Available online at www.sciencedirect.com
ScienceDirect
Surface Science 600 (2006) 3690–3694
SURFACE SCIENCE
www.elsevier.com/locate/susc

# Angular and energy dependences of the surface excitation parameter for electrons crossing a solid surface

C.M. Kwei [a], Y.C. Li [a], C.J. Tung [b,*]

[a] Department of Electronics Engineering, National Chiao Tung University, Hsinchu 300, Taiwan
[b] Department of Nuclear Science, National Tsing Hua University, Hsinchu 300, Taiwan

Available online 17 April 2006

**Abstract**

When fast electrons cross a solid surface, surface plasmons may be generated. Surface plasmon excitations induced by electrons moving in the vacuum are generally characterized by the surface excitation parameter. This parameter was calculated for 200–1000 eV electrons crossing the surfaces of Au, Cu, Ag, Fe, Si, Ni, Pd, MgO and $SiO_2$ with various crossing angles. Such calculations were performed based on the dielectric response theory for both incident (from vacuum to solid) and escaping (from solid to vacuum) electrons. Calculated results showed that the surface excitation parameter increased with crossing angle but decreased with electron energy. This was due to the longer time for electron–surface interaction by glancing incident or escaping electrons and by slow moving electrons. The results were fitted very well to a simple formula, i.e. $P_s = \frac{aE^{-b}}{(\cos\alpha)^c}$, where $P_s$ is the surface excitation parameter, $E$ is the electron energy, $\alpha$ is the angle between the electron trajectory and the surface normal, and $a$, $b$ and $c$ are material dependent constants.


*Keywords:* Electron; Surface excitation parameter; Glancing angle

## 1. Introduction

Quantitative information on inelastic interactions between electron and solid plays an important role in the surface sensitive spectroscopies such as Auger electron spectroscopy (AES), X-ray photoelectron spectroscopy (XPS) and reflection electron energy-loss spectroscopy (REELS), etc. Previous studies showed that surface excitations contributed significantly to the spectra of electrons backscattered from solid surfaces [1–3]. Therefore, an account of surface excitations in the analyses of electron spectroscopies should be established theoretically.

Many authors suggested that surface loss function could be used to estimate the contribution from surface excitations to electron inelastic cross-section [4–7]. This approach, however, was oversimplified and provided limited quantitative information on the characteristic energy loss spectra [8]. Later, the specular reflection model of the dielectric response theory was applied [1,9,10] to calculate the inelastic cross section due to surface excitations for an electron moving (in vacuum or solid) close to the surface. Recently, a surface excitation parameter (SEP) was introduced to characterize the average number of surface plasmons generated by an electron moving across the solid surface [2,11,12]. In the article of Tung et al. [2], they calculated the SEP by assuming that surface excitations occurred right on the surface. But actually surface excitations were possible for an electron moving at the position extending to a few angstroms on both sides of the surface. Chen and Kwei [11] derived the SEP by an integration of the inverse inelastic mean free path (IMFP) for surface excitations over electron path length across the surface on both sides. In their approach, plasmon excitations inside the solid were separated into individual contributions from surface and volume excitations. Because the compensation of surface and volume excitations led to a roughly depth-independent IMFP [12], it was more convenient to deal with surface and volume excitations together rather than separately inside the solid. Kwei et al. [12] then

* Corresponding author. Tel./fax: +886 3 5727300.
*E-mail address:* cjtung@mx.nthu.edu.tw (C.J. Tung).

0039-6028/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.susc.2006.01.071

calculated the SEP by integrating the inverse IMFP over electron path length in vacuum for normally incident and escaping electrons. For tilted crossing electrons, the SEP was approximated by multiplying the SEP for $\alpha = 0°$ (the crossing angle) by $(\cos\alpha)^{-1}$. In their work, however, conservations of energy and momentum were not completely satisfied due to the treatment of momentum transfer in cylindrical coordinates that carried no restriction on the normal component. In order to satisfy conservations of energy and momentum, spherical coordinates [13] should be adopted. The newly developed model by the present authors applied spherical coordinates in the derivation of position-dependent inelastic cross-section for an electron with arbitrary crossing angle [14].

