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MONTE CARLO STUDY OF Ar^+ INDUCED KINETIC ELECTRON EMISSION FROM MgO THIN FILM

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A Monte Carlo program has been developed to investigate the electron emission from 5000 Å thick MgO film for impact of Ar^+ ions having energies in the range of 50 to 1000 eV. The program incorporates the excitation of target electrons by projectile ions, recoiling target atoms and fast primary electrons. It can be used to calculate the kinetic electron yield, distribution of the electron excitation points in the solid and other physical parameters of the emitted electrons. The calculated electron emission yield is compared with the available experimental data, considering the effect of potential emission a good agreement is found. In addition, the effect of projectile energy and incident angle on the longitudinal distribution of the excitation points of electrons emitted from MgO thin film is investigated.

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1. Introduction

It is well reported that the mechanism of kinetic electron emission (KEE) from material surface induced by the impact of energetic ions consists of the following three successive steps [1]: the generation of excited electrons in solid by kinetic energy deposited by the incoming ions, the transport of these electrons towards the solid surface, and finally the escape of electrons through the surface into vacuum. A penetrating ion may generate cascades of recoiling target atoms and electron in the solid. As a result the process of KEE can be split into three parts: one due to collision between primary ions and target electrons, one due to collision between recoiling target atoms and target electrons and one 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 [2,3]. The third part depends only on the target properties, e.g., the electron mean free path inside the target bulk and their escape probability through the surface barrier. KEE is usually characterized by a coefficient γ defined as the average number of electrons ejected per incident ion.

MgO is getting much importance because of its use in the AC Plasma Display Panels (PDPs). These PDPs are used in the development of large, flat and lightweight displays. Electron emission yield plays an important role in plasma display panel's protective layers. Larger the ion induced secondary electron emission coefficient of the protective layer lower will be the driving voltage and power consumption [4]. Presently MgO is used as the protective layer in the PDPs because of its high electron yields and high stability under ion bombardment [4].

In this paper we describe a recently developed Monte Carlo based simulation code, which can be used to simulate a wide variety of phenomena related to ion-induced kinetic electron emission from thin foils of oxides, such as backward and forward electron emission yields, energy and angular distribution, statistical distribution of emitted electrons and the excitation points of the electrons that are emitted from target surface. This program incorporates the electrons excited by projectile ions, recoiling target atoms and primary high energy excited electrons. We report here calculations of the kinetic electron emission yields from MgO thin film for impact of Ar^+ ions having energies in the range of 50 eV to 1000 eV. The calculated electron emission yields are compared with the available experimental data. In addition, we have investigated the effect of the projectile

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incident angle on kinetic electron yield as well as the effect of projectile energy and angle of incidence on the depth distribution of excitation points of the electrons that are emitted from the target. At present the experimental techniques are not capable to measure the distribution of electron excitation points in the target.

2. Monte Carlo Simulation and Procedure

We describe here the main characteristics of the direct Monte Carlo program developed to calculate the ion-induced kinetic electron emission from solid targets of oxides. 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 given energy, position and direction. The ion and recoiling target atom lose its 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 program TRIM [5]. The straight free path length PL is describe as $PL=N^{-1/3}$ where N is the atomic density of the target material. Here compound material MgO is represented by pseudo-atomic solid with average atomic number (z_{avg} =10) [6] and mass density of MgO is taken as 3.58 g/cm^3 [7]. 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), then (nuclear stopping)/(total stopping) is the probability of elastic interaction and if this ratio is less than a random number 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. [5]. 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 [8-12], 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 but limited by band gap energy (E_{BG}) and some randomly selected portion of valence band. The initial direction of electron motion is considered isotropic and randomly selected. After production, the electrons undergo elastic and inelastic interaction 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 is calculated using the screened Rutherford formula where the screening parameter is taken equal to 250 for MgO by interpolation from Fitting and Reinhardt [13]. 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 of the electron is taken from Akkerman et al. [14] and extrapolated to lower electron energies. The energy and direction of incident as well as recoil electron after scattering is calculated on the basis of conservation of energy and momentum. While energy of the electron excited from valence band is limited by band gap energy (E_{BG}) and some randomly selected portion of valence band. The path of every excited electron is followed until it leaves the surface of the target, or its energy becomes less than the apparent surface barrier energy (E_{SB}). In order to leave the surface, normal to the surface component of the electron energy must be greater than the E_{SB}. It means that $E_e\cos^2\theta \geq E_{SB}$ otherwise the electron will be reflected back into target [15], here θ is azimuthal angle of electron determining its direction of motion. The E_{SB} for insulators are taken equivalent to electron affinity (E_A), which plays similar role to the ordinary surface barrier, $U = E_F + \Phi$, for metals where E_F and Φ are the Fermi energy and work function respectively [6]. For MgO E_A=0.85 eV, E_{BG}=7.8 eV and Valence Band=8.5eV are taken [16]. The excitations of inner-shell electron are not taken into account. Each Monte Carlo calculation conducted here for 10^5 projectile ions.

