

NATIONAL INSTITUTE FOR FUSION SCIENCE**Sputtering Yield Calculations Using an Interatomic Potential with the Shell Effect and a New Local Model**

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Sputtering Yield Calculations Using an Interatomic Potential with the Shell Effect and a New Local Model

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In order to test the availability of theoretical screening lengths and a new local electronic energy loss model proposed by Yamamura et al., the sputtering yields due to various ion impacts on monatomic materials were calculated with the ACAT code. It is found that the calculated sputtering yields at normal incidence are in good agreement with experimental data and the Yamamura's empirical sputtering formula without free parameters.

Key words: Monte Carlo simulation, sputtering yield, new local model of electronic energy loss, screening length with shell effect.

1. Introduction

Sputtering of materials is important in the development of a fusion reactor. Sputtering ejects high atomic number materials into a plasma, causing significant contamination and increasing radiation loss of a plasma, and thus results in inefficient heating of a plasma. From the point of view of plasma-wall interaction, sputtering is an undesired process which erodes the surrounding walls. On the other hand, sputtering is useful for many applications. Sputtering allows controlled removal of surface layers on a nearly atomic scale, permitting submicron spatial resolution if a well-focused ion beam is used. At present the mechanism of physical sputtering is well understood [1], and Eckstein calculated sputtering yields for various ion-target combinations, using the TRIM code [2].

In the computer studies on the interaction of a charged particle with solids, authors treated nuclear collisions in terms of the Thomas-Fermi screened Coulomb potential. For better agreement with experiments, they sometimes modified screening lengths used in interatomic potentials [3,4,5]. Recently, Yamamura, Takeuchi and Kawamura [6] proposed a method to determine the screening length of colliding two atoms which includes the shell effect of each element. Yamamura and Kimura [7] also

proposed a new local model of electronic energy loss, based on the Firsov theory [8].

In order to test the screening lengths and a new local model of electronic energy loss proposed by Yamamura et al., we have calculated sputtering yields from monatomic targets at normal incidence, using a Monte Carlo code, ACAT [9], and compared the ACAT sputtering yields with the Yamamura's empirical formula [3] and experimental data. Since high Z materials have recently become ones of the prospective candidates of a divertor plate of a fusion reactor, we pick up Mo and W as target materials and H⁺, D⁺, ³He⁺, He⁺ and Ar⁺ as incident ions are considered. The self-sputtering yields are also calculated.

2. Screening length with the shell effect

The Thomas-Fermi (TF) electron distribution, $n(r)$, shows no shell structure, and is represented as a function of the screening function $\Phi(x)$, i.e., $4\pi r^2 n(r) dr = Zx^{1/2} \Phi(x)^{3/2} dx$, where $x=r/a_{TF}$ (a_{TF} being the TF screening length). Since the analytical screening functions such as the Sommerfeld and Molière approximations are not the exact solutions, Yamamura et al. [6] used the Poisson equation for the TF electron distribution, i.e., $4\pi r^2 n(r) dr = Zx \Phi''(x) dx$, where the prime means the differentiation with respect to x . They

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determined the screening length of an isolated atom so that the average radius of the TF electron distribution be equal to that of the Hartree-Fock electron distribution [10]. Then the screening length for an isolated atom of the species i is obtained by

$$a_{m,i} = \langle r \rangle_{\text{HF},i} / \langle x \rangle_{\text{TF}} \quad (1)$$

where $\langle r \rangle_{\text{HF},i}$ is the average radius of the atomic state HF electron distribution of an atom of the species i , and $\langle x \rangle_{\text{TF}}$ is the average reduced radius of the TF electron distribution. The $\langle x \rangle_{\text{TF}}$ of Molière and Kr-C screening functions are 3.283 and 3.207, respectively. In Table 1 we list screening lengths of present interest which are determined by eq. (1).

