Quantification of Surface Effects in Electron Spectroscopy

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The contribution of surface excitations towards energy spectra of electrons depends on kinetic energy and the direction of motion of electrons. The quantification of influence of surface excitations in electron spectroscopy is investigated through determination of surface excitation parameter (SEP), which indicates the total probability of surface plasmons created by an electron while crossing the solid surface layer. The theoretical treatment to obtain this parameter in this work is based on complex self energy formalism of an electron interacting with the semi-infinite medium, which provides complete information about the position and angular dependence of differential inelastic scattering cross sections. The formulation is based on quantum mechanical approach and uses Drude-Lindhard model bulk dielectric function. SEPs vs electron kinetic energy of range 100-5000 eV for Cu and for different incident/escape angles have been numerically calculated. It is observed that SEP decreases with the increase in electron energy, and, increases with the increasing oblique angles. The calculated SEP was fitted to an empirical equation as a function of energy and angle.

1. Introduction

Comprehensive understanding of electron-solid and electron-surface interactions is an essential step towards quantitative analysis of surface sensitive electron spectroscopies such as AES, XPS and REELS The discrepancies between experimentally measured intensities and theoretical calculations of electron energy loss spectra provide the evidence of surface effects [1-3]. Surface excitations occur at the termination of bulk material and are basically surface version of the corresponding bulk excitation. Tougaard et.al. [1] studied energy loss-spectra of electrons reflected from solid surfaces both experimentally and theoretically and emphasized the importance of inclusion of surface effects for quantitative analysis. The deviations between theory and experiment at low energies were attributed to non uniform scattering properties of medium, i.e., the probability for excitations of surface plasmons is higher when the electron is near surface region. Surface plasmon, a collective excitation of weakly bound solid state electrons as a consequence of coulomb interactions with the incident electron at the surface, was first theoretically predicted by Ritchie [4]. These collective surface waves of the electric field cause dissipation of the energy of the incident electrons while crossing the surface.

Surface effects are commonly neglected in simple formulation of quantitative analysis. However, investigation of surface effects remains an important and interesting area of study and recently has attained a focus of interest as a prerequisite for quantitative evaluation of electron inelastic mean free path (IMFP) through the analysis of electron energy loss spectra. Surface excitations are a competitive phenomenon as it may reduce the yields of other scattering processes [5] e.g., elastic peak intensity [6], intensity of elastic backscattering and of XPS and AES peaks [7]. The intensity of AES and XPS peaks depends both on the inelastic scattering probability inside the solid, as well as on the surface excitations. Therefore, any theory which deals with the intensities and yields of surface sensitive scattering processes should include the effects of surface excitations.

Electrons, which passed through the surface layer of a solid, undergo variety of elastic and inelastic scattering processes. The accuracy of the quantitative analysis of the electron energy spectra depends on the models for these scattering processes. The inelastic interactions in the medium comprise mainly bulk and surface excitations. Electrons near the surface are responsible for surface excitations, while those deep inside the bulk contribute mostly to bulk excitations. The quantification of surface excitations for quantitative analysis can be characterized by the determination of surface excitation parameter (SEP), which provides the information about the number of surface plasmons created by an electron while crossing a solid surface. All electrons detected in these surface sensitive spectroscopies, AES, XPS and REELS, have passed the surface region of the solid once or twice. It is essential to account for surface effects characterized by SEP in order to improve the accuracy of interpretation of electron energy loss spectra.