In the present work, the newly developed model was applied to calculate crossing-angle-dependent and energy-dependent SEPs for 200–1000 eV electrons crossing several solid surfaces. The calculated results were compared with corresponding data of other works [12,15,16]. The presently calculated SEPs were fitted to a simple formula for the convenience of applications. The best-fitted parameters of various materials were listed.

## 2. Methods

Using the dielectric response theory, a modified inelastic-scattering model was developed for an electron moving normally or obliquely across the solid surface [14]. In this model, the SEP was determined by an integration of the inverse IMFP over electron path length in vacuum [12]. Consider a semi-infinite solid ($r > 0$) of dielectric function $\varepsilon(\vec{q}, \omega)$, where $\vec{q}$ is the momentum transfer, $\omega$ is the energy transfer, and $r$ is the radial distance from the crossing point on the surface. The SEPs for escaping (from solid to vacuum: s → v) and incident (from vacuum to solid: v → s) electrons are given by

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

and

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

where $\tilde{\omega} = \omega - qv\sin\theta\cos\phi\sin\alpha$, $Q = q\sin\theta$, $q_z = q\cos\theta$, $q_\pm = \sqrt{2E} \pm \sqrt{2(E-\omega)}$, $v_\perp = v\cos\alpha$, $v$ is electron velocity, and $E = \frac{v^2}{2}$ is electron kinetic energy. The crossing angle $\alpha$ is defined as the angle between surface normal and electron direction. Note that atomic units (a.u.) are used throughout this paper unless otherwise specified. The calculated

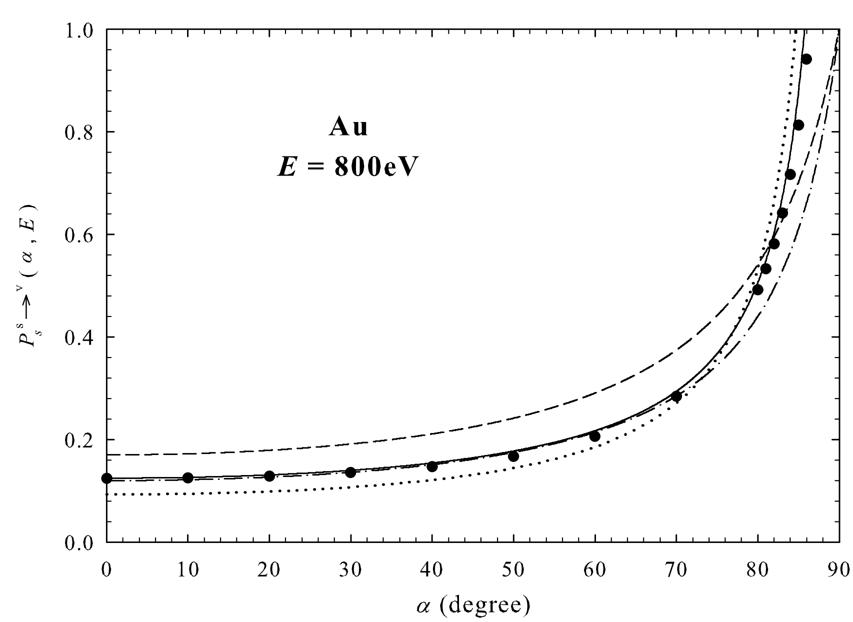


Fig. 1. Crossing-angle-dependent SEPs calculated using Eq. (1) for 800 eV electrons escaping from Au to vacuum (solid circles). The solid curve is a fit of the calculated results using Eq. (3). The dashed, dash–dot and dotted curves are, respectively, the results of Oswald [15], Werner et al. [16] and our previous work [12].

SEPs using Eqs. (1) and (2) were found to follow a simple formula

$$P_s^{s\to v}(\alpha, E) \quad \text{or} \quad P_s^{v\to s}(\alpha, E) = \frac{aE^{-b}}{\cos^c \alpha}, \tag{3}$$

for both escaping and incident electrons.

