Monte Carlo study of the ion-induced electron current tunneling through a metal–insulator–metal junction

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ABSTRACT

A Monte Carlo program is developed to investigate the kinetically excited electrons passing through a realistic Ag–Al$_2$O$_3$–Al junction when Ar$^+$ ions impact on the top Ag layer. The program includes excitation of the target electrons (by projectile ions, recoiling target atoms and fast primary electrons) and subsequent transport of these excited electrons from Ag to bottom Al layer of the metal–insulator–metal (MIM) junction. The calculated tunneling electron yield is consistent with the recently reported experimental results. The simulation, however, enables the calculation of partial tunneling electron yields of the electrons excited by the projectile ions, recoil atoms and cascade electrons, the depth distribution of the electron excitation points in the MIM junction and energy distribution of the tunneling electrons. Our calculation showed that the electrons excited by fast cascade electrons are the major contributor to the tunneling electron yield while the direct contribution of projectile ions to tunneling electron yield is evident only at the projectile energies greater than 10 keV. The tunneling electrons have their origin close to the bottom end of the Ag layer and bulk of the tunneling electrons have energies around 2 eV.

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1. Introduction

When an energetic ion impacts on a solid target its kinetic energy is transferred to the target atoms and electrons. As a result the cascades of recoiling target atoms and electrons are generated in the solid [1]. The mechanism of target electron excitation due to the kinetic energy transfer from the incoming ion can be split into three parts [2,3]: one due to collision between primary ions and target electrons, second due to collision between recoiling target atoms and target electrons and third due to collision between primary excited electrons and target electrons. The first part depends essentially on the electronic stopping power of the penetrating ion, while the second is related to the nuclear stopping power. The third part depends only on the target properties, e.g., the electron mean free path inside the target bulk. The excited electron can be emitted into vacuum if its energy is greater than the surface work function of the target. Consequently, the experimental data is limited only to those secondary electrons, which have the initial energy greater than the surface work function. Recently, Meyer et al. [4,5] and Kovacs et al. [6] have demonstrated the use of metal–insulator–metal (MIM) junction for the detection and internal excitation spectroscopy of hot internal electrons with excitation energies between the Fermi and the vacuum levels. However, several parameters of the tunneling electrons such as partial contributions of the electrons excited by projectile ions, recoiling target atoms and cascade electrons, depth and energy distributions are

still not accessible by the experimental techniques. The aim of the present paper is to describe a Monte Carlo based simulation code, which can be used to simulate these parameters of the electrons flowing through a MIM junction. The dimensions of the MIM junction considered in this work are the same as that of Meyer et al. [4,5] and Kovacs et al. [6]. The top silver layer of 20 nm thickness acts as a target for the ion bombardment that follows a 2.5 nm thick Al$_2$O$_3$ layer. At the bottom of MIM junction, a 20 nm thick Al layer acts as an electron collector (see inset of Fig. 3). The simulated results of Ar$^+$ induced tunneling electron yield, partial contributions of the electrons excited by various mechanisms, depth and energy distribution of the electrons tunneling through a MIM junction are presented and compared with the experimental data published by Meyer et al. [4,5].

2. Simulation model and calculation procedure

We describe here the main characteristics of the direct Monte Carlo program used to calculate the tunneling electron yield induced by impact of the energetic ions on a MIM junction. This Monte Carlo program is based on the classical binary collision approximation such as that used by SRIM for amorphous targets and MARLOW for crystalline targets. The basic idea of the Monte Carlo method is to follow the motion of a large number of individual projectile ions, recoiling target atoms and excited electrons in a target. Each history begins with a given energy, position and direction. The ion and recoiling target atom lose energy as a result of nuclear and electronic stopping. The projectile ion–atom and atom–atom interaction probabilities are determined from nuclear and electronic stopping powers, which are calculated as by the computer