Abundant literature has been published on the surface excitation processes [1-16]. Several attempts have also been made, with different levels of sophistication for quantification of surface effects through determination of SEP either by adopting experimental methods [5-8] or by theoretical treatment based on dielectric theory [17-26]. Ritchie [4] derived differential probability for surface excitations for normal incidence of an electron without considering the recoil effect [36]. Rather [9] obtained the same quantity for obliquely incident electrons under the assumption of small scattering angle. Tung et.al. [17] derived electron differential inverse inelastic mean free paths (DIIMFPs) for volume plasmon excitations as well as for surface plasmon excitations for obliquely incident electrons with the recoil effect included and without the small-angle scattering approximation using dielectric response theory. Their calculations showed that the relative importance of surface to volume excitations depends on the solid material and on the electron energy. Chen et.al. [18] studied the influence of surface excitations on electrons elastically backscattered from Cu and Ag surfaces and found that surface effects significantly reduce the elastic reflection coefficient for low energy electrons and the surface excitations are important for large escape angles measured from surface normal. In another work, Chen [19] investigated the influence of surface excitations for quantitative analysis in XPS by considering differential surface excitation probability (DSEP). Chen and Kwei [20] included surface effects in the electron DIIMFP for surface electron spectroscopy. They studied the case of an electron penetrating into the vacuum from a solid and derived an expression for the position dependent DIMFP, which has contributions both from bulk and surface excitations. Surface term is restricted to a surface layer extending on both sides of the vacuum-solid interface and is considered as position and angle dependent. However, the bulk term is apparently taken as independent of position and emission angle. Kwei et.al. [21] made the argument in another work that both bulk and surface contributions are position-dependent but their sum, i.e., total electron IMFP inside the solid appeared to be spatially non-varying. With these considerations, they described the influence of surface excitations by electrons for the vacuum side in electron spectroscopies for different materials and for electron energy range of 200-2000 eV and calculated SEP from an integration of surface excitation probabilities over electron distance from the surface outside the solid for both incident and escaping electrons by the use of dielectric response theory. Elastic peak electron spectroscopy has been widely used to determine the IMFP in solids. Chen [22] studied the effect of surface excitations in determining the IMFPs for low energy electrons in Cu and Ag by calculating SEP and found that the relative difference between the IMFPs with and without surface excitation may reach 40% for low energy electrons. Gurban et.al. [8] included surface effects for determination of the IMFP of electrons by elastic peak electron spectroscopy through SEP correction factor. Werner et.al. [23-28] measured the REELS spectra for medium energy electrons and extracted SEP from these spectra by fitting the raw data to theory.

In this work, we will concentrate on the numerical calculation of SEP for Cu. We will first describe briefly a full quantum mechanical, non local as well as dispersive formulation of electron self energy using dielectric response theory [10-14] for an electron interacting with the semi-infinite medium. This formalism is particularly applicable also to non-free-electron materials [11-12]. In this theory, loss processes are represented by a complex self energy of electron, which summarizes all the complicated bulk and surface plasmon excitations. The theory is capable to consider the cases of electrons penetrating the solid surface from both solid and vacuum sides at an arbitrary incident or escape angle. The imaginary part of the complex self energy provides differential inelastic scattering cross sections. The numerical integration of these differential inelastic scattering cross sections over energy loss and electron distance from surface layer is performed to compute the SEPs for electron kinetic energy of range 100-5000 eV for Cu. The results are compared for cases of normal and parallel motion of electrons to the solid surface.

2. Self Energy Formalism

A quantum mechanical formulation of Flores and Garcia-Moliner [33] for the electron self energy at a surface using dielectric response function is considered. An extension [11-13] of this formalism provides complete information about the position and angular dependences of the differential scattering cross sections while the imaginary part of self energy gives energy loss cross section. With this formalism the specular surface reflection model [34-35] is used, in which the induced potential is determined by the real charge, its image charge, and the fictitious surface charges fixed by boundary conditions. The image charge and surface charges are responsible for the surface effect of electron inelastic scattering in the surface region. An electron moving in a semi-infinite medium for $z<0$ is considered in this formulation with velocity $\mathbf{v}=(v_{\parallel}, v_{\perp})$, where $v_{\parallel}$ and $v_{\perp}$ are, respectively, the parallel and the normal components of velocity vector $\mathbf{v}$ to the surface. The surface is considered at depth $z=0$ and vacuum side for $z>0$.

Assuming a vanishing surface potential and fast electron approximation, the random-phase-approximation self energy of an inhomogeneous system is expressed in terms of the bulk dielectric function of the specimen, for the cases of an electron moving towards the surface from the vacuum side [33] and from the solid side [11], and for the cases of an electron in the vacuum and in the solid, respectively, as follows:

$$\Sigma(z)=\begin{cases}\Sigma_1(z) & z>0, v_{\perp}<0\\ \Sigma_b+\Sigma_i(z)+\Sigma_S(z)+\Sigma_{i-S}(z) & z<0, v_{\perp}<0\\ \Sigma_1(z)+\Sigma_2(z) & z>0, v_{\perp}>0\\ \Sigma_b+\Sigma_i(z)+\Sigma_S(z) & z<0, v_{\perp}>0\end{cases}, \quad (1)$$

where Σ_b, $\Sigma_i(z)$, $\Sigma_S(z)$, $\Sigma_{i-S}(z)$ are, respectively, the position-independent bulk term, the position dependent image charge term, the surface charge term (see Eqs. (22)-(24) in Ref. [11]) and the term due to interference of the image charge and the surface charges (see Eq. (1) in Ref. [13]] of complex self energy.

