# Spatial distribution of recoiling atoms with a specific momentum generated in a collision cascade

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The spatial distribution of the momentum spectrum of recoiling atoms in an elastic collision cascade, produced by an energetic ion injected into a random solid, is investigated. Recoils are counted when accelerated from rest, or decelerated from above an energy boundary $E_1$ into an energy interval $[E_0, E_0+dE_0]$ in a single collision. Pronounced cascade anisotropies are observed, the magnitude and direction depending on the recoil energy and the depth.

Evidence on the evolution of a collision cascade during ion bombardment of solids can be gained from the differential sputtering yields resolved in energy and direction of the ejected particles.[1–4] Such spectra are images of the momentum distribution in the substrate surface. In the regime of linear cascades, the gross picture is well described by the model of an isotropic cascade and refraction in a planar surface potential.[5] Anisotropies in the cascade have also been considered,[6–10] and the effect of anisotropy on the energy and angular sputtering spectrum has been estimated[11,12] by using momentum spectra, integrated over all depths rather than the spectrum in the surface layer. The depth distribution of the cascade momentum in the limit of completion of the cascade has been thoroughly considered.[8,9] Anisotropy in the cascade also has to be considered in applications of cascade theory to the calculation of damage distributions and atomic mixing.

This Communication reports on the depth distribution of the specified recoil momentum in a linear collision cascade generated in a random solid during self-ion bombardment (ion mass $M_1$ equals target atom mass $M_2$, $M_1=M_2=M$). We consider the average number of recoils $F(E,\vec{e},E_0,\vec{e}_0,x)\,dx\,dE_0\,d\vec{e}_0$ moving in the layer $[x,dx]$ of the target, with energy in $[E_0,dE_0]$ and direction in the solid angle $[\vec{e}_0,d\vec{e}_0] = [\theta_0,d\theta_0;\chi_0,d\chi_0]$, per ion incident on the surface $x=0$ with energy $E$ and direction $\vec{e}=(\theta,\chi=0)$. Several reasonable constraints can be imposed on the counting of the number of recoils $F$ (see, e.g., Ref. 13). We have preferred the following "specific" choice: $F$ includes all recoils excited into $[E_0,dE_0]$ from rest and all recoils deexcited into $[E_0,dE_0]$ from an energy above a boundary value $E_1$ in a single collision. In this way the energy evolution of the cascade is stopped at energy $E_1$ and a "frozen in" picture of the cascade for $E_0<E_1$ is obtained. $E_1$ now acts as a threshold for reproduction of the effects to be described by $F$. We can illustrate the function of $E_1$ at its role in the Kinchin-Pease model[14] for the formation of Frenkel pairs. In this model a crystal atom will generate one and only one Frenkel pair, when it receives an energy between the displacement energy $E_d$ and $2E_d$. If it receives an energy $>2E_d$, it starts a subcascade, which may lead to the formation of more than one Frenkel pair. Thus, for the application of the cascade theory, as discussed here, to the production of Frenkel pairs $E_1=2E_d$. Another application can be found in the production of focusing collision sequences. A focusing collision sequence can be generated, when a recoil in the cascade receives an energy $<E_f$ (focusing energy), provided its direction is in a small angular interval around a low index crystallographic axis.[15] The cascade theory, developed in this paper, lends itself well to calculate the probability of generation of such sequences. Evidently, $E_1=E_f$ in this case. The previous calculations on the depth distribution of the deposited momentum[8,9] have been performed for the case $E_1/E<10^{-7}$ (unspecified deposited momentum).

An expression for $F(E,\vec{e},E_0,\vec{e}_0,x)$ is obtained from a backward transport equation, containing two source terms (see, e.g., Ref. 15). One source term describes the contribution of the direct recoil, the other the contribution of the scattered projectile (we are dealing with self-ion bombardment) to the specified momentum interval. The transport equation is solved by taking spatial averages[16] and using an expansion (in spherical harmonics) in the angular variables. The equation for the zero-order moment is solved following the approach as put forward in Ref. 7 and this solution is used in the recurrence scheme to obtain the higher-order moments.

This results in the following expression for $F$:

$$F(E,\vec{e},E_0,\vec{e}_0,x)=\frac{1}{4\pi}\frac{f(E_0/E_1)}{\psi(1)-\psi(1-m)}\frac{1}{E_1}\left(\frac{F_E(x,E_1,E)}{E_0}+3\frac{\vec{F}_p(x,E_1,E)\cdot\vec{e}_0}{\sqrt{2ME_0}}\right) , \tag{1}$$

with

$$f\left(\frac{E_0}{E_1}\right)=m\left(\frac{E_0}{E_1}\right)^{-m}+\left(1-\frac{E_0}{E_1}\right)^{-m}\left(\frac{E_1}{E_0}-m\right)-\frac{E_1}{E_0}$$

