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ELASTIC AND INELASTIC SURFACE EFFECTS ON ION PENETRATION AND THE RESULTING SPUTTERING AND BACKSCATTERING*

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ABSTRACT

The computer code ITMC (Ion Transport in Materials and Compounds) has been developed to study in detail the transport of charged particles in solid materials and surface related phenomena such as sputtered atoms and backscattered ions. The code is based on Monte Carlo methods to follow the path and the damage produced by the charged particles in three dimension as they slow down in target materials. Single-element targets as well as alloys with possible different surface and bulk compositions or with layered structures of different materials can be used. Various models developed to calculate the inelastic energy losses with target electrons can be used in the code. Most known interatomic potentials can also be used to calculate the elastic energy losses. The major advantages of the code are its ability and flexibility to use and compare various models of elastic and inelastic energy losses in any target with different compounds and different surface and bulk composition.

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1. Introduction

Two major theoretical methods are used to describe ion transport in a solid, i.e., the analytical approach and the Monte Carlo simulation process. The analytical method is based on the transport theory with special simplifying assumptions to make the problem solvable. This approach is usually restricted to certain applications and special cases. The Monte Carlo calculation is simply a theoretical simulation of the three-dimensional trajectory path of the incident ion (and any subsequent primary and secondary knock-on atoms) as it decelerates within the solid target. The trajectory is actually a series of straight line segments connected to each other and the orientation of each segment is determined by the scattering angles associated with the equations that govern the physical processes. The Monte Carlo technique has been extensively applied to the simulation of ion transport and slowing down [1-5]. This increasing popularity of Monte Carlo calculations is due to several factors. Mainly the capability to simulate trajectories in complex configurations such as layered structure and coating materials with different alloy compositions. Another factor is the variety of the processes that can be studied with fine details such as range calculation, sputtering and backscattering coefficients, spatial compositional changes, etc. However, an important factor is the availability of large computers and fast processors that can easily compete with other analytical tools.

A brief description of the methodology of Monte Carlo simulation used in ITMC code for ion scattering and energy dissipation in solid targets is presented. A more detailed analysis and description of the code capabilities and the assumption used in the simulation process are given in Ref. [4]. The code can be used to study ion penetration and damage produced in solids for various ion-target combinations with target materials being a single element or an

alloy and for a wide range of incident ion energies. The alloy may have different surface or bulk compositions due to possible chemical or physical effects that dynamically change the composition. Ion and energy reflection coefficients as well as their angular and energy dependence can also be studied. Sputtered atoms, their energy and angular distribution, and their depth of origin inside the target can be calculated for each atom species of the target. The individual contribution of primary and secondary knock-on atoms, for each atom species, to the total sputtering yield can also be evaluated. Numerous models to calculate the elastic and inelastic energy loss are implemented in the code. Most of the known interatomic potentials can be used to calculate the nuclear scattering cross section. There is a good agreement between certain models in the code and the available experimental results [5]. However, the main purpose of this paper is to study certain applications that would be difficult to measure experimentally. One example is the sputtering performance of a specific fusion reactor first wall or limiter during irradiation. Also, one can study the effect of certain parameters such as the surface and bulk binding energies on the sputtering yield.

2. Methodology and Calculation Procedure

In any Monte Carlo calculation, computer-generated random numbers are used to choose particular values for parameters from the distribution of allowed values. These allowed values are obtained from the physics of ion bombardment and slowing down in target atoms. Physical quantities such as ion penetration depth, backscattering and sputtering yields and their spatial, energy, and angular distributions are evaluated from the simulation of the scattering events occurring in a large number of simulated ion trajectories within the target. The target atoms are assumed randomly distributed and the collision between a moving particle and any target atom is assumed binary with

no influence of neighboring atoms. It is further assumed that the moving particle inelastically loses energy continuously to electrons while traveling in straight lines between successive collisions. During the collision, elastic nuclear losses occur and the particle may then change its direction as schematically shown in Fig. 1. A brief outline of the formalism used to determine the nuclear scattering and the energy losses is presented below. A more detailed description is given in Ref. [4-5].