3. Results and Discussion

The kinetic electron yield γ measured for normal impact of Ar^+ on MgO target is plotted versus ion energy in Figure 1 with the total electron yield measured by S.K. Lee et al. [17]. The total electron yield is sum of kinetic and potential electron yields.

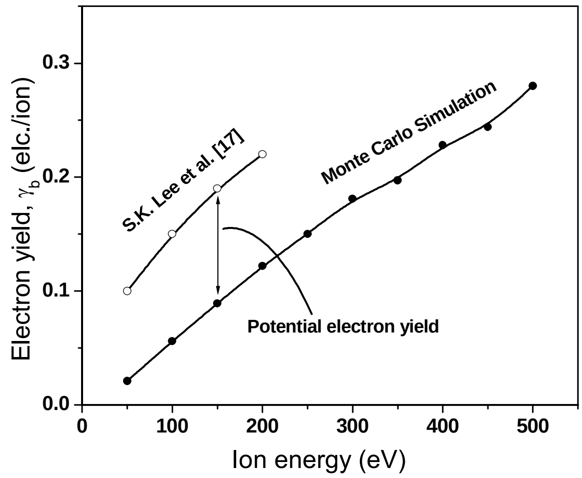

Figure 1. Electron yield from MgO target as a function of Ar^+ impact energy (incident angle=0^o with normal to the target surface).

It can be seen that experimental yield is more than the simulated yield but the difference is almost constant and trend of both the yields is the same. So this difference is a measure of potential electron yield, as Ar^+ has sufficient ionization potential that potential emission is marginally allowed for ion target combination [12, 16]. Kinetic electron yield for 500eV Ar^+ ions as a function of incident angle of the ion with the surface normal is shown in Fig. (2). The backward electron yield increases with the incident angle of ion because the deposition of energy by ions in producing recoil atoms and fast electrons near the surface increases. This increasing trend remains up to about 70^o and then decreases sharply. This decrease is due to very high reflection of ions at these grazing angles as is evident from reflection coefficients calculated by our program also shown in Figure 2. Figure 3 demonstrates depth distributions of excitation points of the emitted electrons from MgO for different impact energies of Ar^+ along with the average depth of emitted electrons. The depth distributions are normalized by the maxima of electron yield in the 1000 eV Ar^+ distribution.

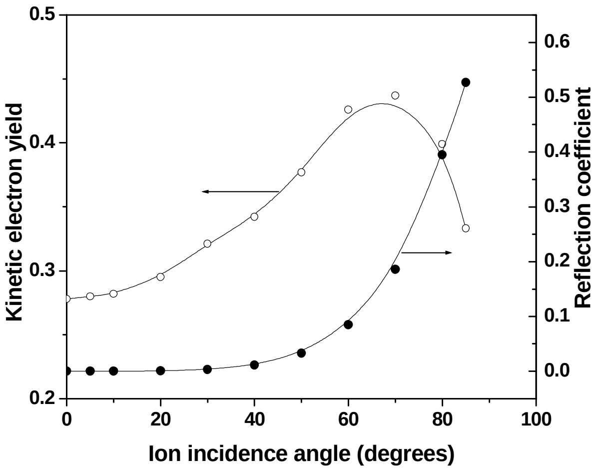

Figure 2. Kinetic electron yield and reflection coefficient of MgO target for 500 eV Ar^+ as a function of incidence angle of ion (angle is taken with the normal to the target surface).

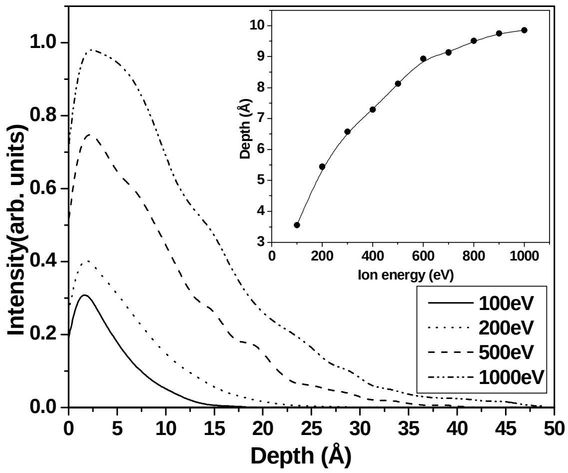

Figure 3. Depth distributions of excitation points of backward emitted electrons from MgO target for 100 eV, 200 eV, 500 eV and 1000 eV energy Ar^+ ions. The inset shows variation of the average depth of electron excitation points as a function of the energy of Ar^+ ions.