## 3. Results and discussion

In the present work, the extended Drude dielectric function was applied to calculate the SEP for an electron incident into or escaping from the solid. The fitting parameters of the dielectric function were taken from our previous work [13,17]. Fig. 1 shows the crossing-angle-dependent SEPs calculated using Eq. (1) for 800 eV escaping electrons moving from Au to vacuum (solid circles). It can be seen that the SEP increases with increasing crossing angle $\alpha$. For $\alpha > 70°$, the SEP increases rapidly, indicating a high probability of surface excitations for glancing emergence electrons. The results of Oswald [15] (dashed curve), Werner et al. [16] (dash–dot curve) and our previous work [12] (dotted curve) are included in this figure for comparisons. These results correspond to calculations based on the simple assumption of a cosine dependence on the crossing angle. The present calculations, however, are based on the derived formulas of the angular dependence using the dielectric response theory. It reveals from the comparisons that the cosine assumption works only approximately. The presently calculated SEPs are fitted to Eq. (3) with fitting results plotted as solid curves. With $E$ in electron-volts, we list best-fitted values of parameters $a$, $b$ and $c$ in Table 1 for all solids studied. These fitting values are different from the corresponding values of our previous work for

Table 1
Fitted values of parameter $a$, $b$ and $c$ in Eq. (3)

| | $P_s^{s\to v}$ | | | $P_s^{v\to s}$ | | |
|---|---|---|---|---|---|---|
| | $a$ | $b$ | $c$ | $a$ | $b$ | $c$ |
| Au | 1.8695 | 0.4052 | 0.80 | 1.8848 | 0.5060 | 1.06 |
| Cu | 1.9994 | 0.4166 | 0.82 | 1.2999 | 0.4664 | 1.13 |
| Ag | 2.1203 | 0.4260 | 0.74 | 1.4260 | 0.4821 | 1.05 |
| Fe | 1.9489 | 0.4321 | 0.80 | 1.2562 | 0.4827 | 1.05 |
| Si | 1.7295 | 0.4201 | 0.83 | 1.1313 | 0.4756 | 1.12 |
| Ni | 2.1712 | 0.4283 | 0.79 | 1.4244 | 0.4786 | 1.03 |
| Pd | 2.0564 | 0.4177 | 0.79 | 1.4934 | 0.4843 | 1.03 |
| MgO | 0.7535 | 0.3771 | 0.85 | 0.6413 | 0.4634 | 1.09 |
| $SiO_2$ | 0.5707 | 0.3764 | 0.85 | 0.5095 | 0.4687 | 1.08 |

$\alpha = 0°$ [12] where conservations of energy and momentum are not completely satisfied by the adoption of cylindrical coordinates there. Fig. 2 shows the energy-dependent SEPs calculated using Eq. (1) for electrons escaping from Ni to vacuum at $\alpha = 60°$ (solid circles). Again, solid, dashed, dash–dot and dotted curves are, respectively, the results of fittings, Oswald, Werner et al., and our previous work. It shows that the SEP decreases with increasing electron energy because of the less interacting time for surface excitations.

Similarly, the SEPs calculated using Eq. (2) as a function of crossing angle for 800 eV electrons incident from vacuum to Fe are plotted in Fig. 3. The SEPs as a function of energy for electrons incident from vacuum to Pd for $\alpha = 60°$ are plotted in Fig. 4. In both figures, symbols and curves have the same meanings as those described above. Note that the SEPs for incident electrons exhibit similar energy and angular dependences as for escaping electrons. However, the SEPs for incident electrons have

