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FLUCTUATION IN THE SPATIAL DISTRIBUTION OF ENERGY DEPOSITED BY ATOMIC PARTICLES

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The standard deviation distribution corresponding to the spatial distribution of energy deposited in the slowing down of atomic particles in solids is calculated. Large fluctuations are found that agree well with Monte-Carlo simulations for fluctuations in the deposited energy and sputtering yields.

The concepts of thermal spike or "non-linear" effects are useful to explain qualitatively those radiation damage and sputtering experiments where the linear collision cascade theory underestimates the observed results. However, when quantitative predictions are desired from thermal models, some difficulties arise. One of them is the calculation of the temperature profile, which usually is assumed to be proportional to the deposited energy distribution corresponding to a single collision cascade [1]. Then a Maxwell–Boltzmann distribution is used to describe the energy spectrum of moving particles inside the "hot" region of the spike [2]. We know the deposited energy distribution corresponding to an average collision cascade [3], but not for an individual one. So, keeping in mind that the average cascade extends over a larger region in space, corrections for individual cascades are applied [1]. At this point, one should notice some short-comings of the model: in the first place, it is not closed, leaving undetermined parameters; furthermore, the individual cascade volume is a rather uncertain quantity; and finally, a three-dimensional gaussian is used to describe the single cascade which is in disagreement with the "Christmas tree" structure that is shown in computer simulations [4,5]. (See also ref. [8].)

We shall not discuss here if the thermal model is well established or not, but we will show a rough estimation of the standard deviation distribution corresponding to the deposited energy distribution. The idea is that, if we are dealing with non-linear effects on the deposited energy, it would be helpful to know its probability distribution. It is, however, an overwhelming task to calculate it, notwithstanding we can get information from its moments. Since the first-order moment of the probability distribution has been obtained [3], our aim is to go over to the second-order moment.

The basic equation has been derived by Winterbon et al. (1970) [3]. They define a function $G(\boldsymbol{r},\boldsymbol{v},P)$ which is the probability distribution just mentioned. That is: $G(\boldsymbol{r},\boldsymbol{v},P)\,\mathrm{d}P$ is the probability that the energy density deposited at $\boldsymbol{r}$, is between P and $P+\mathrm{d}P$ due to a projectile that started its motion at $\boldsymbol{r}=0$ with velocity $\boldsymbol{v}$.

$G(r,\boldsymbol{v},P)$ obeys the equation:

$$-(\boldsymbol{v}/v)\delta G(r,v,P)/\delta r = N\int \mathrm{d}\sigma\left[G(r,\boldsymbol{v},P) - \int_0^P \mathrm{d}Q\, G(r,v',P-Q)\,G(r,v'',Q)\right], \tag{1}$$

with the normalization condition:

$$\int_0^\infty \mathrm{d}P\, G(r,\boldsymbol{v},P) = 1\ . \tag{2}$$

Multiplying by P and integrating, they solved the equation for the average deposited energy distribution: $F_\mathrm{D}(r,\boldsymbol{v})$, where:

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$$F_D(r, \mathbf{v}) = \int_0^\infty P dP \, G(r, \mathbf{v}, P) = \{dE/d^3r\}(r, \mathbf{v}) .$$

In eq. (1) $d\sigma$ is the scattering cross section, and $\mathbf{v}'$ and $\mathbf{v}''$ are the velocity of the scattered projectile and recoil atom, respectively. It is assumed that target and projectile are of the same species, but generalization to different species can easily be done.

Multiplying eq. (1) by P^2 and integrating we arrive at an equation for the average square deposited energy distribution, $F_2(r, \mathbf{v})$:

$$F_2(r, \mathbf{v}) = \int_0^\infty P^2 \, dP \, G(r, \mathbf{v}, P) = \{(dE/d^3r)^2\}(r, \mathbf{v}) ,$$

which, for a one-dimensional case, is:

$$-(v_x/v)\, \delta F_2(x, \mathbf{v})/\delta x = N \int d\sigma [F_2(x, \mathbf{v}) - F_2(x, \mathbf{v}') - F_2(x, \mathbf{v}'')] - 2N \int d\sigma \, F_D(x, \mathbf{v}') F_D(x, \mathbf{v}'') . \quad (3)$$

Assuming a gaussian form for $F_D(x, v)$ and following standard procedures [3,6], the spatial moments for $F_2(x, v)$ are calculated. A power scattering cross section is used: $d = C_m dT/(E^m T^{m+1})$, E and T being the projectile and transferred energy, respectively. Inelastic effects are neglected. Only *averaged* distributions will be described by a gaussian form.

To avoid divergencies, power potentials greater than 2 (that is $m < 1/2$) are used in eq. (3), since for $m > 1/2$, the deposited energy distribution which is proportional to E^{1-2m} goes to infinity when $E \to 0$. This means that the average square deposited energy distribution is sensitive to the low energy part of the cascade and it is not correct to use the same power potential for the whole energy range. These divergencies can be removed by just assuming that F_D is proportional to E for E less than a given E_0, and solving eq. (3) by means of a Laplace transform on the energy [7]. For $E \gg E_0$ this gives a leading term which is independent of E_0 for $m < 1/2$ and is the same as in our calculations with $E_0 = 0$. Otherwise, a smooth E_0-dependence is found.

For power potentials corresponding to $m = 0.2$, 0.3 and 1/3 and for different mass ratios M_2/M_1, M_2 and M_1 being target and projectile masses, respectively, we have calculated the first spatial moments in order to reconstruct the distribution in a gaussian approximation.