The universal differential scattering cross-section given by LSS theory is [6]:

$$d\sigma = \pi a^2 \frac{f(t^{1/2})}{2t^{3/2}} dt \quad , \quad (1)$$

where

$$t^{1/2} = \epsilon \sin\left(\frac{\theta}{2}\right) \quad , \quad (2)$$

$$\epsilon_{ij} = \text{reduced energy} = \frac{a_{ij}}{z_i z_j e^2} \frac{M_i}{(M_i + M_j)} E \quad (3)$$

and θ is the scattering angle in the center of mass system. M and Z are the atomic mass and number respectively, subscript i is for incident particle and subscript j is for target atom. The screening parameter, a_{ij} , can be given by Lindhard [6], Firsov [7].

The universal scattering function $f(t^{1/2})$ may be presented in different forms such as:

$$f(t^{1/2}) = \lambda t^{1/2-m} [1 + (2\lambda t^{1-m})^q]^{-1/q} \quad (4)$$

where the coefficients λ , m , and q are fitting parameters adjusted for different interatomic potentials [5]. At lower energies, the Born-Mayer potential can also be used. The scattering function for this potential is given by

$$f(t^{1/2}) = 24 t^{1/2} \quad . \quad (5)$$

Another form of the scattering function used in ITMC code is derived from the reduced nuclear stopping power, $S_n(\epsilon)$, which can be written as

$$f(t^{1/2}) = \frac{d}{dx} [t^{1/2} \cdot S_n(t^{1/2})] \quad (6)$$

where a universal reduced nuclear stopping has been recently developed in which [8]

$$S_n(\epsilon) = \frac{\ln(1 + a\epsilon)}{2(\epsilon + b\epsilon^c + d\epsilon^{1/2})} \quad (7)$$

where a , b , c , d are fitting coefficients.

The total scattering cross section σ_T is then given by

$$\sigma_T = \int_{t_{\min}^{1/2}}^{t_{\max}^{1/2}} d\sigma \quad (8)$$

where

$$t_{\max}^{1/2} = \epsilon \sin \frac{\pi}{2} = \epsilon \quad (9a)$$

$$t_{\min}^{1/2} = \epsilon \sin \frac{\theta_{\min}}{2} \quad (9b)$$

The minimum angle of scattering θ_{\min} can be determined from Eq. (8) assuming that

$$\sigma_T = \sum_j^{NT} N_j^{-2/3} \quad (10)$$

where N_j is the atom density of type j atom and NT is the total number of atom species. The scattering angle θ_1 after collision (1) is determined from a uniform random number R_1 ($0 < R_1 < 1$), where [4]

$$\sigma(t^{1/2}) = R_1 \sigma_T \quad . \quad (11)$$

The azimuthal scattering angle ϕ_1 is determined from another uniform random number R_2 where

$$\phi_1 = 2\pi R_2 \quad (0 < R_2 < 1) \quad . \quad (13)$$

The nuclear energy loss at each collision is then given by

$$\Delta E_n = \frac{4 M_i M_j}{(M_i + M_j)^2} E_i \sin^2 \frac{\theta_1}{2} \quad . \quad (14)$$

The direction cosines of the particle velocity vector in a fixed frame of reference, must be calculated after each collision to relate the new particle position to a fixed origin in this reference frame [5].

The motion of the incident particle between collisions is simulated as free flights of certain length, δ (as shown in Fig. 1), where the particle continuously loses energy to target electrons. Each step length is assumed proportional to the mean free path, ℓ , where

$$\ell = \sum_j^{NT} N_j^{-1/3} \quad , \quad (15)$$

and to another random number R_3 ($0 < R_3 < 1$). The step length is then given by

$$\delta = -\ell \ln R_3 \sum_j^{NT} N_j^{-1/3} \quad . \quad (16)$$

The electronic energy loss ΔE_e is finally given by

$$\Delta E_e = \delta \sum_j^{NT} N_j S_j \quad , \quad (17)$$

where S_j is the electronic stopping power for atom species j .

Several models can be used to calculate the electronic stopping cross section during particle slowing down [5]. Some of these models are Lindhard stopping formula, Bethe-Block equation, Brice semi-empirical correlation, or Ziegler fitting coefficients. In this calculation the Lindhard stopping formula is used unless otherwise stated.

