DEFOCUSING–FOCUSING COLLISION SEQUENCES

By M. C. E. PETERSEN*

[*Manuscript received October* 28, 1966]

Summary

A defocusing collision sequence with initial energy greater than the focusing energy can be converted into a focused collision sequence. This is demonstrated in the "hard sphere approximation" by taking account of the energy loss due to interaction with neighbouring lattice rows.

It seems fairly well established in the radiation damage of crystalline solids that lattice-correlated collisions are generated at the low energy end of a collision cascade initiated by an energetic primary knock-on (Leibfried 1964). A simple model, proposed by Silsbee (1957), can be used to describe one type of correlated collision. He suggested

1. In almost head-on collisions between two atoms of equal mass, at the point of closest approach we can write

$$V(R) = \tfrac{1}{2}E, \tag{1}$$

where $V(r)$ is the interatomic potential, R is the distance of nearest approach, and E is the energy of the incident atom. The effect of the small impact parameter can be neglected.

2. The repulsive component of the interatomic potential is sufficiently steep to permit the collision of two atoms to be described as a collision between two "hard spheres". The radius of each sphere is $R/2$, where R is determined from equation (1).
3. A sequence of head-on collisions can result in energy transport along close-packed directions in a crystal lattice.

Consider an isolated line of atoms. The separation between each is D. If one atom moves away from the line with an energy E and at a small angle θ_1 and collides with its nearest neighbour, the neighbour will move away from the line with an angle θ_2. For small angles θ_1 and θ_2 the geometry imposes the relation

$$\frac{\theta_2}{\theta_1} = \left(\frac{D}{R} - 1\right), \tag{2}$$

where R is the collision radius, determined by (1). When $R > D/2$, $\theta_2 < \theta_1$. Continuing this process along the line of atoms a series of almost head-on collisions occurs, the angular deviation of successive atoms becoming smaller and the energy transfer at each collision becoming more and more complete. This sequence of collisions has been

* School of Physics, University of New South Wales, Kensington, N.S.W.

called a "focused collision sequence", or, more briefly, a "focuson". The limiting value of the collision radius for this to occur is obtained from (2) when $\theta_2 = \theta_1$, i.e. at $R = D/2$. Collisions of this sort propagating along the $\langle 110 \rangle$ directions of face-centred cubic crystals give rise to the familiar spot patterns obtained in metal single-crystal sputtering experiments (Anderson and Wehner 1960; Nelson and Thompson 1961).

Alternatively, if $R < D/2$ then $\theta_2 > \theta_1$ and the angular divergence of successive atoms along the line increases continuously until the sequence terminates as eventually one atom completely misses its nearest neighbour.

The short-ranged repulsive component in the interatomic potential of a metal is often written in the Born–Mayer form (Huntington 1954)

$$V(r) = A\,\mathrm{e}^{-r/a}. \tag{3}$$

The constants a and A are chosen to fit the elastic constants of the metal. In radiation damage it is usually agreed that the long-ranged, slowly varying, attractive component of the interatomic potential may be neglected (Lehmann and Leibfried 1961). In the almost head-on collisions being considered, equations (1) and (3) may be combined to give

$$E = 2A\,\mathrm{e}^{-R/a}, \tag{4}$$

and the relation between the collision radius and energy is determined. Following Leibfried (1959) we define the limiting energy E_f, called the focusing energy, by substituting $R = D/2$ into equation (4). This gives

$$E_\mathrm{f} = 2A\,\mathrm{e}^{-D/2a}. \tag{5}$$

At energies below E_f a sequence of collisions focuses. Equation (4) can be inverted to give the collision radius as a function of the incident atom's energy. With the aid of (5) it becomes

$$R = \frac{D}{2} - a \ln \frac{E}{E_\mathrm{f}}. \tag{6}$$

Thus, for a given energy a collision radius is determined that will result in a sequence of collisions that are either focusing or defocusing.

In a metal, however, E is not a constant for all the collisions in a sequence propagating along a line of atoms. It is decreased continually by thermal vibrations, non-head-on collisions, and interactions with neighbouring rows of atoms. The most important, for angular deviations less than approximately 5°, is the loss to neighbouring rows of atoms. Dederichs and Leibfried (1962) have shown that this is almost constant at 0·7 eV for the $\langle 110 \rangle$ direction in copper, which confirms an earlier estimate of Leibfried (1959) and agrees well with the result obtained by computer simulation of these events by Gibson *et al.* (1960). Thus, the energy at the nth collision can be written as

$$E(n) = E_\mathrm{f}(1 - n\epsilon), \tag{7}$$

where ϵ ($= 1{\cdot}1 \times 10^{-2}$ for copper (Leibfried 1959)) is the relative loss per collision at E_f. For $n < 0$, $E > E_\mathrm{f}$; and for $n > 0$, $E < E_\mathrm{f}$. According to Leibfried (1959) the small angular changes at each collision permit us to replace θ_n by the continuous function

$\theta(n)$ and, hence, to write $\theta(n+1) = \theta(n)+\theta'(n)$. Using this in equation (2), combined with (6) and (7), we obtain the diffential equation

$$\frac{\mathrm{d}\theta}{\mathrm{d}n} = 2\left\{\frac{1}{1-(2a/D)\ln(1-n\epsilon)} - 1\right\}\theta. \tag{8}$$

