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# Damaging impacts of energetic charge particles on materials in plasma energy explosive events*

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To provide some reference data for estimation of the erosion rates and lifetimes of some candidate plasma facing component (PFC) materials in the plasma stored energy explosive events (PSEEE), this paper calculates the sputtering yields of Mo, W and deuterium saturated Li surface bombarded by energetic charged particles by a new sputtering physics description method based on bipartition model of charge particle transport theory. The comparisons with Monte Carlo data of TRIM code and experimental results are made. The dependences of maximum energy deposition, particle and energy reflection coefficients on the incident energy of energetic runaway electrons impinging on the different material surfaces are also calculated. Results may be useful for estimating the lifetime of PFC and analysing the impurity contamination extent, especially in the PSEEE for high power density and with high plasma current fusion reactor.

**Keywords:** sputtering, bipartition model, transport theory, runaway electron
**PACC:** 2852, 2852F, 2852J

## 1. Introduction

The damaging impacts of the energetic charge particles on material surface in the 'plasma stored energy explosive events' (such as accident of power supply suddenly terminated, major disruption, etc.) are key issues of concern in determining plasma performance and the lifetime of plasma facing components (PFC) in a fusion reactor.[1] Especially for the high power density fusion reactor and with high plasma current during the above-mentioned devastating events, almost about 100–1000MW/m$^2$ average energy fluxes will be dumped on the PFC surface. The divertor target plate surface should endure even much higher peak particle and energy fluxes. Generally speaking, the damaging impacts of the energetic charged particles on material surface refer to several different kinds of fundamental processes, such as melting and vaporizing resulting from high energy flux, physical sputtering of material surface bombarded by energetic ions and electrons, the reflections of ions and electrons from the surface, the secondary electron emission from wall surface induced by ion and electron incidences, ion implantation and re-emission, etc. Among them, the physical sputtering process is one of the most important processes in determining the erosion rate of the divertor plate and the extent of impurity contamination of the fusion core plasma.[2] The impurity concentration makes decisive impact on the particle and energy balances of fusion plasma. The higher the impurity level is, the less fusion power will be produced due to the fuel dilution and the impurity radiation. Therefore, it is important to keep the impurity level as low as possible for an economically competitive fusion reactor. New bipartition model of charged particle transport theory has been developed[3,4] to calculate the sputtering yields of several candidate divertor materials. But it cannot directly solve the above-mentioned problems and can only provide some reference data to the issues in discussion. As we know, the physical sputtering process is that the energetic ions or atoms, escaping from the scrape of layer and impinging on the material surface, undergo a series of elastic collisions and deposit a fraction of their kinetic energies onto the atoms of the target materials. Then the recoiling atoms are pro-

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duced and the recoiling atoms with sufficient energy continue in turn undergoing secondary collisions which give rise to the next generation of recoiling atoms and thereby lead to the formation of a cascade. As a result, it is then possible for both the ions and the energetic recoil atoms to be scattered backward to the surface. If their kinetic energies are high enough to overcome the surface potential barrier they can get out of the surface. This is the so-called sputtering process. The sputtering phenomenon was discovered in the last century, but it had not been explained correctly until Sigmund[5] proposed the sputtering model based on the binary collision cascade concept in 1969. The semi-empirical formula for sputtering yield calculation derived from the Sigmund model could fairly predict the experimental results.[6] However, Sigmund theory still needs to be further improved. In his sputtering theory, a backward transport equation was introduced. This is not beneficial to the description of the cascade atoms going through the surface potential barrier and emitting to the outside surface of the target materials. This is because the backward transport equation is valid only for a homogeneous medium. However, the medium with a surface should also be treated for the sputtering issue. Therefore, the backward transport equation is not appropriate to describe the sputtering process. In order to improve the Sigmund theory, based on a bipartition model of ion transport theory, we have developed a new quantitative physical sputtering theory. In this new model, the Sigmund sputtering model has been retained basically, but the description method of cascade atoms is modified. In brief, the usual ion transport equation is directly utilized to describe the cascade collisions induced by the incident ion. Especially, the detailed description of the process for the cascade atoms passing through surface barrier and emitting out of the surface has been given. Thus the formulation of the sputtering atom is described in more detail. From the viewpoint of the physics mechanism, this method is similar to the application of Monte Carlo simulation for study of the sputtering process. Both this new model and the Monte Carlo method maintain Sigmund's three-step-model of the sputtering process, but the description methods of atom cascade collisions are different. The former solves the transport equation of cascade atoms by using analytical transport theory, while Biersack and Eckstein have developed the statistical random sample method. It is anticipated that this new model and the Monte Carlo method should give very close sputtering yields, if the same input parameters are used.