Once the screening length of an isolated atom is known, we can calculate the screening length

$$\Delta E(p) = \frac{3}{4} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} \frac{\hbar}{a_{m,F}} (Z_1 Z_2)^{2/3} v \int y^2 \left(\frac{\Phi^* \left(\sqrt{y_0^2 + y^2} \right)}{\sqrt{y_0^2 + y^2}} \right)^{4/3} dy, \quad (2)$$

where p is the impact parameter, and v is the velocity of a projectile, $y_0 = p/(2a_{m,F})$. The numerical calculation of the integral term in eq.

$$\Delta E(p) = \frac{S_e(E) \alpha \exp[-\gamma z_0(E, p)]}{a_{m,F}^2 [1 + \beta z_0(E, p)]^6}, \quad (3)$$

where α , β and γ are the fitting parameters depending on the used interatomic potential whose values are listed in Table 2. $S_e(E)$ is the electronic stopping cross section. $z_0(E, p)$ is reduced apsidal distance which is the apsidal distance divided by the screening length $a_{m,F}$. Then, the present local model includes the shell effect of colliding particles, except for the ZBL potential.

4. Sputtering yield calculations by the ACAT code

In order to calculate sputtering yield at normal incidence, we use the ACAT code. The ACAT code is based on the binary collision approximation, and the target atoms are randomly distributed in the simple cubic cell with the average lattice constant, $N^{-1/3}$. The detailed description about the ACAT code is given in ref. 9. In the present calculations we use the Molière, Kr-C and ZBL potentials[14], where the theoretical screening lengths are used for the Molière and Kr-C potentials. For the ZBL

of two-atoms encounter by the equation, $(a_{m,F})^{-3/2} = (a_{m,i})^{-3/2} + (a_{m,j})^{-3/2}$, which corresponds to the Firsov screening length formula [11].

3. A new local model for electronic energy loss

Firsov derived an impact-parameter-dependent formula (local model) of electronic energy loss, assuming that excitation energy of electrons is due to transformation of the kinetic energy of the relative motion of colliding particles[8]. In computer simulations, the empirical Oen-Robinson local model is often used [11], and there are several local models used in channeling simulation [12]. Based on the Firsov electronic energy loss formula and using Sugiyama's potential[13], Yamamura and Kimura derived the following energy loss formula due to the electronic excitation of colliding particles [7]:

(2) gives the following local model for the electronic energy loss:

potential one must use the ZBL screening length which is given as $a_{\text{ZBL}} = 0.4685/(Z_1^{0.23} + Z_2^{0.23}) \text{ \AA}$. The electronic energy loss is estimated by the mixed model, where for low-energy particles we used the present new local model for these three potentials and the path-length-dependent non-local model is used for higher-energy projectiles.

The ACAT sputtering yields at normal incidence are compared with the experimental data and the Yamamura's empirical formula[3] for Mo and W targets in Figs.1 and 2, respectively. The references of experimental data used here are in ref. 3. The ACAT (Molière) and ACAT (Kr-C) sputtering yields show good agreement with the experimental data and the Yamamura's empirical formula for the present ion-target combinations. The ACAT (ZBL) gives slightly larger yields for H^+ and D^+ ions. From these figures we can conclude that the present theoretical screening lengths with the shell effect and the new local model are available for predicting the interaction of charged particles with solids.

5. Conclusion

Sputtering yields at normal incidence by various ion impacts on Mo and W targets were calculated with the ACAT code, using the theoretical screening lengths and the new local model of the electronic energy loss. It is found that the calculated sputtering yields are in good agreement with experiments and the Yamamura's empirical sputtering formula without free parameters. The theoretical screening lengths with the shell effect and the new local model are available for predicting the interaction of charged particles with solids.

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Table 1 The theoretical screening lengths of isolated H, He, Ar, Mo and W atoms for different potentials

| element | screening length (\AA) | |
|---------|-----------------------------------|--------|
| | Molière | Kr-C |
| H | 0.2418 | 0.2475 |
| He | 0.1494 | 0.1530 |
| Ar | 0.1438 | 0.1472 |
| Mo | 0.1218 | 0.1247 |
| W | 0.1017 | 0.1041 |

Table 2 Best-fit parameters of a new local model for the electronic energy loss

| Potential | α | β | γ |
|-----------|----------|---------|----------|
| Molière | 0.01884 | 0.07330 | 0.01101 |
| Kr-C | 0.02623 | 0.08735 | 0.01034 |
| ZBL | 0.03431 | 0.09935 | 0.01365 |

