Memory effect on the inelastic interaction of electrons moving parallel to a solid surface

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It is generally assumed that two successive inelastic interactions between an electron and a solid are independent of each other. In other words, the electron has no memory of its previous interaction. However, the previous interaction of the electron generates a potential that should influence its succeeding inelastic interaction. The aim of this work is to establish a model to account for the memory effect of an electron between two successive inelastic interactions. On the basis of the dielectric response theory, formulae for differential inverse inelastic mean free paths (DIIMFPs) and inelastic mean free paths (IMFPs) considering the memory effect were derived for electrons moving parallel to a solid surface by solving the Poisson equation and applying suitable boundary conditions. These mean free paths were then calculated with the extended Drude dielectric function for a Cu surface. It was found that the DIIMFP and the IMFP with the memory effect for electron energy E lay between the corresponding values without the memory effect for electron energy E and previous energy E_0. The memory effect increased with increasing electron energy loss, $E_0 - E$, in the previous inelastic interaction. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: memory effect; inelastic interaction; surface excitation

INTRODUCTION

Various aspects of the interactions between a fast moving electron and a solid surface have been investigated theoretically and experimentally. Theoretical approaches[1–4] were developed to estimate the inelastic interaction cross sections under the assumption that two successive inelastic interactions between the electron and the solid were independent of each other. In other words, an electron differential inverse inelastic mean free path (DIIMFP) and an inelastic mean free path (IMFP) for the interaction depended on the energy of electron before this interaction, E, but not on its preceding inelastic interaction with the energy, E_0. However, a preceding interaction generates a potential that should influence the succeeding inelastic interaction. The coupling effect because of the induced field caused by the electron before and after the previous interaction should be taken into account in modeling electron inelastic cross sections for the following interaction.

In the present work, analytic formulae are derived to include the coupling effect, or the memory effect, in the inelastic cross sections of electrons moving parallel to a semi-infinite solid surface. Surface excitations by electrons traveling outside the solid were studied using dielectric response theory.[5] A sum-rule-constrained extended Drude

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dielectric function with the dispersion effect[6] was adopted. This function was previously employed to characterize the response of semi-infinite solids[7,8] and overlayer systems.[4,9,10] The formulae with the memory effect for electron DIIMFP and IMFP are applicable to all materials with known dielectric functions. Calculations of electron DIIMFP and IMFP are made here using these formulae for the Cu surface. Calculated results are compared to the corresponding data obtained without the memory effect.

THEORY

Figure 1 illustrates the problem studied in the present work. An electron of energy E_0 before any inelastic interactions moves along the y direction (parallel to the solid surface) at a distance d above the surface. The solid is characterized by the dielectric function $\varepsilon\left(\vec{k}, \omega\right)$, where $\vec{k}$ and ω are the momentum and energy transfers, respectively. At a point $y = 0$, this electron experiences an inelastic interaction and its energy decreases to E. This electron continues to move with the energy E until the occurrence of another inelastic interaction.

By solving the Poisson equation and applying the boundary conditions, the induced potential in the vacuum is given by

$$\varphi_{\text{ind}}(\vec{k}, \omega) = -\frac{4\pi^2}{k^2}[\delta(\omega - \sqrt{2E_0}k_y)$$