The energy of the incident particle after the i th collision can then be calculated as

$$E_i = E_{i-1} - \Delta E_n - \Delta E_e . \quad (19)$$

If the target atom (j) receives an energy $E^j = \Delta E_n > E_b^j$ (binding energy for atom j), this atom will be set in motion with an energy $E^j = \Delta E_n - E_b^j$ and will undergo similar scattering events as the incident particle and hence a cascade is formed. The recoiled atoms in the cascade continue to move, losing energy through both elastic and inelastic scattering, until their energies fall below a cut-off energy E_c^j (usually equal to the surface binding energy E_s^j) or leave the surface as sputtered atoms. For an atom to leave the surface it has to overcome a surface energy barrier, U , where

$$U^j = E_s^j / \cos^2 \theta_j , \quad (20)$$

and θ_j is the ejection angle of the sputtered atom j . If $E_s^j < E^j < U^j$ the atom will be assumed reflected back into the target as if they were reborn again at the surface with incident energy and angle of E^j and θ_j respectively. These atoms will be followed until their energy fall below E_c or successfully leave the surface. But if $E_s^j > E^j < U^j$, these atoms are assumed to be buried in the surface layer. In this calculation the surface energy is usually taken as the heat of sublimation of target material.

3. Applications and Discussion

In this section we examine some of the factors that may affect the

sputtering yield calculation due to surface and other phenomena. The effect of using different interatomic potentials on vanadium sputtering yield bombarded by helium ions with various incident energies is shown in Fig. 2. Vanadium is considered to be an important structural material in fusion reactors. As an example, four different potentials are used, i.e., Thomas-Fermi (TF), Moliève (MOL), Lenz-Jensen (LJ), and the one obtained using the universal reduced nuclear stopping given by Eq. (6). The unpublished experimental data shown are those given in Ref [9]. The differences in the sputtering yield from various interatomic potentials are not as large as in the case of heavier incident ions [5]. The TF potential roughly yields a better agreement with the experimental data at higher energies while the universal form of the nuclear stopping shows a relatively better agreement at lower energies. Whereas for heavier ions, the use of TF potential at high energy and Born-Mayer potential at lower energies provides the best result for the sputtering yield. Although there are no large differences in the electronic and nuclear energy losses and in the average number of primary recoil cascade among the potentials, the larger differences in the sputtering yield are to the fact that some of these cascades are generated closer to the surface. The LJ potential and the universal function result in a slightly longer range of the ion than both TF and MOL potentials. This means that the primary and secondary generated cascades are a little farther away from the surface, leading to a lower fraction of sputtered atoms. However, more data is needed before making a general conclusion. The individual contribution of the primary and the secondary knock-on atoms to the sputtering yield is shown in Fig. 3 for both TF and LJ potentials. It can be seen that the secondary knock-on atoms are the main contribution to the sputtering yield for TF potential over the energy range shown. For LJ and the other interatomic

potentials the primary knock-ons yield becomes larger than the secondary knock-ons contribution at lower energies.

Continuous irradiation and damage to a target material may change the surface properties of the target and consequently change the surface and bulk binding energies. This can be very important in determining, for example, the lifetime of first walls or limiters in fusion reactors which are exposed to intense irradiation. Figure 4 shows the vanadium sputtering yield as a function of surface and bulk binding energies. The decrease in the surface binding energy can substantially increase the sputtering yield and consequently the erosion of the target material. The variation in the sputtering yield is more sensitive to the surface binding energy than to the bulk binding energy.

Another example in which helium is being trapped in a vanadium wall material with vanadium continuously redeposited on the vanadium base material to trap the incident helium. The energy above which the vanadium self-sputtering yield exceeds unity is of interest to the operation and design of a self-pumped limiter concept in a fusion reactor. Figure 5 shows the self-sputtering yield of vanadium for difference helium-vanadium atomic concentrations. For pure vanadium the energy at which self-sputtering becomes unity is roughly 1 KeV. For 50% V + 50% He surface, this energy becomes three times larger (~3 KeV) which may have a substantial effect on the design constraint of this concept.

