loop, the situation will be reversed. In A the local rotation reduces the diffraction and A appears bright, whereas B now appears dark. The loop image will apparently contract, becoming more elliptical, in the situation illustrated. One has next to decide in which sense the loop is inclined to the horizontal, and this is done by observing whether there is a general tendency to become more or less elliptical as a large external rotation is applied in a known direction.

Plate XI shows how these properties can be applied to distinguish between interstitial and vacancy loops. The external rotation is clock-wise so that in a large rotation each image becomes less elliptical as a general trend. Take the situation at (*b*) and (*f*). Just before bend extinction contour crosses the loop, regions A will be dark, since they contain clockwise rotations and anticipate the external rotation. After the contour passes, regions B will be dark since their rotation tries to restore the dark extinction condition. From the diagram it is clear that during the passage of the contour the interstitial loop has apparently become *less* elliptical whereas the vacancy loop has become *more* elliptical. The general tendency of the external rotation was to make the loops appear *less* elliptical. One may generalize to say that when the apparent change as the bend extinction contour passes *enhances* the general trend of ellipticity due to external rotation, one has an *interstitial* loop. When the apparent change *reverses* the general trend one has a *vacancy* loop.

An example of this technique is shown in plate XI where the micrographs show the behaviour of a loop in quenched MgO. As external rotation proceeds the general trend for a *less* elliptical loop is always *reversed* when a bend extinction contour passes through. This is therefore a vacancy loop. It must be emphasized that this simple version of the technique is chosen mainly as an illustration of the physical principle involved. If the Burgers vector were inclined at a small angle to the loop plane the loop behaviour might be difficult to interpret since the regions A and B would be shifted from the positions shown in fig. 33. Further, we have neglected the alteration of Bragg conditions by the local change in lattice spacing and have concentrated only on rotations. Hirsch and his colleagues suggest that the second effect is more important in the vast majority of cases, but some care is necessary in applying the above procedure.

CHAPTER 4

THE PRIMARY EVENT

4.1. Introduction

Having discussed the nature of defects, we now consider how they are produced in a crystal by irradiation. The primary event is the interaction between radiation and solid that leads to an atom recoiling from its lattice site. If the recoil is sufficiently energetic, at least one interstitial-vacancy pair is formed, and in many cases the primary recoil energy will be distributed in a cascade of atomic collisions ejecting secondary atoms from their sites. Such cascades are the subject of Chapter 5.

The simplest primary event is the collision between a charged particle and the atomic nucleus. This can be treated as a two-body collision provided that the mean free path between collisions is much greater than the interatomic spacing. The chance of correlation effects due to neighbouring atoms recoiling almost simultaneously is then very small. The systems treated in this chapter will satisfy this condition, but multiple collisions must be considered in Chapter 5.

The momentum of the recoiling atom is the parameter which determines the damage to the solid structure and it will be our aim to calculate it. The interaction of radiation with atoms is generally considered from the viewpoint of the scattered particle, here however we shall be most concerned with the energy of the recoil atom and the angle between its path and that of the incident particle. First let us derive some general relations governing two-body collisions considering only the asymptotic values of momentum at great distances from the collision. There is then no violation of quantum laws in assigning a sharp momentum to a particle since we are not localizing its position along the path. The Principles of Conservation of Momentum and Energy are all that are required to obtain recoil energy as a function of recoil angle. Initially we shall assume that collisions are elastic and, further, that velocities are small enough for non-relativistic mechanics to apply.

Let the mass, velocity and energy of the incident particle be M_1, u_1 and E_1 before collision; the angle through which it is scattered θ_1 and its final velocity v_1. Let M_2 be the mass of the struck particle, v_2 its final velocity and θ_2 the angle of recoil (fig. 34).

Some simplification is brought about by treating the motion relative to the centre of mass G in what will be referred to as G co-ordinates. The co-ordinate system at rest in the laboratory will be called the L system. The velocity $\mathbf{u}_g$ of G in L co-ordinates is found

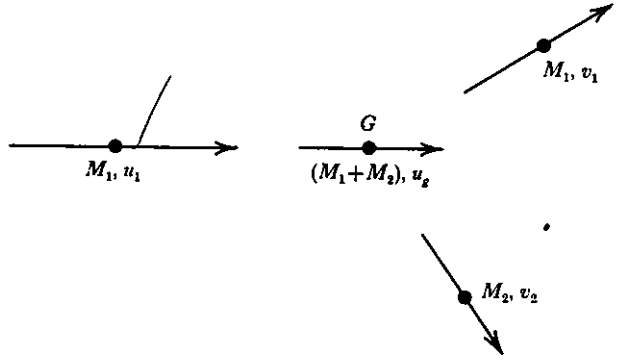

Fig. 34. A two-body collision in laboratory (L) coordinates.

by assuming a particle of mass (M_1+M_2) to be travelling with $\mathbf{u}_g$ and equating its momentum to that of the incident particle: $M_1\mathbf{u}_1$.