3. Surface Excitation Parameter

Electrons impinging on a solid or escaping from it suffer losses in the surface layer due to variety of inelastic scattering events and, thus, the electron energy loss spectra have contributions from surface excitations whose effect may be characterized by the SEP.

The imaginary part of the differential self energy of an electron [13] provides information about the differential energy loss cross section with respect to energy loss ω depending on the distance z from the surface, the velocity vector $\mathbf{v}$ (or the angle α between the velocity vector and surface normal) and energy $E=v^2/2$ (the atomic units, $e=\hbar=m=1$, is used throughout),

$$\sigma(\omega|E,\alpha,z)=-\frac{2}{v}\,\mathrm{Im}\{\Sigma(\omega|E,\alpha,z)\}. \quad (2)$$

The differential energy loss cross section is decomposed into bulk term and surface term in the same manner as that self energy is divided into different terms according to contributions from real charge, image charge and surface charges [10-14]. Therefore, the differential inelastic cross section may be written as

$$\begin{aligned}&\sigma(\omega|E,\alpha,z<0)=\sigma_{bulk}(\omega|E)+\sigma_{surf}(\omega|E,\alpha,z<0)\\ &\sigma(\omega|E,\alpha,z>0)=\sigma_{surf}(\omega|E,\alpha,z>0)\end{aligned}, \quad (3)$$

where σ_{bulk} and σ_{surf} are, respectively, the position independent bulk term, and the position dependent surface term. The net surface term of differential scattering cross section inside the solid ($z<0$) is different for the case of electrons penetrating into the surface from the vacuum side ($v_\perp < 0$), and for the case of electrons moving towards the surface from the interior of the medium ($v_\perp > 0$). The different contributions of image charge term, σ_i, the surface charge term, σ_S, and the term due to interference of the image charge and the surface charges, σ_{i-S}, to net surface terms are given as:

$$\sigma_{surf}(\omega \mid E,\alpha,z<0) = \begin{cases} \sigma_i(\omega \mid E,\alpha,z)+\sigma_S(\omega \mid E,\alpha,z)+\sigma_{i-S}(\omega \mid E,\alpha,z) & v_\perp < 0 \\ \sigma_i(\omega \mid E,\alpha,z)+\sigma_S(\omega \mid E,\alpha,z) & v_\perp > 0 \end{cases} \quad (4)$$

Physically, the directional dependence of scattering cross section is attributed to the asymmetry of space due to the termination of solid material and existence of surface plane [13]. It should be noted that the surface term has different values for the same magnitude of $v_\perp$ but with opposite sign.

SEP indicates the total probability of surface plasmons created by an electron while crossing the solid surface layer once [17-32]. It physically provides an estimation of number of surface excitations for a given electron energy E and incident or escape angle, and, its value is obtained by doubly integrating the surface term of differential inelastic scattering cross section over the energy loss and the distance from the surface both inside and outside the solid. Firstly, the DSEP is defined as [20]

$$p_S(\omega|E,\alpha) = \int_{-\infty}^{+\infty} \frac{dz}{\cos\alpha}\, \sigma_{surf}(\omega|E,\alpha,z), \quad (5)$$

and then, the SEP as,

$$\begin{aligned} P_S(E,\alpha) &= \int_0^E d\omega \int_{-\infty}^{+\infty} \frac{dz}{\cos\alpha}\, \sigma_{surf}(\omega|E,\alpha,z) \\ &= \int_0^E d\omega\, p_S(\omega|E,\alpha) \end{aligned}. \quad (6)$$

The reverse order of integration to obtain SEP from differential inelastic cross section is adopted by Kwei [21]. It's worthwhile to mention that z is the perpendicular distance from the surface boundary and $z/\cos\alpha$ is the distance traveled by an electron incident or escaping at an angle α with respect to the surface normal. Therefore, if we define the normal SEP, $P_{S\perp}$, as the integration of differential inelastic cross sections simply over the perpendicular distance z, then SEP can be obtained by multiplying factor $(\cos\alpha)^{-1}$, as

$$\begin{aligned} P_S(E,\alpha) &= \frac{1}{\cos\alpha} \int_0^E d\omega \int_{-\infty}^{+\infty} dz\, \sigma_{surf}(\omega|E,\alpha,z) \\ &= \frac{1}{\cos\alpha} \int_0^E d\omega\, p_{S\perp}(\omega|E,\alpha) = \frac{P_{S\perp}(E,\alpha)}{\cos\alpha} \end{aligned}. \quad (7)$$