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program SRIM [7]. The straight free path length PL is described as $PL = N^{-1/3}$ where N is the atomic density of the target material. The type of interaction, either elastic or inelastic, is decided on the basis of nuclear and electronic stopping powers. The total stopping power at a given energy is the probability of all the interactions (i.e. equals to unity), the ratio of nuclear stopping to total stopping is the probability of elastic interaction and if this ratio is less than a random number (from 0 to 1) then elastic interaction is considered otherwise the inelastic interaction is taken into account. For the elastic interaction projectile changes its direction as a result of the binary collision with target atom and moves in straight free-flight-paths between the collisions. Consequently a recoil atom is generated after each elastic interaction. The energy and direction of the interacting particles are calculated on the basis of conservation of energy and momentum. The scattering angle is calculated through impact parameter like Ziegler et al. [7]. The impact parameter is determined randomly by $p = \sqrt{R_n} p_{max}$, where R_n is a uniformly distributed random number between 0 and 1 and p_{max} is the maximum impact parameter, which is given by $PL / \sqrt{\pi}$ in amorphous materials. A history is terminated when the energy of projectile ion (or recoil atom) drops below the surface binding energy or when the particle moves out of the target. Like the previous MC programs [8–10], the energy required by target atom (the displacement energy) to leave its lattice site is ignored.

If inelastic interaction is considered, projectile ion (or recoil atom) interacts with a target electron. The energy loss by the projectile ion (or recoil atom) is calculated from conservation of energy. The energy gained by the target electron E_e is equal to the energy loss of the projectile ion. The initial direction of electron motion is considered isotropic and randomly selected. After production, the electrons undergo elastic and inelastic interactions with the target atoms and valence band electrons respectively. For elastic interaction, the direction and energy of scattered electron is calculated by conservation of energy and momentum. The elastic mean free path (EMFP) of the electron is calculated using the screened Rutherford formula (see Fig. 1), where the screening parameter for Ag and Al_2O_3 is taken equal to 2500 and 250 respectively [11]. It can be seen that in the electron energy range of interest, i.e. 1–150 eV, the EMFP of electron is in the range of 0.2–0.3 nm. In every inelastic interaction an additional electron from valence band is excited and as a result an electron cascade is generated in the solid. The inelastic mean free paths (IMFP) of the electron in Ag is taken from Ashley et al. [12] and in Al_2O_3 is taken from Akkerman et al. [13] and extrapolated to lower electron energies (see Fig. 1). Recently, Kovacs et al. [14] used almost similar energy dependence of electron IMFP in the Monte Carlo simulation of the MIM junction. For thorough discussion on the Monte Carlo simulation of

the electron transport in solids, reader is referred to a report by Shimizu and Ze-June [15].

The energy and direction of incident as well as recoil electron after scattering is calculated on the basis of conservation of energy and momentum. The path of every excited electron is followed until it leaves the surface of the MIM target from Ag side, or its energy becomes less than half of the Fermi energy (E_F) in Ag and electron affinity (E_A) in Al_2O_3 or it is collected at Al electrode. In order to leave the surface of metal or insulator, the electron's energy component normal to the surface must be greater than the apparent surface barrier potential (E_{SB}). It means that $E_e cos^2 \geq E_{SB}$ otherwise the electron will be reflected back into target [16], here   is azimuthal angle of electron determining its direction of motion. The E_{SB} for Ag to vacuum is taken as $0.5 \times E_F + \Phi$ [8], for Ag to Al_2O_3 is taken as $0.5 \times (E_F + E_{JB})$ and for Al_2O_3 to metal (i.e. Al or Ag) is taken as $0.5 \times (E_A + E_{JB})$ where E_F, Φ, E_A and E_{JB} are Fermi energy, work function, electron affinity and junction barrier potential respectively. The barrier potentials for electron at various interfaces of MIM junction are shown in Fig. 2. For Ag $E_F = 5.49$ eV and $\Phi = 4.74$ eV [17]. For Al_2O_3 $E_A = 1.0$ eV and band gap energy, $E_{BG} = 9.8$ eV are taken from Ref. [18]. In order to simulate the junction barrier potential, E_{JB}, the tunneling electron yield is calculated for the values of E_{JB} in the range of 0 to 2.4. Half of the E_{JB} is applied at each Ag–Al_2O_3 and Al_2O_3–Al interface. The best fit to the experimental data resulted $E_{JB} = 1.2$ eV (see Fig. 3), which is in good agreement with experimentally determined value of E_{JB} by Meyer et al. [5]. The excitations of inner-shell electron are not taken into account. The detail description on the interaction mechanisms of projectile ion, recoil atom and cascade electrons are given in [19] for metals and in [20,21] for oxides. In each of the Monte Carlo calculations conducted here the tunneling electron yield are generated for 10^4 incident projectile ions.