In the present paper, the sputtering yields for energetic $H^+$, $D^+$, $T^+$ and $He^+$ ion bombardments on Mo, W and deuterium saturated Li of the candidate materials of PFC are calculated by using this new model.

The main ideas of Sigmund's three-steps-model are as follows. (1) An impinging ion undergoes a series of elastic collisions in the target medium, and continuously deposits its energy to the target atoms. (2) The target atom acquiring sufficient energy breaks from the lattice, and becomes a recoiling atom, which can move among the lattices. The recoiling atom with sufficient energy continues in turn undergoing secondary elastic collisions giving rise to another generation of recoiling atoms thereby leading to the formulation of cascade atoms. (3) A fraction of the cascade atoms move to nearby material surface, and if their kinetic energies in the normal direction of surface are greater than surface potential barrier, then these atoms can get out of the surface and become the sputtered atoms.

According to experimental study on the sputtering phenomenon, the sputtering process usually happens within only 10–20-atom layers or so near the surface. It is possible to explore an important simplified approach for sputtering yield calculation. That means actual sputtering yield is only dependent on the distribution function of incident ions near the surface, and independent of incident ion transport deep in target materials. Based on this fact, we have developed the new description model of sputtering.

## 2. New theoretical model

As mentioned above, the sputtering phenomena take place within only 10–20-atom layers or so close to the surface. This is the so-called emission thickness. Under most circumstances, the energies of incident ions are greater than 100eV. The ranges of incident ions in the target medium are usually more than 100Å. However, the thickness of the 10–20-atom layer is about 10Å in order of magnitude. The distribution function of incident ions changes exiguously within the emission thickness and is quite close to the distribution function of incident ions at the surface. Therefore, it is reasonable to substitute the distribution function of incident ions at the surface for the distribution function within the emission thickness. The distribution function at the surface $f_0^{(\mathrm{i})}(0, \mu, E)$ con-

sists of two parts: one is the distribution function of primary incident ions at the surface, and the other is the distribution function of reflected ions at the surface. Thus the ion distribution function at the surface can be written as

$$f_0^{(\mathrm{i})}(0,\mu,E) \approx \delta(E-E_0)\delta(1-\mu)/2\pi + N(0,\mu,E). \quad (1)$$

The first term of Eq.(1) refers to the distribution function of directional incident ions with mono-energy and the second term is the distribution function of the reflected ions at the surface.

The number of first generation cascade atoms with energy $E \pm \mathrm{d}E$ per unit volume and per unit energy interval generated by elastic collisions between the target atom and the primary incident ion or reflected ion can be given by

$$\begin{aligned} S^{(\mathrm{ia})} =& N \int\limits_{(E+E_\mathrm{d})/\gamma}^{E_0} \mathrm{d}E' \int\limits_{4\pi} \mathrm{d}\boldsymbol{u}' f^{(\mathrm{i})}(0,\mu',E') \\ & \times \sigma_\mathrm{n}^{\mathrm{ia}}(E', E+E_\mathrm{d}) \\ & \times \delta\left(\boldsymbol{u}\cdot\boldsymbol{u}' - \frac{M_1+M_2}{2M_1}\sqrt{\frac{M_1(E+E_\mathrm{d})}{M_2E'}}\right)/2\pi. \end{aligned} \quad (2)$$