This figure illustrates that depth distribution as well as the average depth increases with the ion impact energy but the maxima of the depth distributions remains the same for all the energies of Ar^+ i.e. 2 Å. Also the rate of increase of the average depth decreases with the ion impact energies. Similarly depth distributions of excitation points of the emitted electrons from MgO with the average depth for different incident angles of the 500eV Ar^+ ion are shown in Figure 4. These distributions are normalized by the maximum electron yield at 80^o incident angle. The average escape depth decreases with incident angle of ion while the

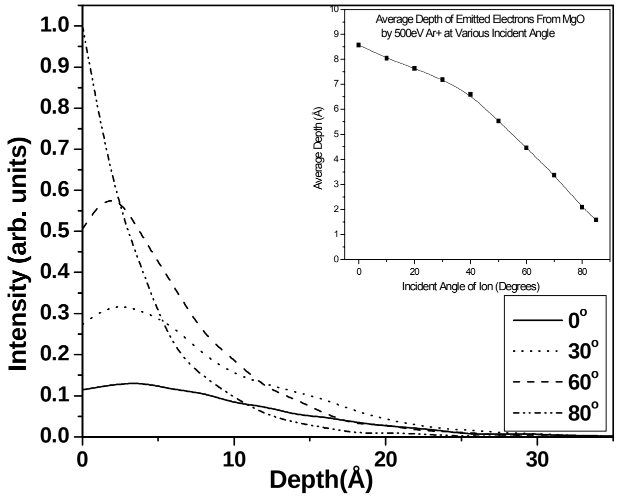

Figure 4. Depth distributions of excitation points of emitted electrons from MgO target by 500 eV Ar^+ for incidence angle=0^o, 30^o, 60^o and 80^o with the surface normal. In the inset variation of the average depth of the electron excitation points is plotted as a function of incidence angle.

maxima of the distribution shifted towards the surface of the target. The distributions of excitation points of the emitted electrons by normal impact of 200eV Ar^+ on MgO in two dimensions are shown in Figure 5. Trends deduced from these distributions are:

1. The average escape depth of excitation points of emitted electrons from MgO for ions and cascade electrons is less than that of recoil atoms. The reason is that the electrons excited by ions move mostly in forward direction to conserve momentum. But only those electrons, which are close to surface have more chance of deflecting towards surface and overcoming the surface barrier. Similarly high-energy electrons excited by ions or recoil atoms inside the target have very high chance of losing its energy in exciting another cascade electron. Energies of these cascade electrons are low and these electrons will be able to overcome the surface barrier only when they are produced near the surface. While the recoil atoms produced primarily by ions are forward directed and the electrons excited by them are produced deeper inside the target with high enough energy to overcome the surface barrier.

2. It is also visible that average lateral spread of excitation points of the emitted electrons in target by the ions is less than that of recoil atoms. This shows that ions follow almost a straight path and undergo fewer deflections in the target, while recoil atoms are deflected more than ions. Large lateral spread of the excitation points for cascade electron shows that these electrons are more frequently deflected.

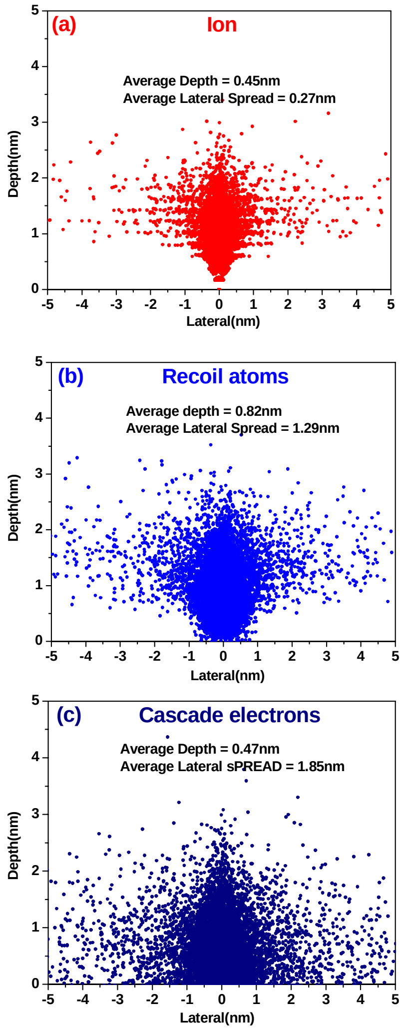

Figure 5. 2-D Plots of the excitation points of electrons generated by (a) ions (b) recoil atoms and (c) cascade electrons for 200 eV Ar^+ impact on MgO.

In conclusion, we described a recently developed Monte Carlo code for investigation of ion-induced kinetic electron emission from solid surfaces. The program is used to study kinetic electron emission from MgO surface induced by Ar^+ ions. It is worth noting that the program can generate partial electron yield of electrons excited by ions, recoiling target atoms and cascade electrons, and distributions of electron excitation point in the solid. These parameters are not accessible by the present day experimental techniques.

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