(i.e., scattering from a potential $V(r)\propto r^{-1/m}$, $0<m<1$). $F_E(x,E_1,E)$ and $\vec{F}_p(x,E_1,E)$ are defined as the specified deposited energy and specified deposited momentum, respectively, at depth $x$, i.e., for a particular value of $E_1/E$ and are independent of $E_0$. $F_E(x,E_1,E)$ and $\vec{F}_p(x,E_1,E)$ are constructed from the spatial averages. A construction of $\Phi_E=F_E(x,E_1,E)/E$ using the method of Padé approximants[8,13] is shown in Fig. 1(a). Evidently $\Phi_E$ depends only weakly on $E_1/E$, and, even for larger values of $E_1/E$, differs very little from the unspecifed (i.e, $E_1/E=0$) deposited energy.[16] For $E_1=\alpha E_0$, $\alpha>1$ the isotropic ($F_E$) term constitutes an $E_0^{-2}$ spectrum.[17] A construction of $\vec{\Phi}_p=\vec{F}_p(x,E_1,E)/\sqrt{2ME}$ is shown in Fig. 1(b). Quite opposite to $\Phi_E$, $\vec{\Phi}_p$ depends strongly on $E_1/E$. For $E_1=\alpha E_0$, $\alpha>1$ this anisotropic term in Eq. (1) leads to a $E_0^{-3/2}$ spectrum.

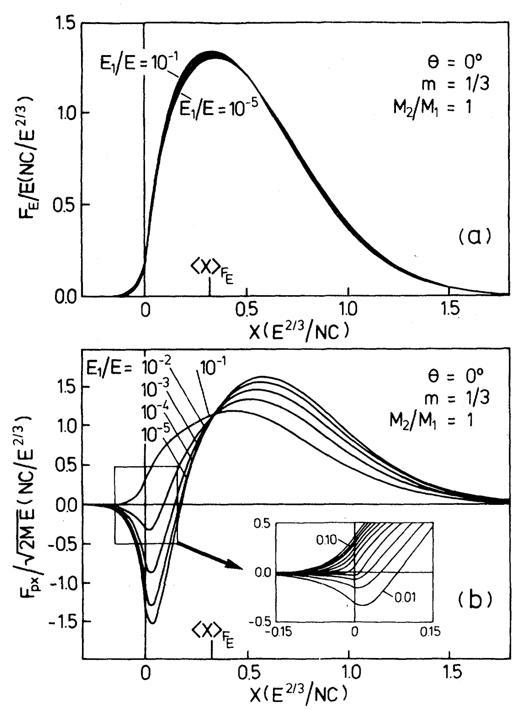


FIG. 1. Depth distribution of the specified deposited energy (a) and the specified deposited momentum (b). The units are scaled to the used power potential ($m=\frac{1}{3}$). Indicated is the mean value $\langle x\rangle_{F_E}$ of the specified deposited energy. The inset in (b) gives the detailed specified momentum near the surface $x=0$ for values of $E_1/E$ ranging from 0.01 (bottom curve) to 0.11 (top curve). Step width in $E_1/E$ is 0.01. ($N$ is the target density, $C$ the constant of the power cross section.)

For an assessment of the relative weight of the two contributions inspect the anisotropy parameter $A$ (Fig. 2):

$$A=1+3\sqrt{E_0/E}\,\vec{\Phi}_p\cdot\vec{e}_0/\Phi_E . \tag{2}$$

We will briefly discuss $A$ at the surface ($x=0$), for normal incidence ($\theta=0$) and $E_1=2E_0$. For $E_1/E\approx 0$ we obtain an isotropic distribution. An increase of $E_1/E$ leads to preferred outward momentum, which reduces again to an isotropic distribution for $E_1/E\approx 0.045$. If $E_1/E>0.045$ the momentum is

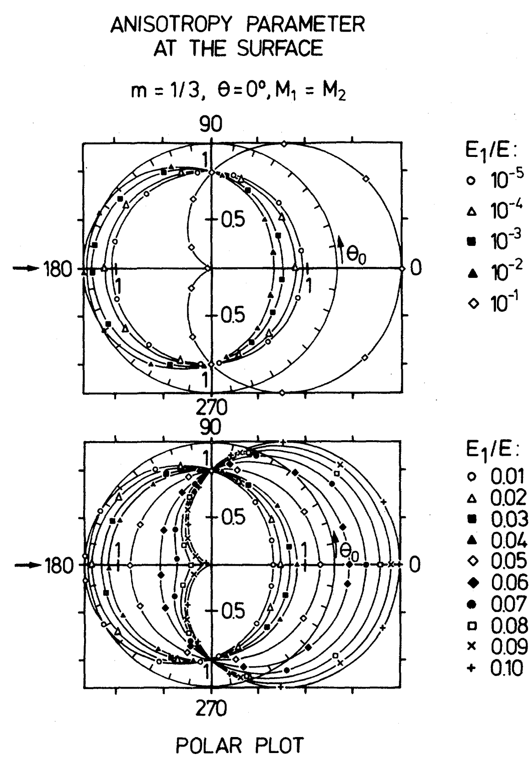


FIG. 2. Polar plots of the anisotropy parameter $A$ for $\theta=0$, $m=\frac{1}{3}$ at $x=0$. For an explanation, see text.

preferably directed inwards [see also Fig. 1(b)].

In conclusion, the anisotropy parameter $A$ represents the modification of the cascade with respect to complete isotropy and is seen to be strongly dependent on the recoil energy both absolutely as well as relatively to the projectile energy. Applied to sputtering it will result in an overcosine distribution when $A > 1$, a cosine distribution when $A = 1$, and an undercosine distribution when $A < 1$ (see Ref. 18). This makes it the first calculation, which potentially predicts both observed distributions of sputtered particles.

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