The intensity of new generation of cascade atoms generated by elastic collisions between the target atoms and the cascade atoms knocked off from lattices is

$$\begin{aligned} S^{(\mathrm{aa})} =& N \int\limits_{E+E_\mathrm{d}}^{\gamma E_0 - E_\mathrm{d}} \mathrm{d}E' \int\limits_{4\pi} \mathrm{d}\boldsymbol{u}' f^{(\mathrm{a})}(x,\mu',E') \\ & \times \sigma_\mathrm{n}^{\mathrm{aa}}(E', E+E_\mathrm{d}) \\ & \times \delta\left(\boldsymbol{u}\cdot\boldsymbol{u}' - \sqrt{\frac{E+E_\mathrm{d}}{E'}}\right)/2\pi, \end{aligned} \quad (3)$$

where $N$ is the target atom number per unit volume; $\sigma_\mathrm{n}^{\mathrm{ia}}$ is the differential cross section of elastic collision between the incident ions and the target atoms. $\sigma_\mathrm{n}^{\mathrm{aa}}$ is the differential cross section of elastic collision between the target atoms and the cascade atoms. $E_\mathrm{d}$ is the averaged displacement energy of target atoms and $\gamma = 4M_1M_2/(M_1+M_2)^2$. $M_1, E_0$ is the mass and initial energy of the incident ions respectively, $M_2$ is the mass of the target atoms. $\boldsymbol{u}$ and $\boldsymbol{u}'$ are the solid angles. $\mu$ is the directional cosine of $\boldsymbol{u}$.

Based on the statistical balance principle, we find that the distribution function of cascade atoms obeys the following transport equation:

$$\begin{aligned} & -\frac{\partial \rho_\mathrm{e}^{(\mathrm{a})}(E) f^{(\mathrm{a})}(x,\mu,E)}{\partial E} + \mu \frac{\partial f^{(\mathrm{a})}(x,\mu,E)}{\partial x} \\ =& N \int\limits_{E}^{\gamma E_0 - E_\mathrm{d}} \mathrm{d}E' \int\limits_{4\pi} \mathrm{d}\boldsymbol{u}' f^{(\mathrm{a})}(x,\mu',E') \\ & \times \sigma_\mathrm{n}^{\mathrm{aa}}(E', E'-E)\delta\left(\boldsymbol{u}\cdot\boldsymbol{u}' - \sqrt{\frac{E}{E'}}\right)/2\pi \\ & - N f^{(\mathrm{a})}(x,\mu,E) \int\limits_0^E \mathrm{d}\tau \sigma_\mathrm{n}^{(\mathrm{aa})}(E,\tau) \\ & + S^{(\mathrm{ia})}(x,\mu,E) + S^{(\mathrm{aa})}(x,\mu,E), \end{aligned} \quad (4)$$

where $\rho_\mathrm{e}^{(\mathrm{a})}(E)$ is the electronic stopping power of the cascade atoms. Because the cascade atoms undergo many times of collisions, the angular distribution of cascade atoms approaches relatively isotropic distribution, hence the $P_n$-approximation is applicable, then we have

$$f^{(\mathrm{a})}(x,\mu,E) \approx \sum_{l=0}^{n} \frac{2l+1}{4\pi} P_l(\mu) N_l^{(\mathrm{a})}(x,E). \quad (5)$$

Similarly, $P_n$-approximation can also be made for $S^{(\mathrm{ia})}(x,\mu,E)$ and $S^{(\mathrm{aa})}(x,\mu,E)$ as

$$\begin{aligned} S^{(\mathrm{ia})}(x,\mu,E) &\approx \sum_{l=0}^{n} \frac{2l+1}{4\pi} P_l(\mu) S_l^{(\mathrm{ia})}(x,E), \\ S^{(\mathrm{aa})}(x,\mu,E) &\approx \sum_{l=0}^{n} \frac{2l+1}{4\pi} P_l(\mu) S_l^{(\mathrm{aa})}(x,E). \end{aligned} \quad (6)$$

In Eq.(5), $N_l^{(\mathrm{a})}$ is the $l$th spherical harmonic moment of $f^{(\mathrm{a})}(x,\mu,E)$, and satisfies the following equation:

$$\begin{aligned} & -\frac{\partial \rho_e^{(\mathrm{a})}(E) N_l^{(\mathrm{a})}}{\partial E} + \frac{1}{2l+1} \\ & \times \left[(l+1)\frac{\partial N_{l+1}^{(\mathrm{a})}(x,E)}{\partial x} + l\frac{\partial N_{l-1}^{(\mathrm{a})}(x,E)}{\partial x}\right] \\ =& -\varphi_l^{(\mathrm{a})}(E) N_l^{(\mathrm{a})}(x,E) + S_l^{(\mathrm{ia})}(0,E) \\ & + S_l^{(\mathrm{aa})}(x,E), \quad l \le n, \end{aligned} \quad (7)$$