4. Summary and Conclusions

The three-dimensional Monte Carlo computer code ITMC has been developed to study ion transport in materials and compounds and its related phenomena. The code includes variety of models to calculate the elastic and inelastic energy losses during ion slowing down in targets. The code can be used to study certain applications that would be difficult to measure experimentally

and/or for a complicated target structure with different components. The ITMC code, which is highly optimized, fast to run, and very easy to use, provides good agreement with available experimental data.

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List of Figures

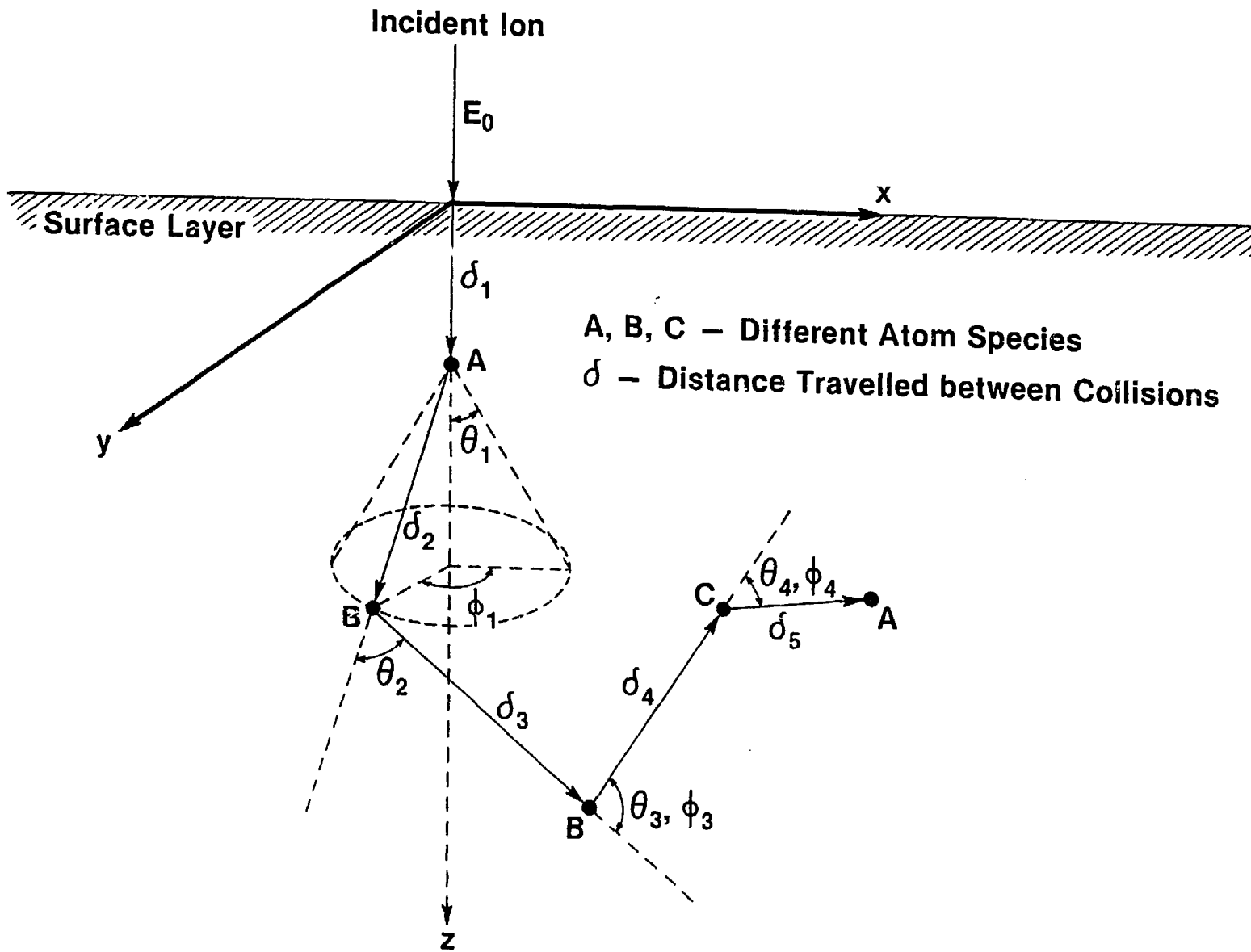
Figure 1 Schematic diagram of the initial steps of ion penetration in a solid target.