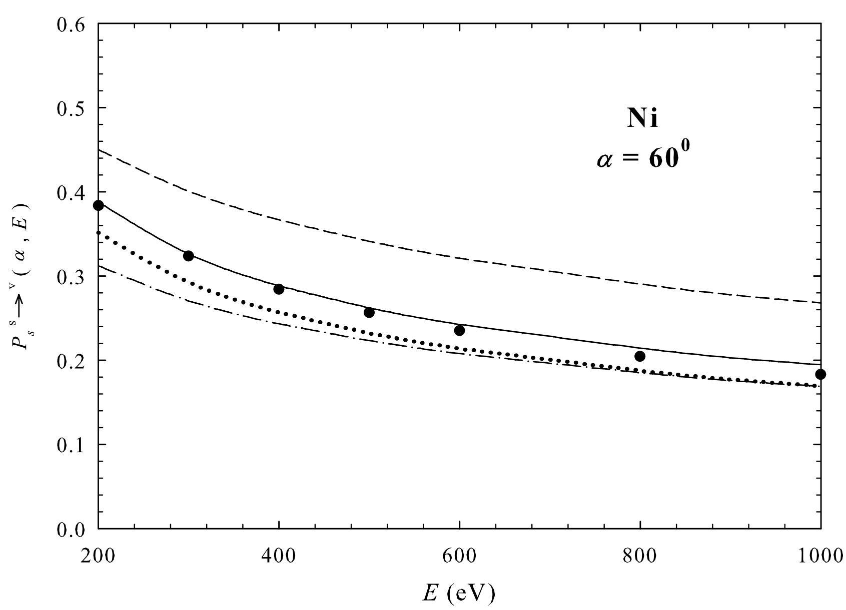


Fig. 2. Energy-dependent SEPs calculated using Eq. (1) for electrons escaping from Ni to vacuum at $\alpha = 60°$ (solid circles). The solid curve is a fit of the calculated results using Eq. (3). The dashed, dash–dot and dotted curves are, respectively, the results of Oswald [15], Werner et al. [16] and our previous work [12].

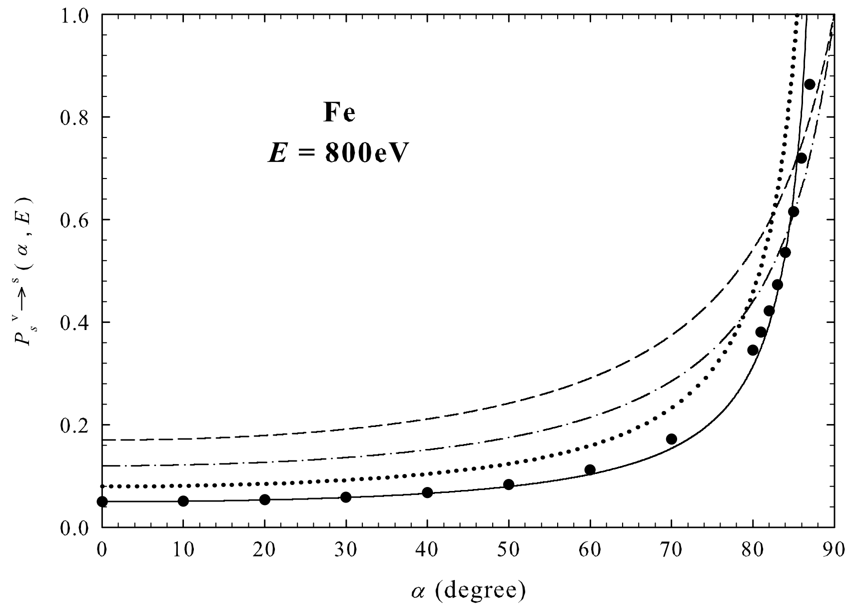


Fig. 3. Crossing-angle-dependent SEPs calculated using Eq. (2) for 800 eV electrons incident from vacuum to Fe (solid circles). The solid curve is a fit of the calculated results using Eq. (3). The dashed, dash–dot and dotted curves are, respectively, the results of Oswald [15], Werner et al. [16] and our previous work [12].