All electrons detected in a reflection electron energy loss spectroscopy (REELS) must pass through the surface region of the solid twice. Therefore the total surface excitation parameter (SEP) for REELS is given as:

$$\begin{aligned} &P_S^{total}(E,\alpha_{in},\alpha_{out}) = P_S(E,\alpha_{in}) + P_S(E,\alpha_{out}) \\ &= \frac{P_{S\perp}(E,\alpha_{in})}{\cos\alpha_{in}} + \frac{P_{S\perp}(E,\alpha_{out})}{\cos\alpha_{out}} \end{aligned}. \quad (8)$$

4. Results and Discussion

The self energy formalism is considered in this work for interaction of probing electrons with semi-infinite Cu medium to study contributions of surface effects in electron energy loss spectra through the determination of SEP. The dependence of SEP on electron kinetic energy E, direction of movement (i.e., the angle α between the surface normal and the moving direction of incident and escape electrons), the position of electrons (i.e., inside and outside of the solid), as well as DSEP on energy loss ω will be presented below.

Figure 1 illustrates the normal SEP as a function of electron energy E ranging 100-5000 eV and angle α for the case of electron moving towards Cu surface from solid side (escaping case, $v_\perp > 0$). It shows that normal SEP decreases with the increase of electron energy. Moreover, it can be observed that normal SEP

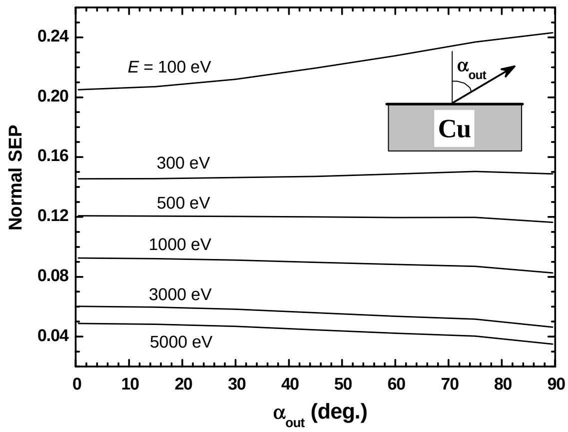

Fig. 1 A plot of normal SEP as a function of angle between electron velocity and surface normal escaping from Cu surface at different energies.

has higher values for larger oblique angles and at low electron energies. The figure also explains that the variation of normal SEP for smaller angles is weak but it increases for α very close to $\pi/2$ for low energy electron. However, in order to obtain SEP along the distance traveled by electron during its course of motion, the computed values of normal SEP are multiplied by the factor $(\cos\alpha)^{-1}$.

Figure 2 describes the variation of SEP as a function of electron energy for electrons escaping from Cu surface at different α angles ranging from 0.5° (i.e. electrons move nearly normal to the surface) to 89.5° (i.e. electrons move nearly parallel to the surface). This SEP has strong angular dependence particularly for α very close to $\pi/2$. The comparison of normal SEP and SEP shows that the factor $(\cos\alpha)^{-1}$ is significant at large oblique angles. For parallel motion of probing electrons along the surface boundary (i.e., $\alpha \sim \pi/2$), the actual distance traveled by electrons (i.e., $z/\cos\alpha$) is much larger than the perpendicular distance z from the surface. Moreover, this factor is an indirect way to account for the time spent by the probing electron near the surface. The larger the distance traveled by electron, longer the time spent in the vicinity of the surface boundary and therefore higher the probability of surface excitations. This observation is prominent particularly for low energy electrons.

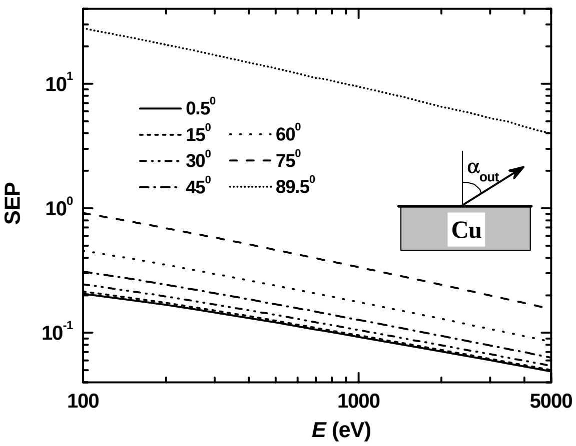

Fig. 2 A variation of SEP as a function of electron energy for electrons escaping from Cu at several typical angles. The large discrepancy between SEP values for small and large angles are due to $(\cos\alpha)^{-1}$ factor.