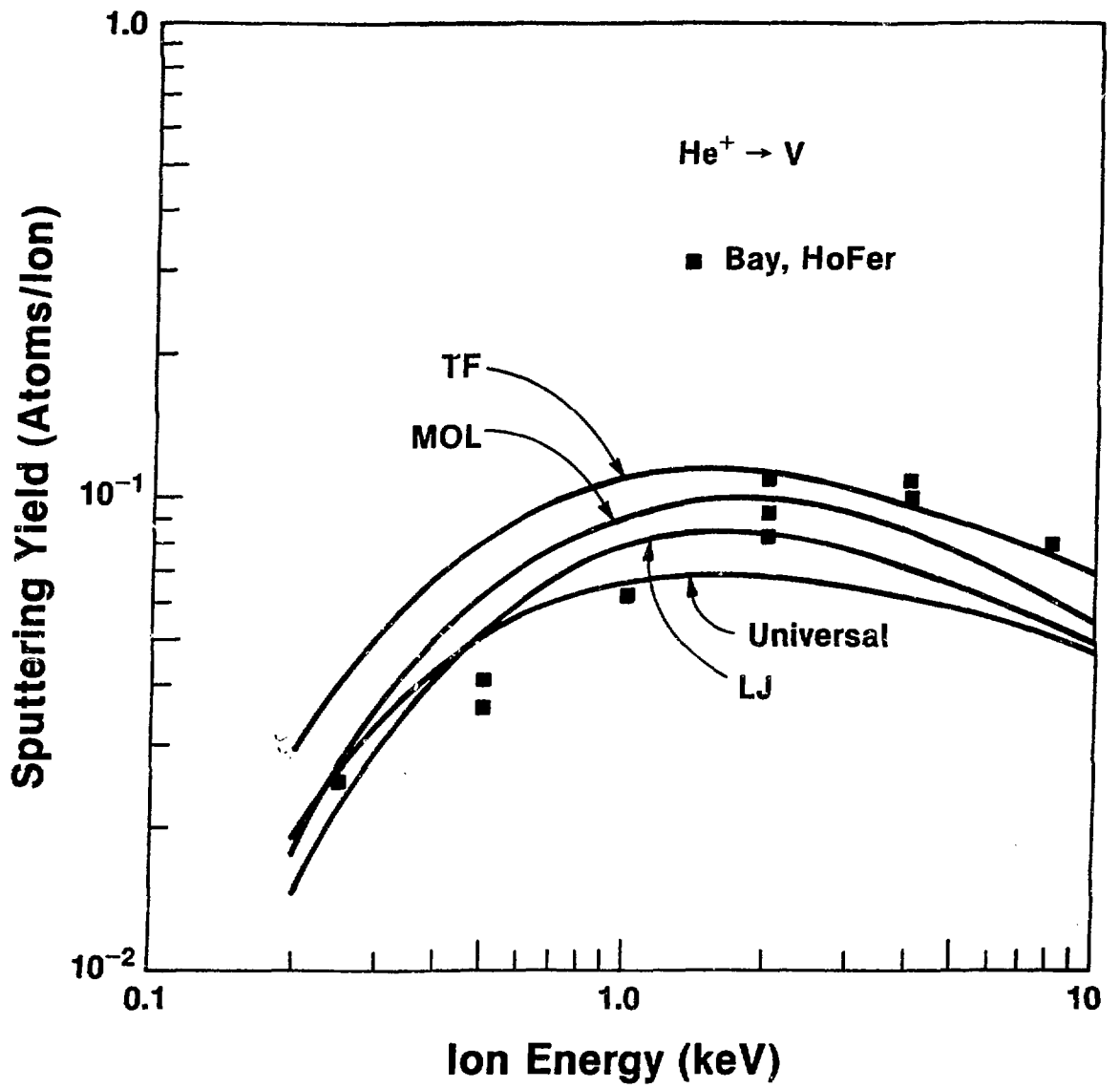
Figure 2 Vanadium sputtering yield for various interatomic potentials.