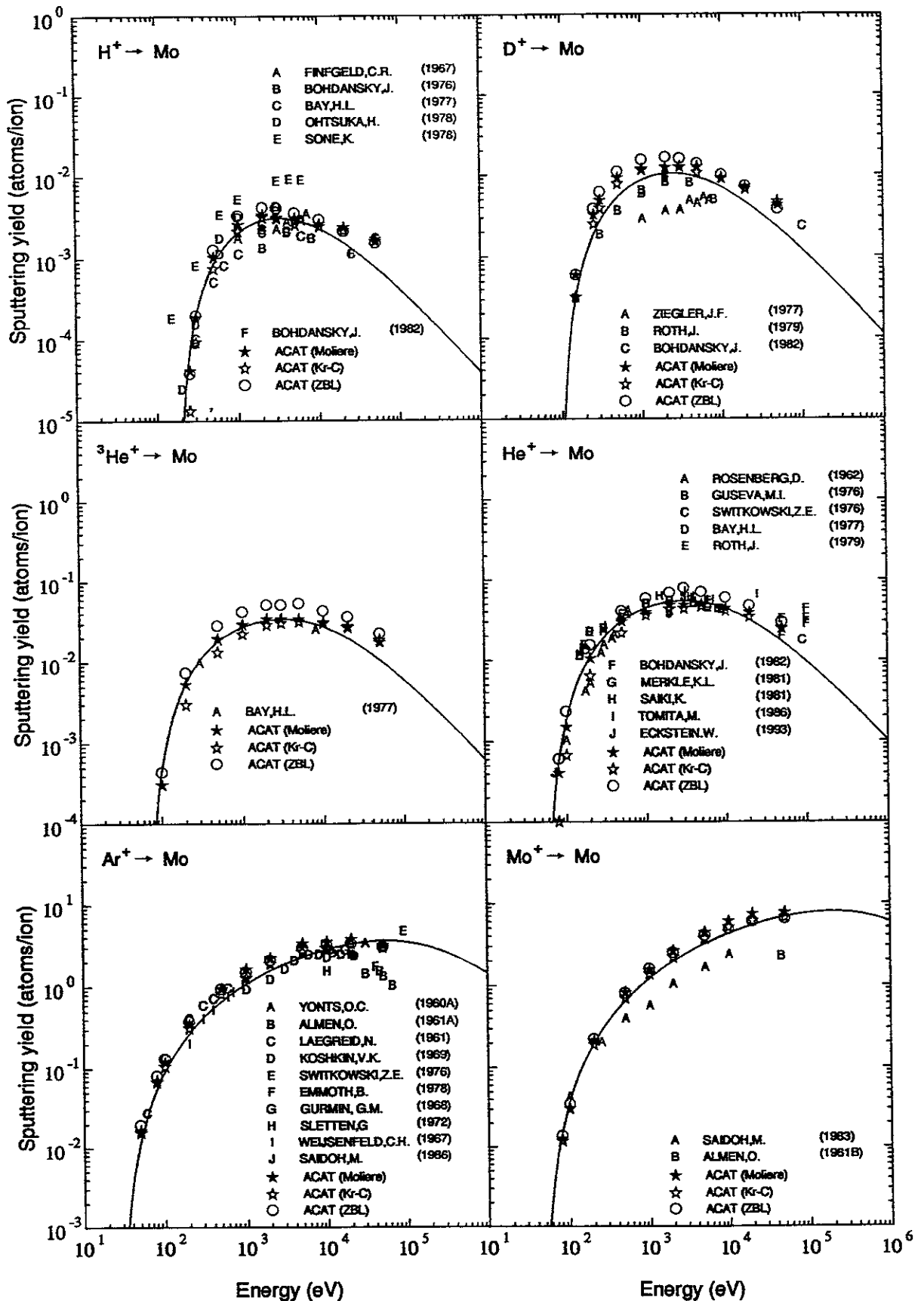


Fig. 1 : The energy dependence of the sputtering yield for H^+ , D^+ , $^3He^+$, He^+ , Ar^+ and Mo^+ ion normal impact on Mo targets. The solid line is Yamamura's empirical formula.