$$+ \delta(\omega - \sqrt{2E}k_y)] \cdot \left[e^{-K \cdot d}\frac{\varepsilon(\vec{K}, \omega) - 1}{\varepsilon(\vec{K}, \omega) + 1}\right] \quad (1)$$
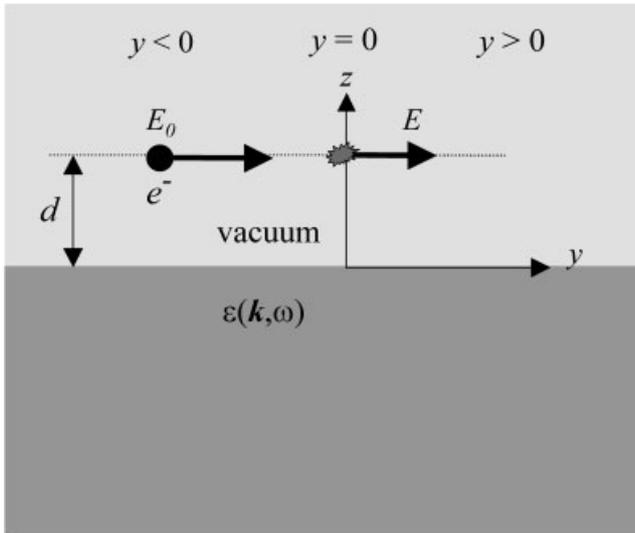
Figure 1. A sketch of the problem studied in the present work. An electron of energy E_0 moves along the y direction (parallel to the surface) at a distance d above the surface of a solid of dielectric function $\varepsilon(\vec{k}, \omega)$. At a point $y = 0$, this electron experiences an inelastic interaction and its energy decreases to E. Special interest is on the induced potential, the DIIMFP and the IMFP at $y > 0$.

where $\vec{k} = (k_x, k_y, k_z) = (\vec{K}, k_z)$. Here, the dependence of ε on k_z is neglected.[11–13] Considering the memory effect, the position-dependent DIIMFP for the succeeding interaction is given by[14]

$$
\mu(\omega, y) = \frac{\sqrt{2}}{\pi^2 \sqrt{E_0}} \int_{k_{\min}}^{k_{\max}} dk \int_{\omega/\sqrt{2E_0}}^{k} dK \frac{K}{k} \frac{1}{\sqrt{k^2 - K^2} \sqrt{2E_0 K^2 - \omega^2}}
$$
$$
\times \cos(d\sqrt{k^2 - K^2}) \cdot \left\{ \mathrm{Im} \left[e^{-K \cdot d} \frac{\varepsilon(K, \omega) - 1}{\varepsilon(K, \omega) + 1} \right] \right.
$$
$$
\times \cos \left(\frac{\sqrt{E} - \sqrt{E_0}}{\sqrt{2E_0 E}} \omega y \right) + \mathrm{Re} \left[e^{-K \cdot d} \frac{\varepsilon(K, \omega) - 1}{\varepsilon(K, \omega) + 1} \right]
$$
$$
\left. \times \sin \left(\frac{\sqrt{E} - \sqrt{E_0}}{\sqrt{2E_0 E}} \omega y \right) \right\} + \frac{\sqrt{2}}{\pi^2 \sqrt{E}}
$$
$$
\times \int_{k_{\min}}^{k_{\max}} dk \int_{\omega/\sqrt{2E}}^{k} dK \frac{K}{k} \frac{1}{\sqrt{k^2 - K^2} \sqrt{2E \cdot K^2 - \omega^2}}
$$
$$
\times \cos(d\sqrt{k^2 - K^2}) \cdot \mathrm{Im} \left[e^{-K \cdot d} \frac{\varepsilon(K, \omega) - 1}{\varepsilon(K, \omega) + 1} \right] \quad (2)
$$

where $k_{\max} = \sqrt{2E} + \sqrt{2(E - \omega)}$ and $k_{\min} = \sqrt{2E} - \sqrt{2(E - \omega)}$ are obtained from the conservation of energy and momentum. Taking $E_0 = E$, Eqn (2) reduces to the formula without the memory effect.[4] Note that all quantities in this work are expressed in atomic units (a.u.) unless otherwise specified.

According to the Poisson law, the probability for an inelastic interaction of an electron at a distance y is proportional to $(y/\lambda(y))e^{-y/\lambda(y)}$,[5,11] where $\lambda(y)$ is the position-dependent IMFP calculated by the inverse integration of $\mu(\omega, y)$ overall energy transfers. Thus the DIIMFP with the memory effect may be obtained by averaging overall

electrons paths

$$
\mu(\omega) = \frac{\int_0^\infty (y/\lambda(y))e^{-y/\lambda(y)} \mu(\omega, y) \mathrm{d}y}{\int_0^\infty (y/\lambda(y))e^{-y/\lambda(y)} \mathrm{d}y} \quad (3)
$$