where $\varphi_l^{(\mathrm{a})}(E)$ is the scattering parameter for the cascade atom with energy $E$, $S_l^{(\mathrm{ia})}(0,E)$ and $S_l^{(\mathrm{aa})}(x,E)$ are the $l$th spherical harmonic moments of the source terms in the $P_n$-approximation of $S^{(\mathrm{ia})}(x,\mu,E)$ and $S^{(\mathrm{aa})}(x,\mu,E)$ respectively, they are given by

$$S_l^{(\mathrm{ia})}(0,E) = \frac{N}{\mu_0}\sigma^{(\mathrm{ia})}(E_0, E+E_\mathrm{d}) \times P_l\left(\frac{M_1+M_2}{2M_1}\sqrt{\frac{M_1(E+E_\mathrm{d})}{M_2E_0}}\right)P_l(\mu_0) + N\int\limits_{(E+E_\mathrm{d})/\gamma}^{E_0} \mathrm{d}E'\sigma_\mathrm{n}^{(\mathrm{ia})}(E', E+E_\mathrm{d}) \times P_l\left(\frac{M_1+M_2}{2M_1}\sqrt{\frac{M_1(E+E_\mathrm{d})}{M_2E'}}\right)N_l^{(\mathrm{i})}(0,E'), \tag{8}$$

$$S_l^{(\mathrm{aa})}(x,E) = N\int\limits_{E+E_\mathrm{d}}^{\gamma E_0-E_\mathrm{d}} \mathrm{d}E' N_l^{(\mathrm{a})}(x,E)\sigma_\mathrm{n}^{(\mathrm{aa})}(E', E+E_\mathrm{d}) \times P_l\left(\sqrt{\frac{E+E_\mathrm{d}}{E'}}\right). \tag{9}$$

In order to calculate the sputtering yield, a proper boundary condition is required to match Eq.(7), which is different from the Mark boundary condition; the latter condition is valid only for free surface case. The effects of surface barrier should be taken into account in this boundary condition by introducing a critical angle $\vartheta_\mathrm{c}$, which is determined by the relation:

$$\cos\vartheta_\mathrm{c} = \mu_\mathrm{c} = \sqrt{\frac{U}{E}}, \tag{10}$$

where $U$ is the surface binding energy ( or barrier potential ). The proper boundary condition is

$$f^{(\mathrm{a})}(0,\mu_i,E) = \begin{cases} f^{(\mathrm{a})}(0,-\mu_i,E), & 0<\mu_i<-\mu_\mathrm{c}, \\ 0 & -\mu_\mathrm{c}<\mu_i<1, \end{cases} \tag{11}$$

where $\mu_i (i = 0,1,\cdots,n)$ are the roots of Legendre polynomial $P_{n+1}(\mu)$. The above boundary condition refers to the following physical picture of cascade atoms in the vicinity of the surface. The cascade atoms in the angular interval of $\mu_\mathrm{c} < \mu < 0$ would be reflected back into the materials by the surface barrier, while only the atoms moving in the angular interval of $-1 < \mu < \mu_\mathrm{c}$ would get out of the surface. Solving Eq.(7) with boundary condition Eq.(11), we find that the sputtering yield can be calculated by

$$Y = \int\limits_0^{\gamma E_0} N_1^{(\mathrm{a})}(0,E)\mathrm{d}E. \tag{12}$$

## 3. Deuterium saturated surface

However, in the most realistic circumstance, the material surface is often saturated by the fuel atoms of deuterium (or tritium) in fusion device. It can be regarded as a multi-component surface. In this case the expression derived by Sigmund[7] based on the linear cascade theory can be used to calculate the partial sputtering yield

$$\frac{Y_\mathrm{Li}}{Y} = \frac{c_\mathrm{Li}}{c_\mathrm{D}}\left(\frac{M_\mathrm{D}}{M_\mathrm{Li}}\right)^{2m}\left(\frac{U_\mathrm{D}}{U_\mathrm{Li}}\right)^{1-2m}. \tag{13}$$

