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Ion Deposition Profiles**

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W.G. Wolfer and M.E. Benchikh-Lehocine

Fusion Technology Institute
University of Wisconsin
1500 Engineering Drive
Madison, WI 53706

<http://fti.neep.wisc.edu>

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W. G. Wolfer and M. E. Benchikh-Lehocine
Department of Nuclear Engineering, University of Wisconsin,
Madison, WI 53706, USA

Abstract

Using the transport theory for the distribution of deposited energy or deposited ions, it is shown that the effect of density changes on these distribution profiles can be obtained from the distribution profiles in a medium with constant density by a simple coordinate transformation, provided the distribution functions depend only on one spatial coordinate.

1. Introduction

In studies of sputtering, blistering, radiation damage, and ion implantation of solids, the range distribution of both deposited ions and deposited energy are of primary interest. These distribution profiles are commonly computed according to the transport theory developed by Sigmund and Sanders.^(1,2) In their original formulation, the density of atoms in the solid was considered to be constant. It is a trivial matter, however, to generalize it to include nonuniform atom densities.

Variations in density and composition with depth are often encountered in ion bombardment studies. These variations may be due to the initial surface contamination and segregation of alloying elements to the surface. Or, more often, the variations are due to void and bubble formation as a result of the ion bombardment itself.

The effect of density variations as caused by radiation-induced voids on the range of ions and damage was earlier considered by Odette et al.⁽³⁾ in an ad hoc fashion. They argued that the effect of voids can simply be included into the range by adding the distance traveled through the voids to the distance traveled through the void-free solid. They considered this procedure an approximate one, however, since void-induced straggling was not accounted for.

In the present paper we prove rigorously, starting from the transport theory, that density correction to the entire profiles for both ion and damage distribution can be made immediately if one knows these profiles in the solid with constant density and if one knows the density variation with depth. This can be achieved by a simple transformation of the depth coordinate. It follows further from the proof that density corrections can be made in this

manner whenever the transport problem can be formulated as a one-dimensional one, be it planar, cylindrical or spherical.

2. Transport Equation for Range and Damage Distribution

Let $F(\vec{r}, \vec{v})$ denote the distribution function for either the deposited energy (damage) or the deposited ions (range). More specifically, $F(\vec{r}, \vec{v}) d^3r$ is either the recoil energy or the ions deposited in the volume element d^3r about \vec{r} when these ions enter the solid at $\vec{r} = 0$ and with initial velocity \vec{v} .

This distribution function satisfies the following transport equation:

$$\begin{aligned}
 & - \frac{\vec{v}}{|\vec{v}|} \cdot \vec{\nabla}_r F(\vec{r}, \vec{v}) - N(\vec{r}) \frac{S_e}{|\vec{v}|} \frac{\partial}{\partial |\vec{v}|} F(\vec{r}, \vec{v}) \\
 & = \int N(\vec{r}) d\sigma \{F(\vec{r}, \vec{v}) - F(\vec{r}, \vec{v}') - \xi \bar{F}(\vec{r}, \vec{v}'')\} .
 \end{aligned}
 \tag{1}$$

Here, $N(r)$ is the local atom density, $d\sigma(\vec{v}', \vec{v}'')$ is the differential cross section for elastic nuclear scattering, the integration being carried out over all velocities \vec{v}' of the scattered ion and over all velocities \vec{v}'' of the recoiling target atom, and S_e is the electronic stopping power per target atom. The parameter $\xi = 0$ for the range distribution, and $\xi = 1$ for the damage distribution, respectively. $\bar{F}(\vec{r}, \vec{v})$ is the recoil distribution. If the target atoms differ from the projectile atoms, then $\bar{F}(\vec{r}, \vec{v})$ satisfies an equation like Eq. (1) in which all the distribution functions refer now to target atoms.

Equation (1) is identical to those derived by Sigmund and Sanders^(1,2) and others^(4,5,6) with the trivial modification that the number density of target atoms, $N(\vec{r})$, is a function of the position.

3. Transformation to Constant Density

For a plane ion source with a lateral ion flux profile that changes little over distances of the order of the ion range, the transport problem becomes one-dimensional. Then F depends only on the depth coordinate x if the density is also only a function of x . Let us then define a new space coordinate

$$\bar{x} = \frac{1}{\bar{N}} \int_0^x N(x') dx' \quad (2)$$

where

$$\bar{N} = \frac{1}{R} \int_0^R N(x') dx' \quad (3)$$

is the number density of atoms average over at least the entire range or beyond.