Subsequently, the IMFP with the memory effect may be calculated from

$$
\lambda = \frac{1}{\int_0^E \mu(\omega) \mathrm{d}\omega} \quad (4)
$$

RESULTS AND DISCUSSION

DIIMFPs with the memory effect were calculated for electrons moving parallel to the Cu surface. In these calculations, the sum-rule-constrained extended Drude dielectric function was applied with parameters determined by a fit of this function to the optical data.[6] Figure 2 shows a plot of the DIIMFP with the memory effect as a function of energy transfer for electrons with $d = 1$ a.u., $E_0 = 800$ eV and $E = 500$ eV. Corresponding DIIMFPs without the memory effect for $E_0 = E = 800$ eV and $E_0 = E = 500$ eV are plotted for comparison. It is seen that the DIIMFP with the memory effect exhibits a similar shape to that of the DIIMFP without the memory effect. The magnitude of the DIIMFP with the memory effect for preceding and succeeding electron energies E_0 and E lies between the DIIMFPs without the memory effect for constant electron energies E_0 and E. This result indicates that the moving electron keeps some memory of its previous energy E_0 in the next interaction. A plot of the DIIMFP with the memory effect is shown in Fig. 3 for electrons with $E_0 = 500$ eV, $E = 300$ eV and $d = 1, 2$ and 3 a.u. above the Cu surface. These curves show that the DIIMFP decreases with increasing distance of the electron above the surface owing to the weaker response by the solid.
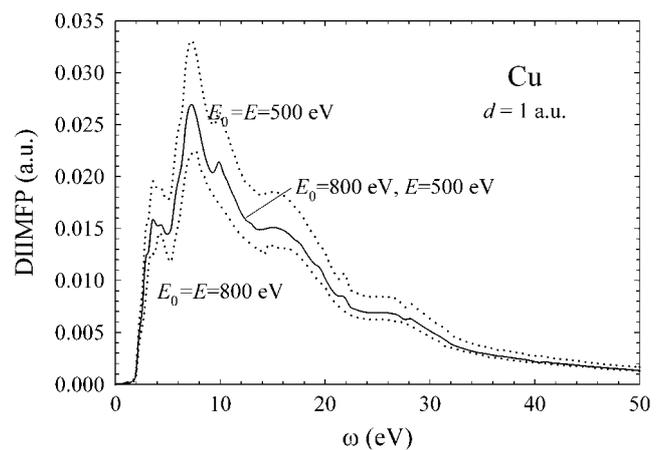

Figure 2. A comparison of the DIIMFPs with (solid curve) and without (dotted curves) the memory effect for electrons moving parallel to the Cu surface at a distance $d = 1$ a.u. The DIIMFP with the memory effect is calculated for preceding and succeeding electron energies $E_0 = 800$ eV and $E = 500$ eV. The DIIMFPs without the memory effect are calculated for constant electron energies $E_0 = E = 500$ eV and $E_0 = E = 800$ eV.
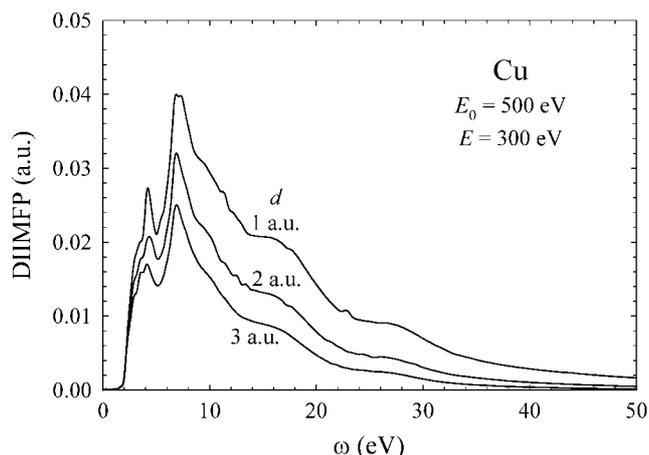
Figure 3. A plot of the DIIMFPs with the memory effect for electrons of preceding and succeeding energies $E_0 = 500$ eV and $E = 300$ eV. These electrons are moving at various distances d from the Cu surface.
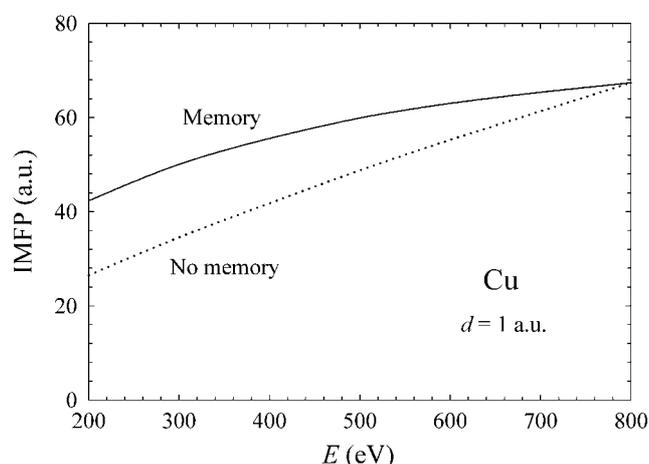

