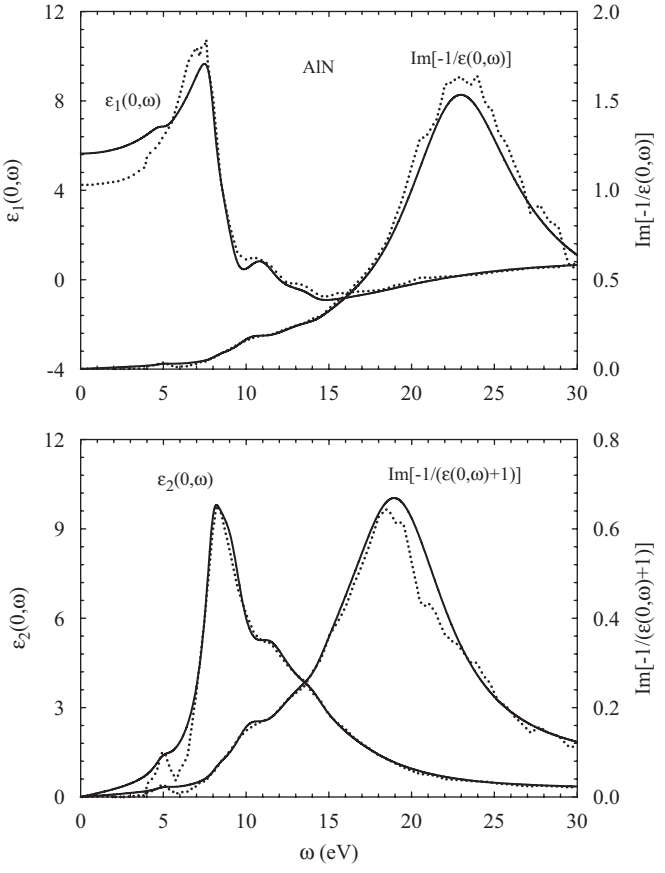

Fig. 1. A plot of the real and imaginary parts of the dielectric function, $\varepsilon_1(0,\omega)$ and $\varepsilon_2(0,\omega)$, and the volume and surface loss functions, $\mathrm{Im}\left[-1/\varepsilon(0,\omega)\right]$ and $\mathrm{Im}\left[-1/(\varepsilon(0,\omega)+1)\right]$, for AlN. Solid and dotted curves are, respectively, calculated results of the present work and experimental data [18,19].

where a, b, and c are the fitting coefficients. With E in electron volts, the best-fitted values of the parameters are $a = 1.2938$, $b = 0.4491$, and $c = 0.9173$ for escaping electrons, and $a = 0.6617$, $b = 0.4480$, and $c = 1.1551$ for incident electrons. Fig. 2 is a plot of the SEP as a function of the crossing angle for 800 eV electrons moving from AlN to vacuum. Solid circles, solid curve, dashed curve, and dotted curve are, respectively, calculated results using Eq. (1), Eq. (4), our previous model [4], and the Oswald's model [26]. It is seen that the fitting results using Eq. (4) are in good agreement with the calculated data using Eq. (1). It is also seen that the SEP increases with increasing crossing angle since glancing electron has longer interaction time with the surface. The difference between results of present (solid curve) and previous (dashed curve) models is due to the simplified $(\cos\alpha)^{-1}$ dependence of the SEP on crossing angle and no restriction on the normal component of momentum transfer in the previous model. A large discrepancy is found between the results calculated using present and Oswald's models. This is because Oswald's model is valid only for free-electron-like materials. AlN, however, is a semiconductor with wide band gap and complex band structure.