Figure 3 shows the plot of SEP vs electron energy for the cases of incoming and escaping electrons moving normal to the surface (α= 0.5°) and moving parallel (α= 89.5°) to the surface. The plot also compares the present SEP with the results of Chen et.al. [18] and Kwei et.al. [21]. The figure shows that SEP is higher for the case of electron escaping from the bulk region as compared to the case of an electron incident on solid with the same electron energy but with opposite direction of movement. The difference in SEP for the two opposite directions (i.e. incident and escape) of motion of electron is obvious for higher electron energies. This is due to the fact that surface terms involved in the calculation of differential energy loss cross section have different values for the same magnitude of vertical velocity $v_\perp$ but with opposite sign. Physically it can be explained in terms of asymmetry of space due to presence of surface boundary.

Figure 3(a) shows that our results for SEP almost coincide with that of Kwei et.al. [21] at low energies for normally escaping electron and at higher energies for normally incident electrons. The surface excitation parameter as reported by Chen et.al. [18] for normally incident electron also has similar variation with electron energy. Fig. 3(b) presents the results for electron moving nearly parallel to the surface (α= 89.5°) for an electron moving towards surface layer from solid side ($v_\perp > 0$) and vacuum side ($v_\perp < 0$). The increase of SEP at large angles reveals that surface excitations are more probable for glancing angles. This confirms the experimental observations [5-8] as well as the tendency agrees with the results of Chen et. al. [18] and Kwei et.al. [21].

Figure 4 explains the phenomenon of surface excitations in terms of DSEP as a function of energy loss ω at typical electron energy of 100 eV for incoming and escaping electron direction of motion and for normal and parallel movement of electron to the solid surface. The surface excitation mode for Cu metal constitutes a continuous distribution peaked at 3.5 and 7 eV. The DSEP decreases with the increase of electron energy. This is obvious because low energy electrons can spend more time near the surface region. The difference in the surface excitation probability for cases of escaping and incoming

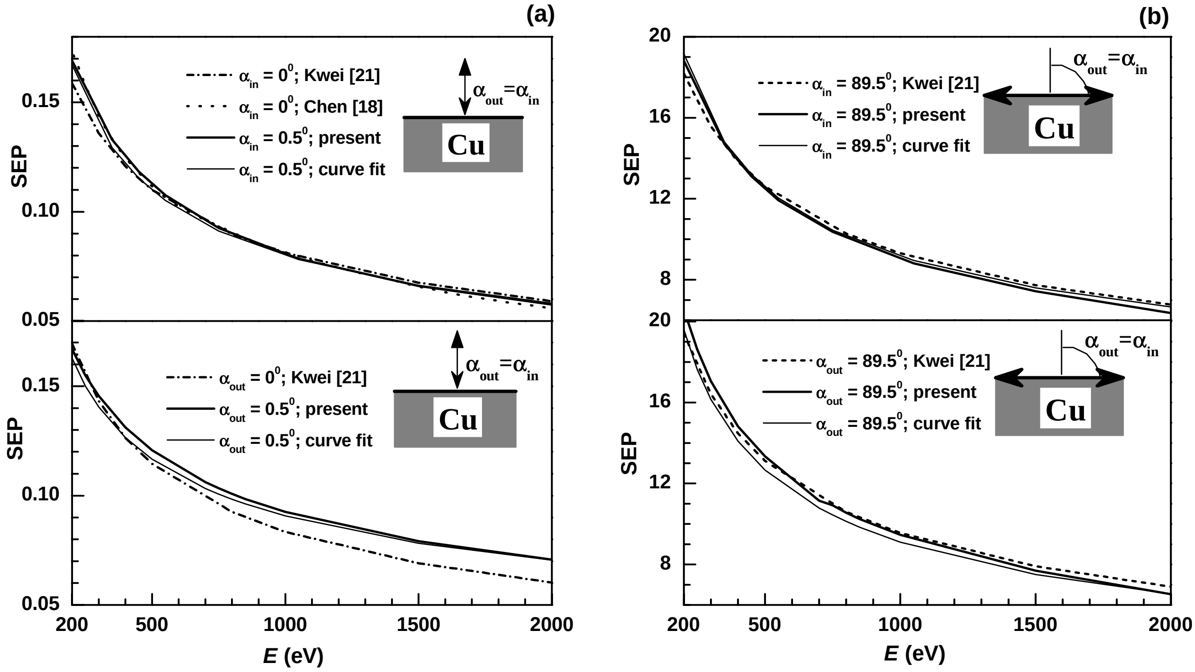

Fig. 3 SEP vs electron energy for nearly normal and parallel incident/escape electrons from Cu.