Hence

$$\mathbf{u}_g = M_1\mathbf{u}_1/(M_1+M_2). \tag{4.1}$$

By subtracting this vector from all velocities in the problem one transforms from L to G co-ordinates, as shown in fig. 35 where the meaning of $\mathbf{V}_1$, $\mathbf{V}_2$ $\mathbf{U}_1$ and ϕ are defined. Because G remains at rest, $\mathbf{V}_1$ and $\mathbf{V}_2$ are in opposite directions. A further simplification arises from conservation of energy and momentum which require:

$$M_1U_1^2+M_2u_g^2 = M_1V_1^2+M_2V_2^2, \tag{4.2}$$

$$M_1U_1+M_2u_g = M_1V_1+M_2V_2. \tag{4.3}$$

In L co-ordinates the equations would include trigonometric functions and would not possess the simple form of this pair. Because (4.2) and (4.3) are similar to the extent that where (velocity)^2 appears in (4.2) the corresponding (velocity) appears in (4.3) they

can only be simultaneously satisfied by each particle leaving G with the same speed with which it approached, i.e.

$$U_1 = V_1 \quad \text{and} \quad u_g = V_2. \tag{4.4}$$

Then, calculating V_1 from figure 35 and (4.1):

$$V_1 = M_2u_1/(M_1+M_2) \tag{4.5}$$

the simplified collision is represented in fig. 36.

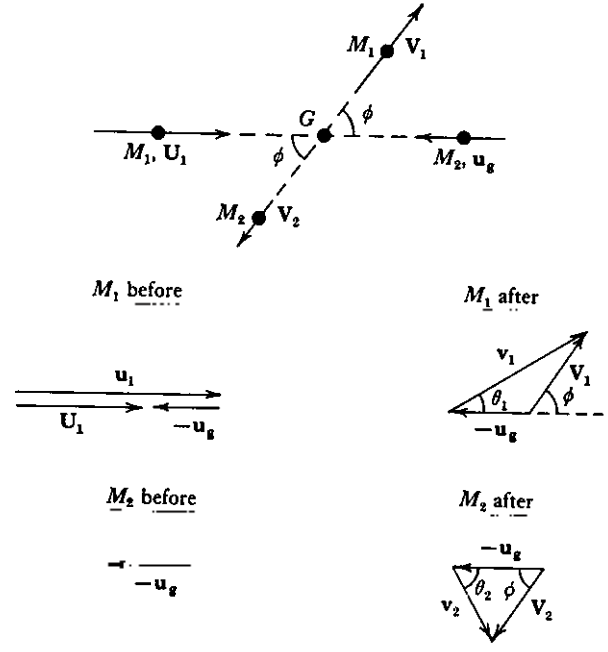

Fig. 35. The transformation to centre-of-gravity (G) coordinates.

An important quantity is the sum kinetic energy, either before or after collision, in the G system. This is easily shown to be:

$$M_2E_1/(M_1+M_2). \tag{4.6}$$

It is easily verified that this, when added to the kinetic energy of the centre of mass $\frac{1}{2}(M_1+M_2)u_g^2$ is just E_1 confirming that the total energy of the two bodies is unchanged by the new description in G co-ordinates.