The moments of the average square deposited energy distribution which are defined as follows:

$$F_2^0(\mathbf{v}) = \int F_2(x, \mathbf{v}) \, dx ,$$

$$\{x\}_2(\mathbf{v}) = \int F_2(x, \mathbf{v}) \, x \, dx / F_2^0(\mathbf{v}) ,$$

$$\{\Delta x^2\}_2(\mathbf{v}) = \int F_2(x, \mathbf{v}) x^2 dx / F_2^0(\mathbf{v}) - \{x\}_2^2(\mathbf{v}) ,$$

are compared with those of the deposited energy distribution $\{x\}_D$ and $\{\Delta x^2\}_D$ defined in the same way, and also called average damage depth and spatial straggling, respectively.

It is found that:

$$\{x\}_2/\{x\}_D \approx 1 , \quad (4a)$$

$$0.7 < \{\Delta x^2\}_2/\{\Delta x^2\}_D < 0.9 . \quad (4b)$$

These are almost constant over M_2/M_1, but the spatial straggling ratio increases monotonically with m.

From the above results we can say that the distributions $\{(dE/dx)^2\}$ and $\{dE/dx\}^2$ are not strictly proportional. For them to be proportional, instead of the results (4a) and (4b), $\{x\}_2/\{x\}_D = 1$ and $\{\Delta x^2\}_2/\{\Delta x^2\}_D = 1/2$ is required.

Let us define the standard deviation of the deposited energy distribution as follows:

$$\Omega(x, \mathbf{v}) = |F_2(x, \mathbf{v}) - F_D^2(x, \mathbf{v})|^{1/2} ,$$

and the relative standard deviation:

$$|\Omega/F_D|(x, \mathbf{v}) = \Omega(x, \mathbf{v})/F_D(x, \mathbf{v}) .$$

The facts just discussed, lead us to conclude that the relative standard deviation will have a minimum around the average damage depth.

Results are shown in figs. 1 and 2. In fig. 1 the relative standard deviation for different power potentials is plotted as a function of the mass ratio and at $x = 0$. For comparison, the relative fluctuation in the sputter coefficient is also shown; such a quantity is defined as the standard deviation of the number of sputtered particles relative to the sputtering yield. These data have

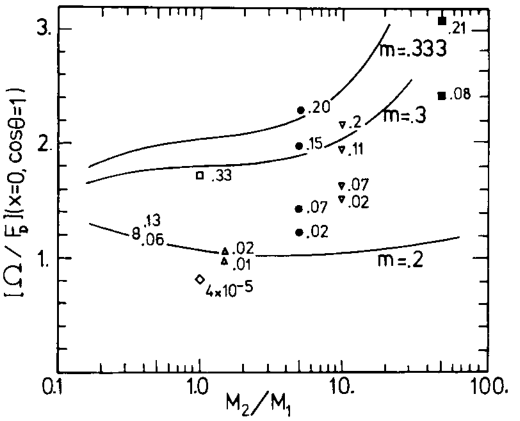

Fig. 1. Solid line: relative standard deviation of the deposited energy calculated for m = 0.333, 0.3 and 0.2 power cross sections. And relative fluctuation of the sputtering yield coefficient from TRIM-SP Monte-Carlo Code for the following projectile–target combination: ○ As on Si; ▽ Ne on Au; □ Si on Si; ◇ Au on Au; △ Xe on Au; ● Ar on Au; and ■ He on Au. Beside each point is depicted the projectile energy in reduced units.

been obtained from the TRIM-SP Monte-Carlo Code, originally used for sputtering due to ions in random solids [8], which was modified by us to deal with fluctuation problems. Large fluctuations in sputtering yields were already predicted by Westmoreland et al. [9] qualitatively from their study of the correlation between deposited energy and particle range. In fig. 2 we can see the relative standard deviation of the deposited energy as a function of depth calculated from

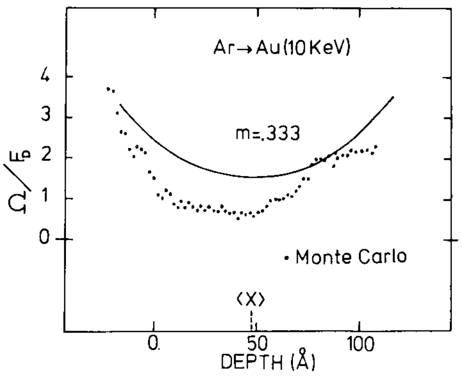

Fig. 2. Depth profile of the relative standard deviation of the deposited energy distribution calculated for m = 0.333 and the same from the TRIM-SP Monte-Carlo Code for 10 keV Ar incident upon Au.

eq. (3) and from the Monte-Carlo Code and for Ar bombardment of gold at 10 keV. In this case the numerical model simulates the history of particles which started their motion inside the solid, and the surfaces are located far from the origin compared with the projectile range.

The main features of the numerical simulation are reproduced by our calculation. A monotonically increasing function of the mass ratio is obtained for the relative standard deviation at the surface, except for m = 0.2 and low mass ratios where our results become meaningless because the gaussian approximation fails. The reader should be also aware that the gaussian approximation is not good outside the half-width region.

A word should be said about the meaning of what is calculated. The origin of the fluctuations on the deposited energy according to our model is due to a spatial effect. In other words, it is due to the fact that the cascade could grow in a certain region at one time and in another the next time. We have not included fluctuations due to a displacement threshold energy or to energy lost through processes which do not contribute to the phenomena under study. These processes should be important for fluctuations of the total amount of displaced atoms or for the energy left in excitation and ionization when energetic particles are slowed down in matter. Fano [10] and Lindhard et al. [11] have considered these effects some years ago.

In conclusion, the deposited energy density has a rather broad probability distribution supporting the idea that there are strong differences between each individual collision cascade. Therefore, one has to be careful in using averaged quantities to deal with nonlinear effects.

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