Fig. 3 shows a plot of the SEP as a function of electron energy for the crossing angle 60°. Solid and open circles are the calculated data using Eqs. (1) and (2) for escaping and incident electrons, respectively. Solid and dashed curves are the corresponding results calculated using the fitting formula, i.e. Eq. (4), for escaping and incident electrons. Also, results calculated using the Oswald's model (dotted curve) are included for comparisons. It is seen that the results using the formula of Eq. (4) are in good agreement with the calculated results using Eqs. (1) and (2). Again, the SEP decreases with increasing electron energy due to the shorter time for electron–surface interactions. Note that

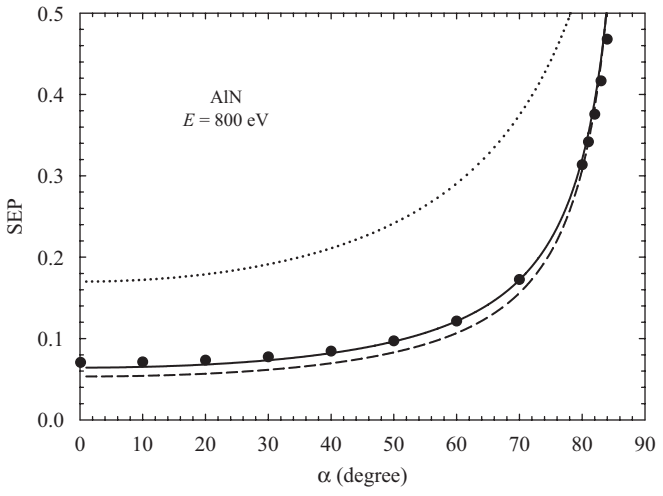

Fig. 2. A plot of the SEP as a function of crossing angle for 800 eV electrons moving from AlN to vacuum. Solid circles are the data calculated using Eq. (1). Solid, dashed, and dotted curves are, respectively, the results calculated using Eq. (4), our previous work [4], and the Oswald's model [26].

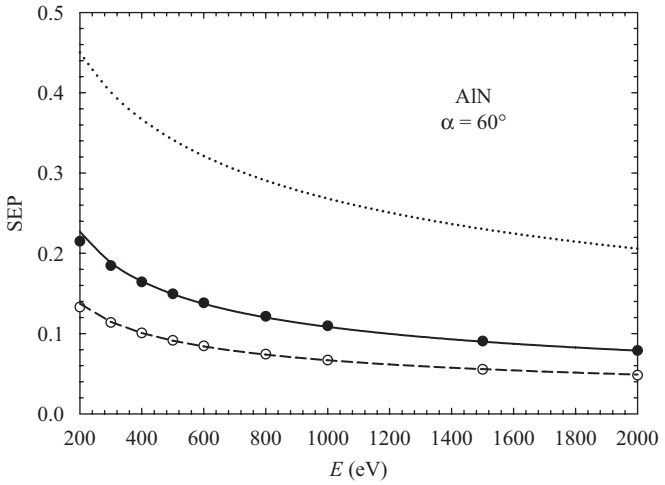

Fig. 3. A plot of the SEP as a function of electron energy for 60° crossing angle electrons across the AlN surface. Solid circles and solid curve are the results calculated using Eqs. (1) and (4) for escaping electrons, respectively. Open circles and dashed curve are the corresponding results calculated using Eqs. (2) and (4) for incident electrons. The dotted curve is the data calculated using the Oswald's model [26].

the Oswald's free-electron-gas model works poorly for AlN. The different results for escaping and incident electrons are due to the different attractive forces on the electron by the surface-induced charges, which decelerate and accelerate the escaping and incident electrons, respectively. Therefore, the probability of surface excitations for escaping electrons is larger than that for incident electrons.

4. Conclusions

The high thermal conductivity of AlN, a ceramic semiconductor, makes it an important material in the application of high power, high temperature electronics. In the present work, surface excitations were studied for energetic electrons passing through the AlN surface. The SEP for electrons crossing the AlN surface, either incident on or escaping from the solid, was calculated. These calculations were performed for various electron energies and crossing angles using the sum-rule-constrained extended Drude dielectric function with parameters obtained by a fit of this function to the experimental optical data and electron energy-loss data. A simple formula was proposed for the fitting of SEP as a function of electron energy and crossing angle.

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