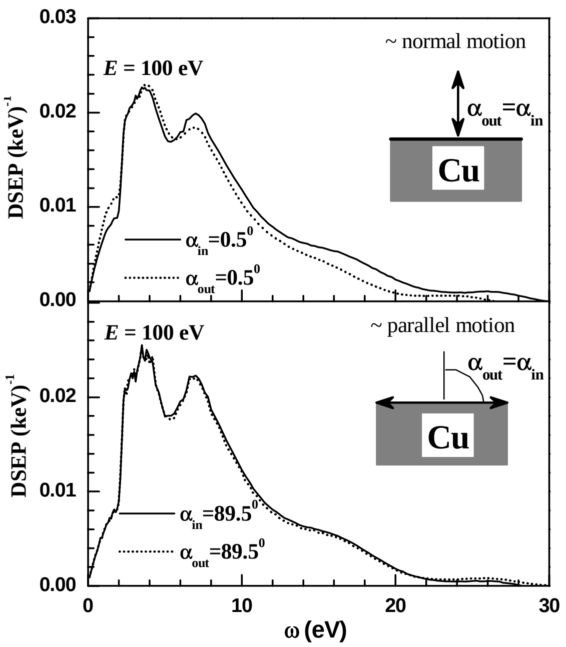

Fig. 4 Plot of energy loss dependence of DSEP for different conditions of electron motion.

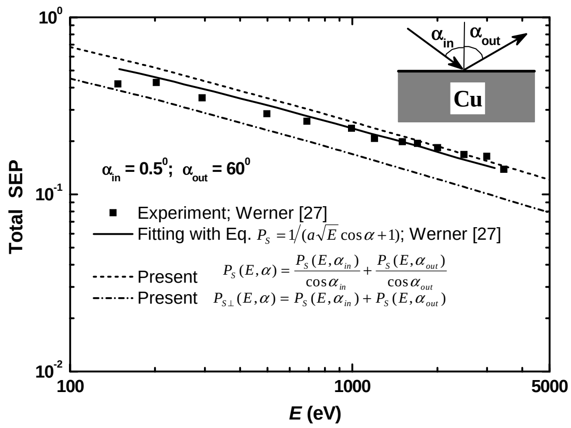

Fig. 5 A comparison of total SEP and total normal SEP as a function of electron energy with the results of Ref [27].

electron is expected due to the asymmetry of surface excitation mode.

Figure 5 provides a comparison of total SEP and normal SEP as a function of electron energy with the experimental results of Werner et.al. [27]. The total SEP is evaluated by computing the SEP for normal electron incidence (α_{in} = 0.5°) and for electron emission at angle α_{out} = 60° for Cu surface. Werner et.al. experimentally extracted the total SEP from REELS spectra by evaluating the ratio of the number of electrons which induced a surface excitation to the intensity of elastic peak. This quantity provides average number of surface excitations caused by an electron while crossing the solid surface in whole. The present result is in good agreement with experimental data at higher energies and also the overall tendency of calculated SEP with electron energy is similar to the experimental results.

The inverse inelastic mean free path (IIMFP) is obtained by numerically integrating differential energy loss cross section $\sigma(\omega \mid E, \alpha, z)$ as given in Eq. (3) over energy loss ω. Fig. 6 illustrates the E, α and z dependence of total IIMFP and surface term of IIMFP. Fig. 6(a) demonstrates the plot of IIMFP as a function of distance from the surface and electron energy for the case of an electron moving towards surface from bulk side (escaping case). The total IIMFP has contributions from both bulk and surface excitations in bulk region ($z < 0$), whereas in vacuum region ($z > 0$) contributions towards inelastic scattering events are due to surface excitations. In bulk region, the surface charge term cancels the contribution of image charge term (according to Eq. 4), which leads to negligible surface term of IIMFP. In contrary to this behavior in the bulk, there is a net surface term which peaks at the surface boundary and decays into the vacuum over distance of several Angstroms. Fig. 6(b) more clearly illustrates this tendency of surface IIMFP as a function of distance z from the surface for electron energy range 100-5000 eV. Surface excitations are more probable in vacuum region for equal distance from the surface boundary ($z = 0$). The surface term of IIMFP is peaked at the surface boundary and the peak value decreases with increasing electron energy. This is also observed in the calculations of SEP, which explains the importance of SEP for quantification of surface effects. The surface IIMFP has negative values near the vicinity of surface boundary in the bulk side due to begrenzung effect [37-39]. However, when the bulk term is added, the total IIMFP is positive as it can be observed in the plot of IIMFP shown in Fig. 6(a). A work is under process in which authors will consider the begrenzung effect in detail and results will be published elsewhere.

