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Abstract

A Monte Carlo simulation of the secondary electron emission from beryllium is combined with a model of bowl structure for surface roughness, for analyzing the difference between the electron emissions for normal and oblique incidences. At normal incidence, with increasing the roughness parameter $H/W$, the primary energy $E_{pm}$ at which the maximum electron yield occurs becomes higher, and at more than the $E_{pm}$, the decrease in the yield is slower; where $H$ and $W$ are the depth and width of the bowl structure, respectively. The dispersion of incident angle to the microscopic surface causes a small increase in the yield at oblique incidence, whereas the blocking of primary electrons from bombarding the bottom of the structure causes an opposite trend. The strong anisotropy in the polar angular distribution with respect to the azimuthal angle is calculated at oblique incidence.

Keywords:
beryllium, secondary electron emission, surface roughness, Monte Carlo simulation, plasma surface interaction.

1. Introduction

In magnetic confinement fusion devices, secondary electron emission from plasma-facing material (PFM) surfaces is particle-surface interaction process of considerable importance for the determination of plasma sheath potential, which strongly influences the impurity production due to sputtering of the PFM [1]. The existing experimental data on the secondary electron emission are relatively less voluminous than those for ion backscattering and sputtering; furthermore, the data on the secondary electron yield involve larger scatter among experiments [2]. This may be because the secondary electron emission is more sensitive to the experimental conditions (e. g., surface cleanliness and roughness, measurement method and so on).

Surface morphology changes, induced by high-fluence plasma irradiation, strongly modify the surface roughness, which is an important parameter for the secondary electron emission dynamics. In fact, such modifications of surface morphology (e. g., ripple, cone, pyramid, terrace and self-affine fractal and so on) by ion irradiation were observed in many experiments [3,4], and then projectile backscattering and sputtering, as well as secondary electron emission, were modified [5-10]. In order to investigate the effect of surface roughness on the particle emission processes, some calculations have carried out and been compared with the ex-
experimental results [11-16]. In a previous paper [17], we presented a Monte Carlo calculation of the secondary electron emission from beryllium, which is one of candidate materials for the PFM [18], with a ripple-structured surface at normal incidence of low-energy (≤ 1keV) electrons. By introducing the roughness into the calculation, the secondary electron yield was increased, and a low-energy shift of the energy distribution of secondary electrons and their angular distribution, being different from the cosine distribution, were calculated. However, since the bombarding plasma particles have an energy of wide range and the bombardment may not be normal to the PFM surface, the secondary electron yield (as well as the energy and angular distributions of emitted electrons) is needed not only as a function of primary energy, but also as a function of incident angle. Furthermore, the secondary electron emission is more sensitive to the rough surface for oblique incidence than for normal incidence. Therefore, the dependences of the secondary electron emission properties on incident angle and primary energy, which were not discussed in the previous paper [17], should be explored, systematically. Furthermore, we are concerned about the fact that, in the previous model, the surface roughness was described in an oversimplified way by assuming the two dimensional ripple-structured surface, in spite of three-dimensional and complicated topography of real surfaces. Therefore, in this study, a three-dimensional surface model of bowl structure is designed, and the dependences of the secondary electron emission properties on the incident angle and the energy of primary electrons are investigated.

2. Brief Description of the Model

Figure 1 (a) shows the bowl-structured surface used here. The profile is constructed with the Gaussian distribution. The depressions have a constant width W (25, 100 or 250nm) and depths H varied from 0 to 4μm. The bombardment points of primary electrons on the surface are randomly chosen within the ranges of x (0 ≤ x ≤ 4W) and y (0 ≤ y ≤ 4W). The incident angle (φ) of the primary electron and polar angle (θ) of emission of secondary electrons are measured from the normal line to the z = 0 plane; the incident angle is changed in the x-z plane. For oblique-angle incidence, since the polar angular distribution of secondary electrons may depend on the azimuthal angle of emission, electrons emitted in the direction of the zones A-F in Fig. 1 (b), which shows the top view of the surface bombarded at the point (x, y) = (0, 0) by the primary electron, are distinguished from each other.

The basic idea of the Monte Carlo model of secondary electron emission used here is to simulate trajectories of primary and secondary electrons in a solid with given cross sections for active scattering processes. The trajectory of each electron is chosen using a series of random numbers representing the path length between scattering events, the type of scattering that takes place, and energy loss and/or scattering angle. The primary and second-
ary electrons interact with the solid through elastic collisions with the solid atoms, and through inelastic collisions, i.e., excitations of conduction electrons, bulk plasmons and K shell electrons. The bulk plasmon is assumed to decay giving one or two electron emissions immediately after the excitation. In each inelastic process, new secondary electrons are generated, and as a result, a cascade electron multiplication is generated. Some of the secondary electrons are emitted to the vacuum with reduced energy in a refracted direction due to the surface potential barrier [19], which conforms to the microscopic boundary of the surface structure. Due to the topographic features of the surface, re-entrance (and re-emission) of electrons emitted should be taken into account. Details of the model and the cross sections for the elastic and inelastic collisions are given in Ref. 17.