Now, for $n\epsilon < 1$, expansion of the first term in the brackets in a Taylor series gives

$$\frac{\mathrm{d}\theta}{\mathrm{d}n} = 2\left\{-\frac{2a}{D}\epsilon n - \frac{a}{D}\left(1-\frac{4a}{D}\right)\epsilon^2 n^2 + \ldots\right\}\theta. \tag{9}$$

Integrating this equation and using the condition that, at $E = E_\mathrm{f}$, $n = 0$ and $\theta = \theta_\mathrm{f}$ gives

$$\frac{\theta}{\theta_\mathrm{f}} = \exp\left\{-\frac{2a\epsilon}{D}n^2 - \frac{2a\epsilon^2}{3D}\left(1-\frac{4a}{D}\right)n^3 + \ldots\right\}, \tag{10}$$

which can be written in terms of energy using equation (7).

Neglecting the term in n^3 in equation (10) we see that the angular divergence of successive atoms, as a momentum pulse travels along a line, is a Gaussian relation centred at $n = 0$, i.e. at $E = E_\mathrm{f}$. Thus, for $n < 0$, i.e. for $E > E_\mathrm{f}$, the angular deviation increases to a maximum at θ_f, and thereafter the deviation decreases as one expects in a usual focused collision sequence with $E < E_\mathrm{f}$. As an example of the effect in copper we calculate the values of n and E that give $\theta = \frac{1}{2}\theta_\mathrm{f}$ and $\theta = \frac{1}{5}\theta_\mathrm{f}$. The values $a = D/13$ and $A = 22{\cdot}5$ keV are used in the interatomic potential (Lehmann and Leibfried 1961). When $\theta = \frac{1}{2}\theta_\mathrm{f}$, $n = \pm 20$ and $(E-E_\mathrm{f})/E_\mathrm{f} = \pm 0{\cdot}22$; similarly, at $\theta = \frac{1}{5}\theta_\mathrm{f}$, $n = \pm 31$ and $(E-E_\mathrm{f})/E_\mathrm{f} = \pm 0{\cdot}34$.

Duesing and Leibfried (1965) have given an analysis of a collision sequence propagating along a close-packed line of atoms correct to second-order terms in the impact parameter. The exact relation of the angular deviation of an atom to its energy at each collision in a sequence was obtained iteratively and included angular losses, the calculation being valid to $\theta \approx 12°$. The results given above are in general agreement with that of Duesing and Leibfried apart from the overestimation of E_f in the "hard sphere" model used here.

In taking explicit account of the energy dependence of the collision radius this calculation, within the confines of the "hard sphere" approximation, has two important results.

1. For energies $E > E_\mathrm{f}$ a focused collision sequence may be created by conversion of a defocusing collision sequence at $E = E_\mathrm{f}$. This is in contrast to the result obtained when a constant collision radius is used (Leibfried 1959).
2. For $E > E_\mathrm{f}$, $R < D/2$, the incident particle is closer to the equilibrium site of the target atom than its own site at the instant of the collision. The incident atom will replace the target atom when it moves off after the collision. From the values given in the preceding paragraph it is clear that a succession of replacement collisions may transport an interstitial some 20–30 lattice spacings. Further, replacement collisions can occur down to

an energy $E = \frac{1}{4}E_f$, this being due to the "non-hard-sphere" character of the interatomic potential (Thompson 1964). Using $E = \frac{1}{4}E_f$ in equation (7) with the above results it is seen that an interstitial may be dynamically transported through the lattice by correlated collisions and separated by up to 100 lattice spacings from the vacancy at the beginning of the sequence of collisions.

The author thanks Dr. J. C. Kelly of the University of New South Wales for his critical comments.

References

Anderson, G. S., and Wehner, G. K. (1960).—*J. appl. Phys.* **31**, 2305.
Dederichs, P. H., and Leibfried, G. (1962).—*Z. Phys.* **170**, 320.
Duesing, G., and Leibfried, G. (1965).—*Phys. Status Solidi* **9**, 463.
Gibson, J. B., Goland, A. N., Milgram, M., and Vineyard, G. H. (1960).—*Phys. Rev.* **120**, 1229.
Huntington, H. B. (1954).—*Phys. Rev.* **93**, 1414.
Lehmann, Chr., and Leibfried, G. (1961).—*Z. Phys.* **162**, 203.
Leibfried, G. (1959).—*J. appl. Phys.* **30**, 1388.
Leibfried, G. (1964).—*In* "The Interaction of Radiation with Solids". p. 1. (Eds. R. Strumane *et al.*) (North Holland: Amsterdam.)
Nelson, R. S., and Thompson, M. W. (1961).—*Proc. R. Soc.* A **259**, 458.
Silsbee, R. H. (1957).—*J. appl. Phys.* **28**, 1246.
Thompson, M. W. (1964).—*In* "The Interaction of Radiation with Solids". p. 84. (Eds. R. Strumane *et al.*) (North Holland: Amsterdam.)