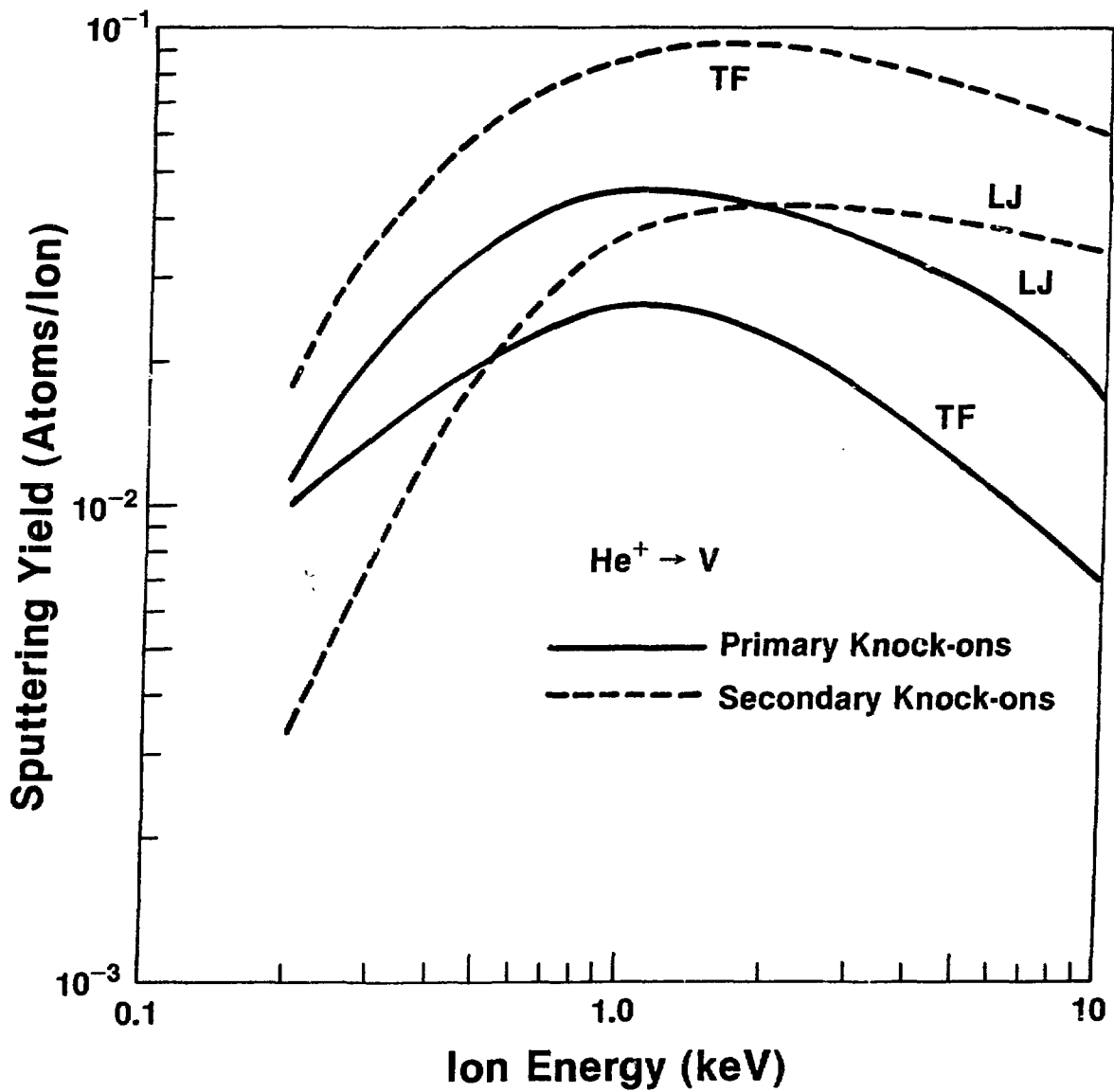
Figure 3 Contribution of the primary and secondary knock-ons to the sputtering yield.