In each of the Monte Carlo calculations conducted here, the secondary electrons are generated by $10^5 - 10^6$ projectiles.

3. Results and Discussion

At first, the calculated secondary electron yields $\sigma$ at normal incidence are shown in Fig. 2 as a function of the roughness parameter $H/W$ for surface roughness of the bowl structure, along with that for the previous ripple-structured one. The yield $\sigma$ includes backscattering electrons ($\geq 50eV$); for a flat surface, the maximum yield $\delta$ of true or slow secondary electrons ($\leq 50eV$) is calculated as 0.58 at primary energy $E_p = 200eV$ ($\sigma = 0.65$), whereas the backscattering coefficient $\eta$ is less than 0.1 at $E_p \leq 1keV$. As long as the primary electron is incident normal to the macroscopic surface (the $z = 0$ plane) the following effects of surface roughness on the physical process in secondary electron emission are considered. One is that low-energy electrons, which cannot escape from a flat surface due to the energy loss during their transport to the surface and the refraction of the electron trajectory by the surface potential barrier, can escape from an inclined plane of the rough surface. We henceforth call this as the 'effect of the inclined surface'. The other is that secondary electrons emitted from the surface with large emission angles re-enter into the adjacent part of the topographic surface. This effect is henceforth called the 'effect of re-entrance'.

Fig. 2 Variations of the secondary electron yield $\sigma$ at normal incidence with the roughness parameter $H/W$ for surface roughness of bowl structure (a) and ripple structure (b). The data points are calculated by changing the depth $H$ under the condition that the width $W$ is constant.

For small $H/W$, the effect of the inclined surface causes an increase in $\sigma$. With increasing $H/W$, some secondary electrons emitted near the bottom of the surface structure re-enter into the neighboring part of the surface; this causes a peak in the $\sigma$-variation with $H/W$. For large $H/W$, this effect of re-entrance is dominant so that the $\sigma$ becomes smaller than that for the flat surface. For the ripple-structured surface, secondary electrons emitted in perpendicular to the rippled direction never re-enter into the surface, whereas for the bowl-structured surface, the microscopic surface is partially flat (e.g., the area near the point of $(x, y) = (2W, 2W)$). The former causes a higher peak in the $\sigma$-variation with $H/W$ for the ripple structure, and the latter causes a lower peak and a slower change in the $\sigma$-variation due to change in $H/W$ for the bowl structure.

Figure 3 shows the primary energy dependence of calculated $\sigma$ for normal incidence on flat and

As described in the previous paper [17], however, the surface roughness of target materials will be one of the possible reasons for the large scatter in the experimental data.

The incident angle has a strong influence on secondary electron emission. The secondary electron yield is directly related to the amount of electronic excitation generated by a projectile within an electron escape depth of the solid. Thus, by changing the incidence from normal to oblique angles, the path length of the projectile within the electron escape depth is prolonged and thereby its deposition of energy with excitation of secondary electrons (also the secondary electron yield) increases. A simple geometric model [24], which assumes constant excitation of electron along the projectile trajectory in the electron escape depth and disregards elastic scattering of the projectile, leads us to a simple law in the form, \( \sigma(\phi) = \sigma(0) \cos^{-1}\phi \) (i.e., inverse cosine law); \( \sigma(\phi) \) and \( \sigma(0) \) are the secondary electron yields at an incident angle \( \phi \) and at normal incidence, respectively. At keV or less energy range, due to the breakdown of the assumptions in the model, the incident-angle dependences deviate from the inverse dependency on aluminum. As described in the previous paper [17], however, the surface roughness of target materials will be one of the possible reasons for the large scatter in the experimental data.