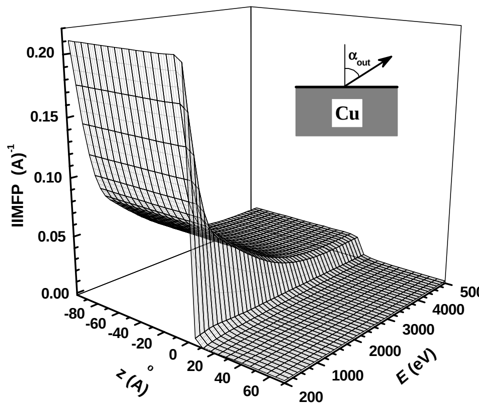

Fig. 6(a) A perspective view of IIMFP as a function of distance from the surface and electron energy for normally escaping electrons.

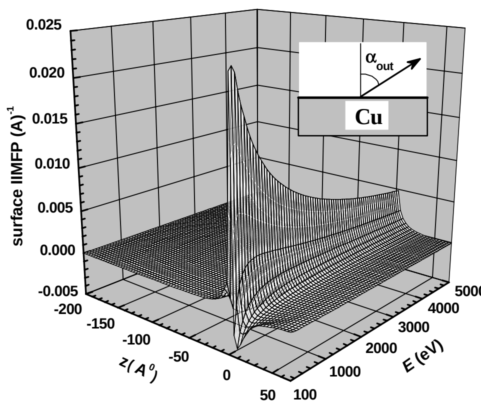

Fig. 6(b) A plot of surface IIMFP as a function of distance from the surface and electron energy for normally escaping electrons.

Fig. 7 presents total IIMFP for an electron escaping normally from the solid into vacuum region for electron energies of 500 eV, 800 eV and 1000 eV. The results are compared with the work of Kwei et.al. [21] and Chen et.al. [29, 32]. In vacuum region, IIMFP is solely due to surface excitations and it decays with sharp slope. This tendency of IIMFP in vacuum part is also observed in calculations of Kwei et.al. [21]. However, the decay behavior of IIMFP with the distance from surface in vacuum region for 500 eV in the work of Chen et.al. [32] is much slower than our present results as well as with their own results for 1 keV calculated by the same model [29]. In bulk region, our calculated IIMFPs for these typical electron energies are higher, which is due to the difference in calculating the position independent bulk term.

For practical usage the calculated SEPs vs electron energy at different incident or escaping angles are fitted by the following empirical equation,

$$P_S = \frac{a(\alpha)}{\cos\alpha} E^{-b(\alpha)}, \tag{9}$$

where

$a(\alpha) = a_1 - a_2 \cos\alpha; \quad b(\alpha) = b_1 - b_2 \cos\alpha$.

This fitting equation is capable to reproduce calculated data exactly for SEP at all possible values of angle α and for electron energy range 100-5000 eV. The values of parameters in curve fit are

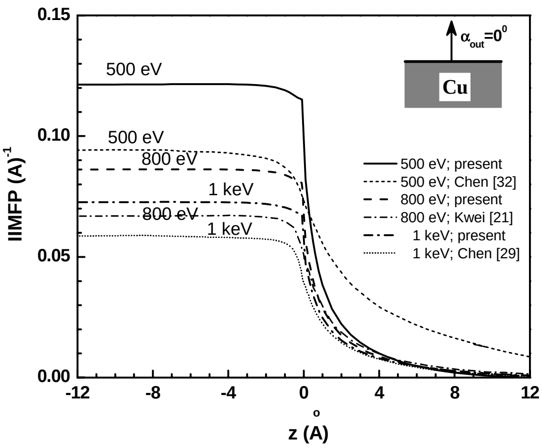

Fig. 7 A comparison of results for IIMFP as a function of distance from the surface at typical electron energies for normally escaping electrons.