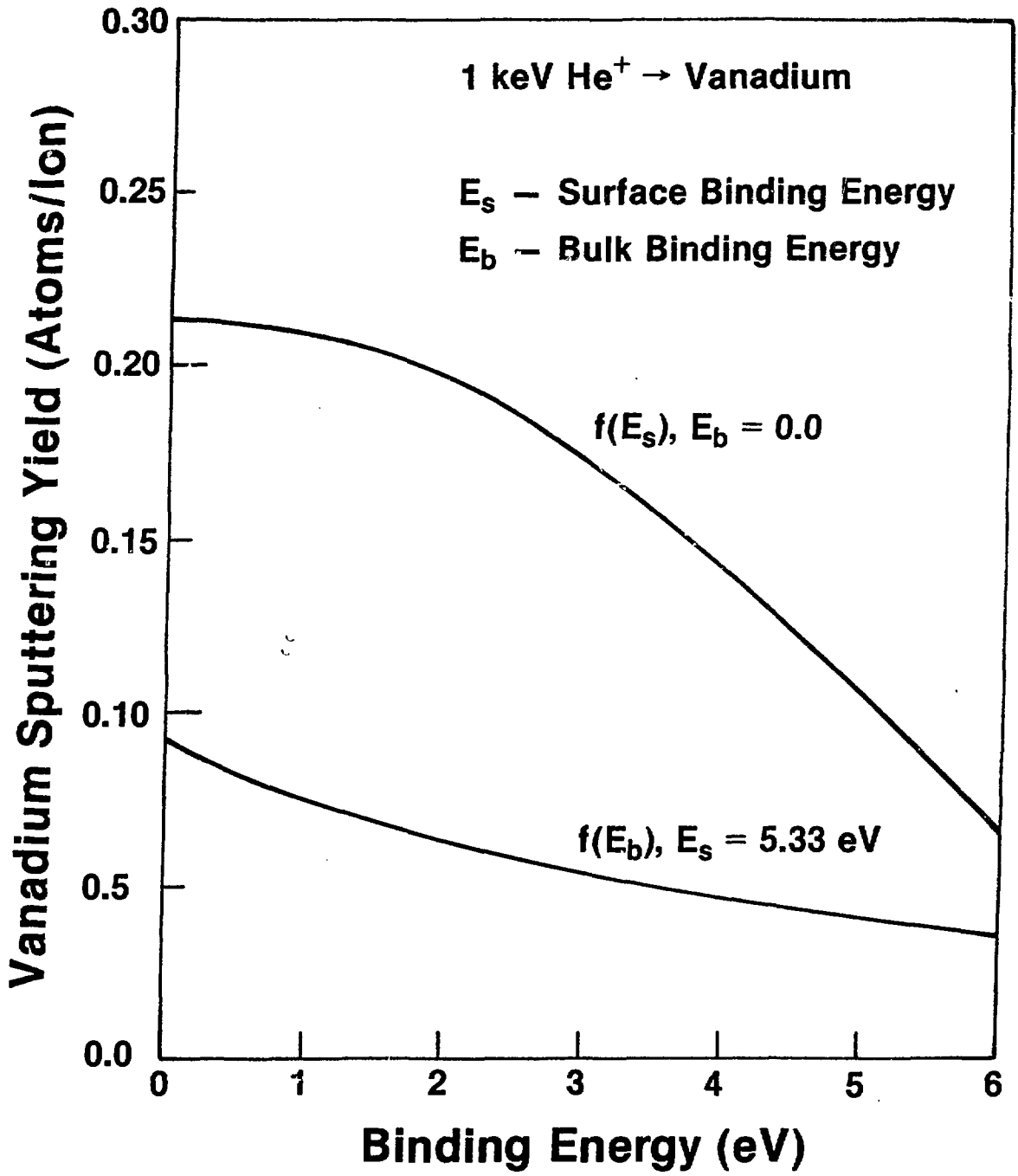
Figure 4 Sputtering yield as a function of both surface and bulk binding energies.

Figure 5 Vanadium self-sputtering yield for different V-He target composition.









Vanadium Sputtering Yield (Atoms/Ion)