bowl-structured surfaces. For small \( H/W \), due to the dominant effect of the inclined surface, \( \sigma \) becomes larger than that for the flat surface at all the energies \( E_p \) calculated. On the other hand, for large \( H/W \) \( \sigma \) becomes smaller (larger) at low (high) \( E_p \) due to fast (slow) decrease in \( \sigma \) with increasing \( H/W \); and hence, the energy \( E_{pm} \) at which the maximum yield occurs becomes higher, and the decrease in \( \sigma \) at more than the \( E_{pm} \) is slower than that for the flat surface. In the figure, the calculated \( \sigma \) is compared with some experimental data [20-22]. Since the majority of the secondary electrons have an energy below 20eV, the calculated \( \sigma \) is strongly affected by the surface potential barrier, the magnitude of which is taken as 19.06eV in this study. As a result, an important effect on the large scatter in the experimental data on \( \sigma \) may be the surface contamination, which leads to the change in the surface potential barrier (i.e., the work function). For example, Suleman and Pattinson [22] observed that, due to the oxidation of a Be surface, the maximum yield changed from 0.68 to 4.16 and the \( E_{pm} \) shifted from 200eV to 410eV. Furthermore, the calculated \( \sigma \) is sensitive to the cross sections for elastic and inelastic interactions in a solid; Dubus et al. [23] studied the effect of the cross sections on the calculated yield in the case of
cosine law, as shown in Fig. 4. In the figure, the $\sigma$ ($\phi$) multiplied by $\cos\phi$ is used, because it might be kept at a fixed value (equal to $\sigma(0)$) for all the angles of incidence if the inverse cosine law is correct. The calculated incident-angle dependence is consistent with the dependence observed for $\phi \geq 60^\circ$ by Bronshtein and Dolinin [20], although the calculated $\sigma(0)$ at normal incidence, which largely depends on $H/W$, is different from the observed one. The following effects of surface roughness on the incident-angle dependence of the secondary electron yield can be expected. One is the dispersion of incident angle to the microscopic boundary of the rough surface; this effect is dominant for small $H/W$. This results in a small increase in $\sigma$ with increasing $\phi$ in comparison with that for the flat surface. The other effect is the blocking of the primary electrons from bombarding near the bottom of the rough area. This results in a suppression of the re-entrance of once-emitted electrons in the case of oblique incidence, so that for large $H/W$ the incident-angle dependence is enhanced, except for grazing angles: the $\sigma$ for $\phi \approx 0^\circ$ largely decreases due to larger effect of re-entrance, whereas the $\sigma$ for oblique angles decreases less (or increases).

The backscattering of primary electrons, which produces a small contribution ($\eta < 0.1$) to total electrons emitted from the beryllium surface at normal incidence, becomes large at oblique incidence. With increasing $H/W$, due to dominant effect of re-entrance, the backscattering coefficient decreases, whereas the yield $\delta$ of true secondary electrons increases due to dominant effect of the inclined surface; e.g., at $E_p = 300$eV, $\phi = 60^\circ$ and $W = 25$nm, for $H/W = 0$ (flat), 0.4, 2.4 and 12, $\eta$ is 0.23, 0.22, 0.19 and 0.16, respectively, while $\delta$ is 0.78, 0.84, 0.98 and 1.07. The small effect of re-entrance on $\delta$ for oblique incidence does not produce the decrease in $\delta$ with large $H/W (= 12)$, being different from that for normal incidence ($\delta$ is 0.54, 0.61, 0.86 and 0.75, for $H/W = 0$ (flat), 0.4, 2.4 and 12, respectively).

In Figs. 5 (a), 5 (b) and 5 (c), the doubly differential electron yields $d^2\sigma/dE_d\theta$ calculated with respect to the energy $E_s$ and polar angle $\theta$ of electrons emitted in the A-direction at 60° interval of the azimuthal angle (see Fig. 1 (b)) from flat and bowl-structured surfaces for normal incidence. For the flat surface, the calculated energy distribution of secondary electrons has a peak at $2 - 3$eV and the full width at half-maximum (FWHM) is $7 - 8$eV, whereas the polar angular distribution agrees with the well-known cosine distribution [25]: the number of electrons emitted in a unit solid angle is proportional to $\cos\theta$. By introducing the surface roughness, the shape of the energy distribution shifts towards the low-energy side due to the effect of the inclined surface (the peak position $\approx 1 - 2$eV, the FWHM $\approx 5 - 6$eV), although, for large $H/W$, the energy distribution slightly broadens towards high energy. This changes result in better agreement with the observed energy distribution in comparison with the calculated one for the flat surface, the same as the previous paper [17]. The effect of re-entrance increases the contribution of

![Fig. 5 Doubly differential secondary electron yield $d^2\sigma/dE_d\theta$ at normal incidence ($\phi = 0^\circ$) with respect to the energy $E_s$ and polar angle $\theta$ of electrons emitted at an interval of 60° in the azimuthal angle (the zone A in Fig. 1 (b)) from a flat surface (a) and bowl-structured surfaces; (b) $H/W = 3$ and (c) $H/W = 30$ ($E_p = 300$eV, $W = 25$nm).]
secondary electrons emitted with small θ to the angular distribution.