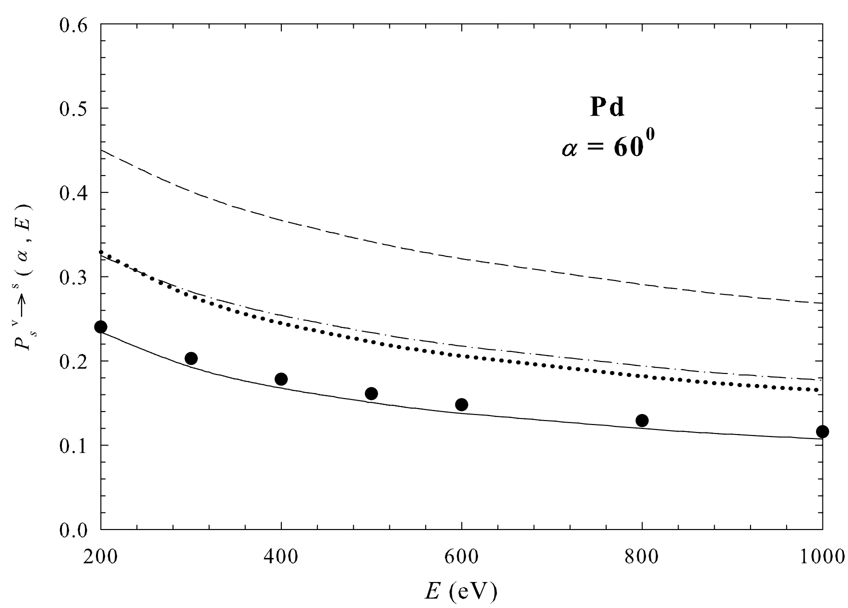


Fig. 4. Energy-dependent SEPs calculated using Eq. (2) for electrons incident from vacuum to Pd at $\alpha = 60°$ (solid circles). The solid curve is a fit of the calculated results using Eq. (3). The dashed, dash–dot and dotted curves are, respectively, the results of Oswald [15], Werner et al. [16] and our previous work [12].

smaller values than for escaping electrons. This is because the attractive force acting on the incident electron (in vacuum) by the surface induced charges accelerates the electron. On the other hand, the attractive force on the escaping electron (in vacuum) decelerates the electron. Therefore, the time spent near the surface for incident electron is less than for escaping electron, thus leading to less surface excitations for incident electron.

## 4. Conclusions

Applying the recently constructed dielectric model for inelastic cross sections, we calculated the crossing-angle-dependent and energy-dependent SEPs for electrons crossing solid surfaces, such as Au, Cu, Ag, Fe, Si, Ni, Pd, MgO and $SiO_2$. Calculations were performed using the extended Drude dielectric functions derived from optical data. The calculated results showed that the SEP increased with crossing angle due to the longer time for electron–surface interaction by glancing incident or escaping electrons. Also, the SEP decreased with electron energy due to the shorter time for electron–surface interaction by fast moving electrons. The presently calculated SEPs were fitted very well to a simple formula. This formula may be applied to the analyses of the intensity reduction for reflected or emitted electrons in surface and interface analyses.

## Acknowledgement

This research was supported by the National Science Council of the Republic of China under Contract No. NSC94–2215–E–009–080.

## References

[1] F. Yubero, S. Tougaard, Phys. Rev. B 46 (1992) 2486.
[2] C.J. Tung, Y.F. Chen, C.M. Kwei, T.L. Chou, Phys. Rev. B 49 (1994) 16684.
[3] Y.F. Chen, P. Su, C.M. Kwei, Phys. Rev. B 50 (1994) 17547.
[4] G. Chiarello, E. Colavita, M. De Cresenzi, S. Nannarone, Phys. Rev. B 29 (1984) 4878.
[5] Y. Ohno, Phys. Rev. B 39 (1989) 8209.
[6] J.C. Ingham, K.W. Nebesny, J.E. Peemberton, Appl. Surf. Sci. 44 (1990) 279.
[7] F. Yubero, J.M. Sanz, E. Elizalde, L. Galan, Surf. Sci. 237 (1990) 173.
[8] F. Yubero, S. Tougaard, Surf. Interf. Anal. 19 (1992) 269.
[9] F. Yubero, J.M. Sanz, B. Ramskov, S. Tougaard, Phys. Rev. B 53 (1996) 9719.
[10] A.C. Simonsen, F. Yubero, S. Tougaard, Phys. Rev. B 56 (1997) 1612.
[11] Y.F. Chen, C.M. Kwei, Surf. Sci. 364 (1996) 131.
[12] C.M. Kwei, C.Y. Wang, C.J. Tung, Surf. Interf. Anal. 26 (1998) 682.
[13] C.M. Kwei, S.J. Hwang, Y.C. Li, C.J. Tung, J. Appl. Phys. 93 (2003) 9130.
[14] Y.C. Li, Y.H. Tu, C.M. Kwei, C.J. Tung, Surf. Sci. 589 (2005) 67.
[15] R. Oswald, Ph.D. thesis, University of Tübingen, Tübingen, 1997.
[16] W.S.M. Werner, W. Smekal, C. Tomastik, H. Störi, Surf. Sci. 486 (2001) L461.
[17] C.M. Kwei, Y.F. Chen, C.J. Tung, J.P. Wang, Surf. Sci. 293 (1993) 202.