Assuming that the function $\bar{x}(x)$ can be inverted in principle to obtain $x(\bar{x})$, the distribution function becomes now a function of \bar{x} . Since

$$\frac{\partial F}{\partial x} = \frac{d\bar{x}}{dx} \frac{\partial F}{\partial \bar{x}} = \frac{N(x)}{\bar{N}} \frac{\partial F}{\partial \bar{x}}, \quad (4)$$

the transport Eq. (1) for the one-dimensional case can now be written as

$$\begin{aligned} & - \frac{v_x}{|v|} \frac{N(x)}{\bar{N}} \frac{\partial}{\partial \bar{x}} F(\bar{x}, \vec{r}) - N(x) \frac{S_e}{|v|} \frac{\partial}{\partial |v|} F(\bar{x}, \vec{r}) \\ & = \int N(x) d\sigma \{ F(\bar{x}, \vec{r}) - F(\bar{x}, \vec{v}') - \xi F(\bar{x}, \vec{v}'') \} . \end{aligned} \quad (5)$$

If this equation is multiplied by $\bar{N}/N(x)$ we obtain a transport equation for $F(\bar{x}, \vec{v})$ in a medium with constant atom density \bar{N} .

Therefore, we have shown, that if the transport equation is solved for a constant uniform atom density \bar{N} and the solution is $F(\bar{x}, \vec{v})$, then the distribution function in a medium with nonuniform atom density $N(x)$ is given by $F[x(\bar{x}), \vec{v}]$, where $x(\bar{x})$ can either be obtained from the inversion of the function defined in Eq. (2), or from the equation

$$x = \bar{N} \int_0^{\bar{x}} \frac{d\bar{x}}{N(\bar{x})} . \quad (6)$$

When we apply these results to density changes caused by void or bubble swelling, it is more convenient to employ the number density N_0 in the theoretically dense material rather than \bar{N} . If $S(x) = \Delta V/V$ and $S_0(\bar{x}) = \Delta V/V_0$ denote then the void volume fraction per unit volume of the voided and void-free material, respectively, then

$$N(x) = N_0 (1 - S(x)) \quad (7)$$

and

$$N(\bar{x}) = N_0 (1 - S_0(\bar{x})) . \quad (8)$$

Hence, the depth coordinate transformation is given by

$$\bar{x} = x - \int_0^x S(x') dx' \quad (9)$$

or by

$$x = \int_0^{\bar{x}} \frac{d\bar{x}'}{[1 - S_0(\bar{x}')] } . \quad (10)$$

Experimentally, the swelling is usually measured as a function of depth x , so that Eq. (9) is the more appropriate one to use.

4. Discussion

We have shown from the transport theory applicable to range and damage distribution as produced by a planar ion beam that density variations with depth can simply be accounted for once the distribution functions have been obtained for the fully dense and uniform material. Although this was shown explicitly only for the planar, one-dimensional distributions, the same result is obtained, whenever the transport equations depend only on one coordinate. It applies then also to ion-bombardment from a spherical or a cylindrical source in a solid. Spherical ion sources in the form of boron-rich precipitates have recently been considered by Gelles and Garner⁽⁷⁾ as a tool to study void formation in steels under simultaneous production of damage and helium. The void density around the precipitate particles was found to depend only on the radial distance.

As mentioned in the discussion, a variation in the composition of alloys or compounds with depth may be produced by the ion bombardment due to preferential sputtering, radiation-induced segregation and recoil mixing.

To compute the redistribution of the various elements in an alloy or compound as a result of ion bombardment, a set of transport equations for each species need to be solved simultaneously.⁽⁸⁾ When electronic losses can be neglected each transport equation depends on only one number density. If the number densities for the various species depend on the depth we can again apply the above coordinate transformation for each species separately, and we obtain transport equations which depend only on an average constant density of one particular species.

Unfortunately, when electronic losses are included each transport equation depends now on all number densities, and the above transformation no longer generates equations for uniform atom densities.

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References

1. P. Sigmund and J. B. Sanders, Proc. of the Intern. Conf. on "Application of Ion Beams to Semiconductor Technology," ed. by P. Glotin (Editions Oplins, Paris, 1967), p. 215.
2. P. Sigmund, Phys. Rev. 184, 383 (1969).
3. G. R. Odette, D. M. Schwartz, and A. J. Ardell, Rad. Effects 22, 217 (1974).
4. K. B. Winterbon, P. Sigmund, and J. B. Sanders, Mat. Fys. Medd. Dan. Vid. Selsk. 37, No. 14, 1970.
5. P. Sigmund, M. T. Matthies, and D. L. Phillips, Rad. Effects 11, 39 (1971).
6. K. B. Winterbon, Rad. Effects 30, 199 (1976).
7. D. S. Gelles and F. A. Garner, J. Nucl. Materials 85 & 86, 689 (1979).
8. K. B. Winterbon, Rad. Effects 48, 97 (1980).