In order to compare with experimental data, only deuterium saturated lithium is calculated in this work. In Eq.(13) $Y$ is the absolute sputtering yield, as given in Eq.(12), if no any deuterium atoms were present on the lithium surface. $c_\mathrm{D}$ is the concentration of deuterium atoms in a lithium matrix and $c_\mathrm{Li} = 1 - c_\mathrm{D}$. The $U_\mathrm{Li}$ and $M_\mathrm{Li}$ correspond to the surface binding energy and mass of lithium respectively. We assumed a 50%Li–50%D surface coverage and with homogeneous composition profile. The surface binding energies are taken from Fig.5 of Ref.[8]. The $U_\mathrm{D}$ should be replaced by the surface binding energy of Li–D component rather than pure solid phase deuterium.

## 4. Results and discussions

The sputtering yields of W, Mo bombarded normally by the energetic fusion charged particles $H^+$, $D^+$, $T^+$ and $He^+$ can be obtained. The results are shown in Fig.1 and Fig.2 respectively. For comparison, the Monte Carlo data[9] with $D^+$ and $T^+$ bombardments are also plotted together on the same figures. Figure 3 shows the sputtering yields of deuterium saturated Li bombarded by $He^+$ and $D^+$ at normal incidence, and the comparisons with experimental data provided by Allain and Ruzic.[10] We can find that the results obtained from this new model are reasonably consistent with the Monte Carlo results from TRIM code and experimental data, but the calculation of this new model is much faster and more effective in comparison with Monte–Carlo calculations. We find that the TRIM code data is a little higher than that obtained from bipartition model in the region of higher incident energy, this may be resulted from neglect of

the contributions from the atoms farther away from emission thickness in this model. These results can provide some reference data for estimation of the lifetime of PFC, and some reference data of the source terms for analysis of the impurity transport in the core plasma of fusion reactor.