Figure 4. A comparison of the IMFPs with (solid curve) and without (dotted curve) the memory effect for electrons moving parallel to the Cu surface at a distance $d = 1$ a.u. The IMFP with the memory effect is calculated for a preceding electron energy $E_0 = 800$ eV as a function of succeeding electron energy E. The IMFP without the memory effect is calculated for constant electron energy $E_0 = E$.

A comparison of IMFPs with (solid curve) and without (dotted curve) the memory effect is shown in Fig. 4 for electrons moving parallel to the Cu surface at $d = 1$ a.u. The IMFP with the memory effect is calculated for preceding electron energy $E_0 = 800$ eV as a function of succeeding electron energy E. The IMFP without the memory effect is calculated for constant electron energy $E_0 = E$. At $E = 300$ eV, for instance, the solid and dotted curves correspond to $E_0 = 800$ eV (with memory effect) and $E_0 = 300$ eV (without memory effect), respectively. It should be noted that there is a significant difference between the solid and dotted curves. When the energy difference, $E_0 - E$, for the solid curve is large, the difference between solid and dotted curves is also large. At $E = 700$ eV, on the other hand, the solid and dotted curves correspond to $E_0 = 800$ eV and $E_0 = 700$ eV, respectively. In this case, the energy

difference is small, and the difference between the curves is also small. Thus the memory effect, proportional to the difference between solid and dotted curves, decreases with decreasing $E_0 - E$ and approaches zero at $E = E_0$. Moreover, the IMFP with the memory effect for given preceding energy E_0 and succeeding energy E is between the IMFPs without the memory effect for these given energies. The IMFP with the memory effect for $E_0 = 800$ eV and $E = 500$ eV (solid curve in Fig. 4), for instance, is between IMFPs without the memory effect for 500 eV and 800 eV (dotted curve). This result indicates that the previous electron energy has also an effect on the succeeding inelastic interaction.

CONCLUSIONS

On the basis of the dielectric response theory, analytic formulae for the DIIMFP and IMFP including the memory effect were derived for electrons moving parallel to a solid surface. The extended Drude dielectric function was employed to calculate electron DIIMFPs and IMFPs using these formulae for a Cu surface. It was found that the influence of the surface effect on the DIIMFP became significant as electrons moved closer to the surface. Without the memory effect, the DIIMFP and IMFP are determined by E, without reference to E_0. With the memory effect the DIIMFP and IMFP are affected by both E and E_0. The influence of the memory effect on DIIMFP and IMFP increases as the difference between preceding and succeeding electron energies, $E_0 - E$, becomes larger.

However, since a small energy loss is more probable than a large energy loss in the inelastic interaction, the memory effect on DIIMFP and IMFP is practically unobvious. In applications, theoretical models[11,12,15–17] of the inelastic cross section without the memory effect can still be used in electron transport theory near solid surfaces. Any attempt to measure the memory effect should be carefully designed to account for the rare consecutive surface interactions and the less frequent large energy losses.

The formulae derived in the present work can be applied to any charged particles moving parallel to the surface of solid materials with known dielectric functions. The study of memory effect for any charged particle moving perpendicular to a solid surface is underway.

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