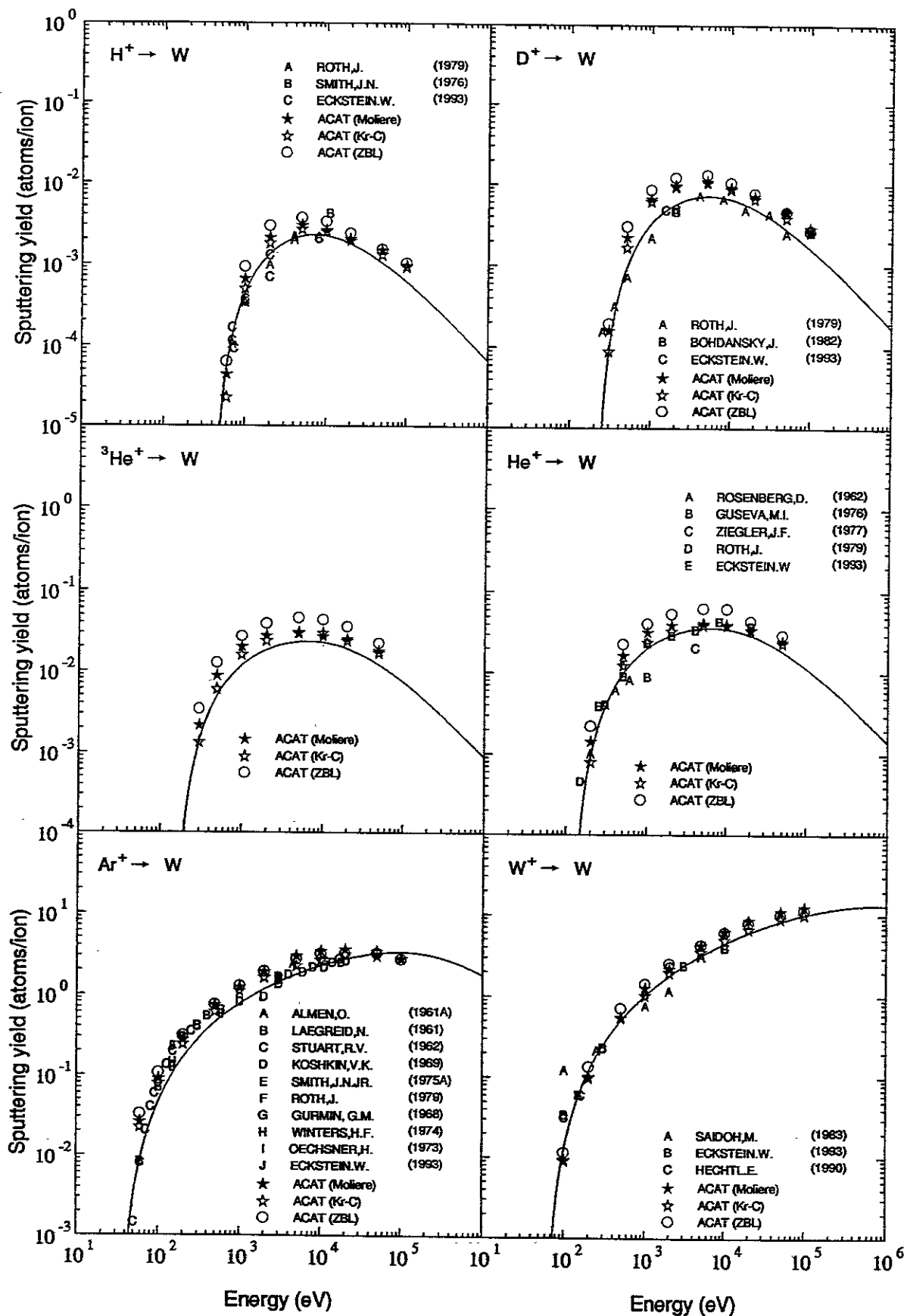


Fig. 2 : The energy dependence of the sputtering yield for H^+ , D^+ , $^3He^+$, He^+ , Ar^+ and W^+ ion normal impact on W targets. The solid line is Yamamura's empirical formula.

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