The calculated energy and polar angular distributions of secondary electrons emitted from a flat surface is almost independent of the incident angle (not shown here). The unchange of the energy distribution with the incident angle is consistent with the experimental data for copper obtained by Koshikawa and Shimizu [26]. This is also due to the fully-developed and isotropic spatial distribution of the electron multiplication process in the solid. The energy and emission angle of secondary electrons do not depend on the energy and angle of 'secondary' electrons excited by the 'primary' electron, but depend only on the transport process of low-energy 'thirdly or higher order' electrons produced by the cascade multiplication of the 'secondary' electrons in the solid [27]. As a result, in spite of the oblique incidence, both the shapes of the energy and polar angular distributions are insensitive to the azimuthal angle of emission.

By introducing the roughness, strong anisotropies in the energy and polar angular distributions (as well as the electron yield) with respect to the azimuthal angle are caused by the topographic features of the surface, as shown in Fig. 6. Due to the dominant bombardment to an inclined plane (2W ≤ α ≤ 3W) of the surface, the increase in the number of secondary electrons emitted in the backward direction (D, E and F in Fig. 1 (b)) is more enhanced in comparison with that in the forward direction (A, B and C in Fig. 1 (b)). It is also found that the enhanced emission in the backward direction is accompanied not only with the low-energy shift of the energy distribution, but also with the revival of the large-angle emission, which is suppressed with the normal incidence on the rough surface. These are due to the emission of low-energy electrons from the inclined plane near the top of the rough area, resulting from the blocking of the projectile bombardment near the bottom of the rough area. With increasing H/W, furthermore, these anisotropies with respect to the

Fig. 6 Doubly differential secondary electron yield $d^2\sigma/dE_d\theta$ at oblique incidence ($\phi = 60^\circ$) with respect to the energy $E_s$ and polar angle $\theta$ of electrons emitted at interval of 60° in the azimuthal angle (the zones A-F in Fig. 1 (b)) from a bowl-structured surface with the roughness parameter $H/W = 3$ ($E_s = 300$eV, $W = 25$nm).
azimuthal angle are enhanced.

It should be noted that the present model calculations do not give evidence of quantitative behavior, but qualitative one for the secondary electron emission properties from the rough surface, because our model of the surface roughness is simplified to describe complicated topography of real surfaces. However, Banouni et al. calculated the energy-resolved polar angular distribution of Auger electrons emitted from Al bombarded by Ar⁺ and obtained strong modifications of polar angular distribution from oblique incidence by surface roughness [11]. Furthermore, their calculations with changing roughness parameter were good agreement with their experimentally obtained ones, while the number of emitted electrons was different between calculations and experiments [8].

4. Conclusions

A Monte Carlo simulation of the secondary electron emission from beryllium was combined with the model of the bowl structure for surface roughness. As long as the primary electron is incident normal to the rough surface, due to topographic features of the bowl structure, the primary energy $E_{pm}$ at which the maximum secondary electron yield $\sigma$ (including backscattering electrons) occurs becomes higher, and the decrease in the yield at the primary energies of more than the $E_{pm}$ is slower than that for a flat surface. By introducing the surface roughness, the shape of the energy distribution of secondary electrons shifts by $1 - 2$ eV towards the low-energy side, whereas the over-cosine angular distribution are calculated for polar emission angle of electrons; for a flat surface, a cosine distribution is calculated.

In this paper, the emphasis was put on the similarity and difference between secondary electron emissions for normal (incident angle $\phi = 0^\circ$) and oblique incidences (incident angle $\phi$) on a rough-textured beryllium as well. The similarity is the dispersion of incident angle due to the surface roughness; this results in a small increase in $\sigma$ with increasing $\phi$. The difference is the blocking of primary electrons from bombarding near the bottom of the rough areas at oblique incidence; this results in a suppression of the re-entrance of electrons emitted at large angles into the adjacent part of the topographic surface.

The calculated energy and angular distributions of secondary electrons emitted from a flat surface is almost independent of the incident angle of primary electrons, except for the absolute magnitude. By introducing the roughness, for oblique incidence, the number of secondary electrons emitted in the forward direction (like a specular reflection of primary electrons) is decreased, whereas in the backward direction it is increased. The secondary electron emission in backward direction is accompanied with the low-energy shift of the energy distribution, as well as the large-angle emission in the same (different) manner as in the case of the flat surface (as in the case of the rough surface at normal incidence).

References