3. Results and discussion

The calculated tunneling electron yield of Ag–Al_2O_3–Al MIM junction for normal impact of Ar^+ is plotted versus ion energy in Fig. 3. The experimental results of Meyer et al. [5] for the same MIM junction are also shown. It can be seen that the agreement between experimental and the calculated results is quite good above 10 keV energy of the incident ion. One of the reasons for the disagreement at low impact energies is that the potential electron excitation is not included in this simulation. The electrons that are excited in the top Ag layer due to the potential energy deposition of the projectile ion and emitted towards the Ag–Al_2O_3 interface may overcome the junction barrier and reach the bottom Al layer. Recently, Peters et al. [22] have experimentally determined that the tunneling electron yield induced by potential energy of the projectile ion is $\gamma / E_{pot} = 1 \times 10^{-3} e^-$ (ions ·eV)$^{-1}$, therefore for singly charged argon ions the expected $\gamma = 0.016$ e$^-$/ion. Considering the indicated error bars in the experimental data the
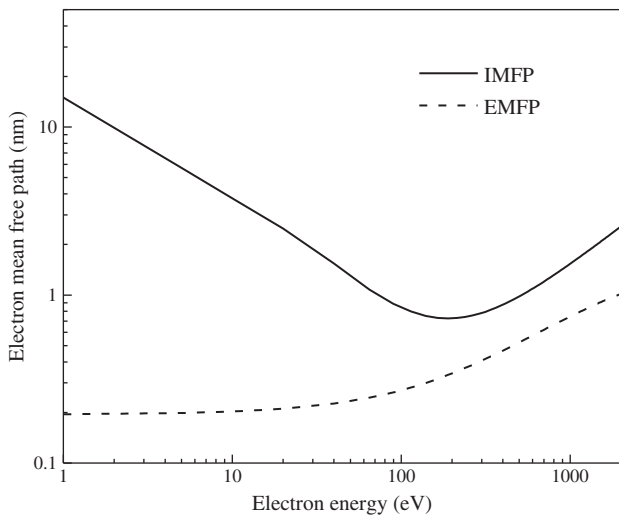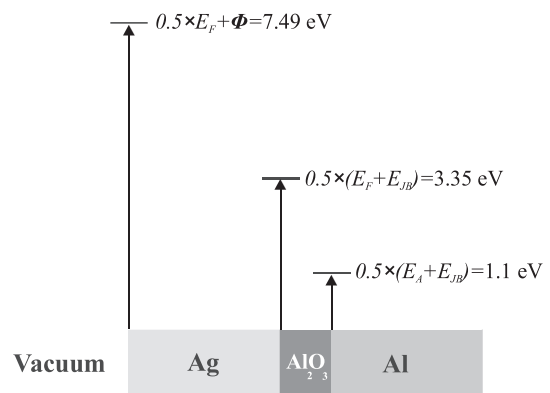

Fig. 1. Elastic and inelastic mean free path of electron in Ag as a function of electron energy. The elastic mean free path (EMFP) was calculated using the screened Rutherford formula and inelastic mean free path (IMFP) was taken from Ashley et al. [12].

Fig. 2. Barrier potentials for electron at various interfaces of MIM junction where E_F is Fermi energy and Φ is work function of Ag, E_{JB} barrier potential and E_A electron affinity of the Al_2O_3.