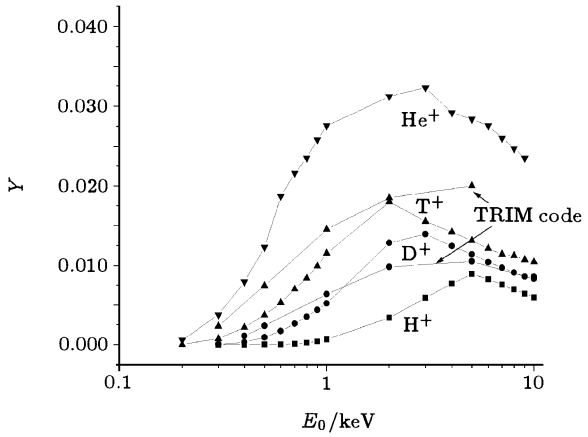



**Fig.1.** Sputtering yield of tungsten bombarded by the fusion charged particles.

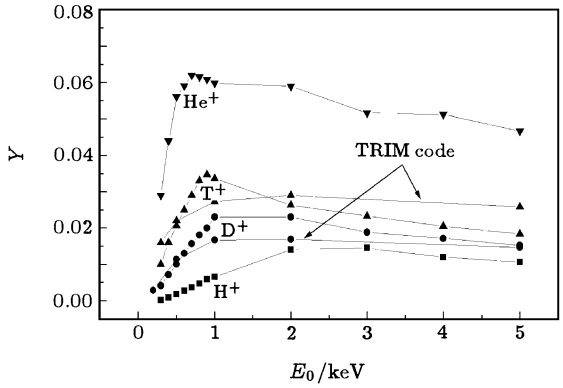



**Fig.2.** Sputtering yield of molybdenum bombarded by the fusion charged particles.

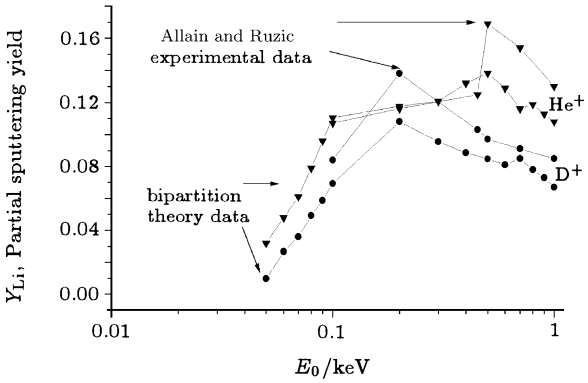



**Fig.3.** Deuterium saturated solid lithium bombarded by $D^+$, $He^+$.

We have also developed a new transport code for energetic electron to calculate the maximum energy depositions on the different material surfaces for different incident energies of the energetic runaway electrons escaped from core fusion plasma during the disruption or plasma current collapse events, which lead to the increase of the impinging heat flux on the wall, meanwhile, some cooperative cascade fortified damage processes, such as vaporizing and melting, might occur especially for the liquid lithium surface. The other important processes will be discussed in our later work. The results are shown in Fig.4 and Fig.5 for different wall materials. $E_0$ refers to the incident energy, $\left.\frac{\mathrm{d}E}{\mathrm{d}x}\right|_{\max}$ is the maximum energy depositions on the different material surfaces for different incident energy of energetic runaway electrons. $R_{\mathrm{N}}$ and $R_{\mathrm{E}}$ are the particle reflection coefficient and energy reflection coefficient of energetic electrons respectively. Since liquid lithium is considered as having a potential application[11,12] to liquid curtain as the first wall of blanket in a high power density reactor, so it is covered in this research.

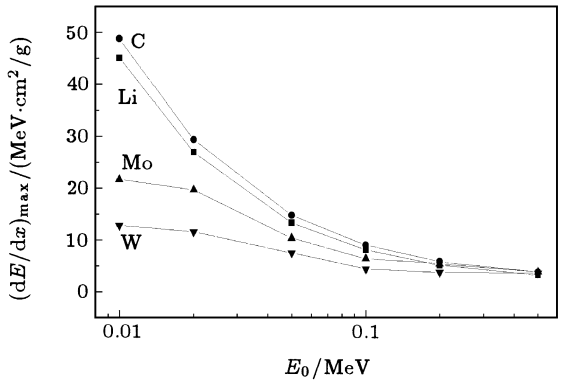



**Fig.4.** Maximum energy deposition versus runaway electron energy for different materials.

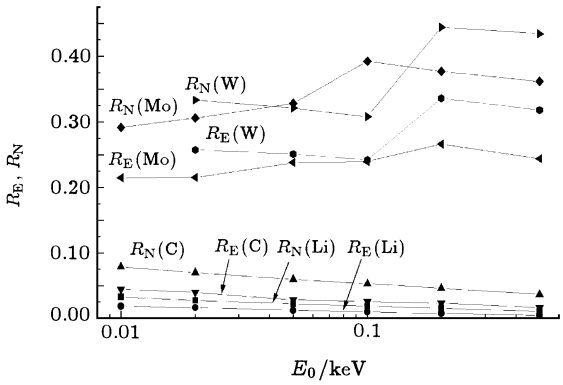



**Fig.5.** Particle and energy reflection coefficients of energetic electron on different material surfaces.

# References


[1] Cracken G and Stott P 1979 *Nucl. Fusion* **19** 889

[2] Roth J 1993 *Impurity Generation Processes in Particle–Surface Interaction: Data Status and Needs, In: Atomic and Plasma–Material Interaction Processes in Controlled Nuclear Fusion* ed. Janev R and Drawin H (Netherlands: Elsevier) Vol.1

[3] Luo Z M and Wang S 1987 *Phys. Rev.* B **36** 1885

[4] Luo Z M and Hou Q 1993 *J. Appl. Phys.* **74** 6007

[5] Sigmund P 1969 *Phys. Rev.* **184** 383

[6] Sigmund P 1981 *Sputtering by Ion Bombardment: Theoretical Concepts, Sputtering by Particle Bombardment* Vol.1 Ed. Behrisch R (New York: Plenum)

[7] Sigmund P 1981 *Appl. Phys.* **47** 466

[8] Roth J 1986 *Physics of Plasma–Wall Interactions in Controlled Fusion* (New York: Plenum) p351

[9] Biersack J and Eckstein W 1984 *Appl. Phys.* A **34** 73

[10] Allain J P and Ruzic D 2002 *Nucl. Fusion* **42** 202

[11] Deng B Q, Huang J H, Yan J C, Peng L L and Wang E Y 2003 *J. Nucl. Mater.* **313-316** 630

[12] Shi B R 2004 *Chin. Phys.* **13** 2097