a_1=2.14086, a_2=1.02271, b_1=0.4772 and b_2=0.1135 . However for incident electron case, the α -dependence of the SEP is found to be weak. Therefore we obtained the best fitting parameters as independent of incident angle α_{in} and the values of these parameters in the curve fit are $a = 1.90497$ and $b = 0.45922$ for the case of incident electron. The angular dependence of exponent b is considered to obtain best fit for numerically calculated SEP for practical use. Any fixed value of exponent for all emission angles such as in the results by other workers [6, 21, 29], does not provide best fit to the data for all emission angles in our present work. Werner et.al. [28] mentioned that in general energy dependence is different in different works. Chen obtained the value $b = 0.5$ by considering free electron gas model [32] in his formalism, which shows inverse square root energy dependence of SEP. Werner et.al. [27] also reported inverse square root energy dependence of SEP for non free electron like materials. Their expressions for SEP formula depicts that surface excitation parameter decreases linearly with the speed of the electron while crossing the surface boundary. The form of our best fitted equation to the surface excitation data shows that inverse square root energy dependence of SEP does not hold exactly. The exponent can be expressed in the form $b(\alpha)$=0.5(0.9544 − 0.227 cos α). Tanuma et.al. [6] and Kwei et.al. [21] also reported similar expressions for fitting equation with $b \neq 0.5$, however, in these cases exponent b is angle independent. For larger oblique angles and decreasing electron speed (lower electron kinetic energy), the probing electron spends more time in the vicinity of surface boundary and therefore may cause more surface excitations. The SEP increase with decreasing electron speed is not linear due to α-dependent exponent in our fitting equation. However, detailed investigation may be needed for physical explanation of α-dependence of exponent b or in other words the variation in the energy dependence of SEP with emission angle.

5. Summary and Conclusions

The influence of surface excitations in electron spectroscopy is investigated by considering the self energy of electron on the basis of quantum approach, which uses Drude-Lindhard model bulk dielectric function and its quantification through determination of surface excitation parameter (SEP). The present method of using self energy formalism makes it possible to compute SEP for non-free-electron materials and for all possible conditions, e.g. the kinetic energy of signal electrons, the direction of motion of electrons, the incident or escaping angle of electron and the material. The SEP is calculated in this work by doubly integrating the surface term of the differential inelastic scattering cross section with respect to the distance z from the surface and the electron energy loss ω, for the material Cu, electron energy of range 100-5000 eV, different values of angle α to the surface normal and for different direction of electron motion, i.e., either an electron is incident on solid target from vacuum side or it is escaped from bulk material into the vacuum.

The results are discussed only for nearly normal and parallel motion of electron to the surface. But a fitted expression of SEP has described all the calculated data as a function of α and E . The behavior of inelastic inverse mean free path (IIMFP) as a function of distance from the surface and differential surface excitation probability (DSEP) is also studied for different conditions of electron motion. The surface term of IIMFP is found to be peaked at the surface boundary, which showed that surface excitations are most probable at the surface layer. The DSEP is higher for lower electron energy loss. It is observed that SEP decreases with the increase in electron energy and increases with the increasing oblique angles.

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Comment by Dr. G. Gergely

The problem of surface excitation is a classical one since the historical work of Ritchie (1957). In 1994 Tung et. al. analysed experiments and improved results by taking into account surface excitation. The SEP parameter has been defined. The problem became the focus of interest since 2000 with the work of Tanuma et. al. (SIA 2000), analysing CMA experiments on Ni by Goto. Many new works have been published by Ding et. al., Werner (Surf. Sci. 2001) and Chen (Surf. Sci. 2002) and other authors. The physical models of Chen and Werner are different. In 2003 Werner et. al. (Phys. Rev. B 64 p155414) applied some results of Chen (2002). The main problem is: no reliable, exact experimental results are available. Good experiments needed for comparing them with calculated values are: The integrated elastic peak in absolute (%) units. Goto's CMA is promising for this purpose, but correction for energy resolution is absolutely necessary. The requirement of % units can be avoided by REELS spectra, measured at very good energy resolution, together with the elastic peak. Useful characteristic experimental parameters are: the intensity ratios of the elastic peak with the first plasmon peak (e.g. Si), or with the maximum of the adjacent minimum of the loss spectrum is of crucial importance, as shown by Nagatomi at PSA-04. These quantities are shown in our previous work J. Toth et. al. Vacuum 50 (1998) 479. According to Figs. 2 and 4, for Ni E=2 keV primary energy, the energy resolution should be better, than 200 meV. The angular variation of the elastic peak supply information on the angular dependence of SEP (cosine?), but absolute intensity (%) values are needed for the SEP parameter.

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