We require the recoil energy E_2 in L co-ordinates and must therefore calculate v_2 from the appropriate vector triangle in fig. 35 using the cosine law to give:

$$v_2^2 - 2(1-\cos\phi)M_1^2u_1^2/(M_1+M_2)^2 \tag{4.7}$$

and hence
$$E_2 = \Lambda E_1 \sin^2(\phi/2)$$
with
$$\Lambda = 4M_1M_2/(M_1+M_2)^2. \tag{4.8}$$

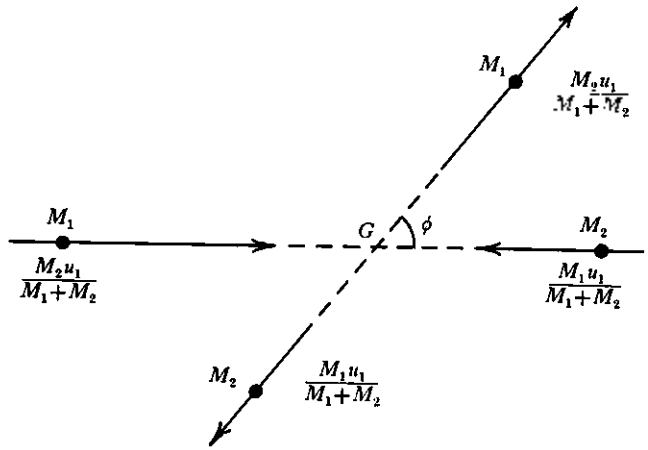

Fig. 36. The two-body collision in G co-ordinates.

Λ has special significance for when $\phi = \pi$ (head-on collision in classical terms) and particles approach and recede along one axis, one has the *maximum possible energy transfer* with:

$$\hat{E}_2 = \Lambda E_1. \tag{4.9}$$

When $\phi - 0$, no scattering occurs and $E_2 = 0$ as one would expect.

In any radiation damage problem there will be a minimum recoil energy, $\check{E}_2$, which is just capable of producing damage. There is also a minimum bombarding energy $\check{E}_1$ which has $\check{E}_2$ as its maximum possible recoil energy, i.e.

$$\check{E}_2 = \Lambda \check{E}_1. \tag{4.10}$$

Clearly, we are only concerned with particles for which $E_1 > \check{E}_1$. Some values of $\check{E}_1$ for various combinations of bombarding particle and target are given in table IX, assuming the $\check{E}_2 = 10\,\text{eV}$.

TABLE IX. *Values of E_1^*, the energy to be greatly exceeded by the product ϕ^2E_1 in order for classical collision mechanics to apply. Also shown are values of $\check{E}_1$, the threshold energy for various particles to produce damage*

Incident particle	Target atom	$\frac{a_0}{a}$	E_1^* (eV)	$\check{E}_1$ (eV)
electron	Li	1·4	—	10^4
electron	U	1·5	—	10^6
proton	Li	1·8	10^{-2}	10^1
proton	U	4·6	10^{-3}	10^3
heavy ion ($M_1 = 100$)	Li	3·8	10^{-4}	10^1
heavy ion ($M_1 = 100$)	U	5·7	10^{-5}	10^3

The relation between θ_2 and ϕ is obtained by considering the components of M_2's velocity parallel and perpendicular to the axis of incidence. The values in L co-ordinates must equal those in G co-ordinates when appropriate components of $\mathbf{u}_g$ are added, i.e.

$$V_2\cos\phi + v_2\cos\theta_2 = u_g, \quad V_2\sin\phi = v_2\sin\theta_2.$$

Hence using expression (4.4) above for V_2 we find

$$\tan\theta_2 = \sin\phi/(1-\cos\phi). \tag{4.11}$$

Before being able to calculate the number of recoils in the energy interval dE_2 at E_2 one must know the angular distribution function giving the probability of recoil into $d\phi$ at ϕ. This can only be obtained with a detailed knowledge of the interaction forces between particles M_1 and M_2. Various types of interaction will be dealt with later, but some general methods of calculation can be established. The primary decision is whether a particular problem requires quantum mechanical solution or if a classical approximation would be valid.

Before applying classical mechanics two criteria must be satisfied:

(1) The particle trajectories must be well defined in relation to some linear dimension and that characterizes the range of the forces between particles. Since the particle should be represented by a wave packet with mean wavelength $\lambda\!\!\!^{-}$, this criterion is expressed as:

$$\lambda\!\!\!^{-} \ll a.$$

(2) The deflexion of the incident trajectory must be well defined. The target particle can be thought of as an obstacle of radius $\sim a$ by which incident particle waves are diffracted. It is well known that strong diffraction exists for small angles of the order $\lambda\!\!\!^{-}/a$ and the second criterion is therefore

$$\phi \gg \frac{\lambda\!\!\!^{-}}{a}.$$

For a particle of energy E_1 the wavelength is:

$$\lambda\!\!\!^{-} = \hbar \sqrt{\left(\frac{2}{M_1 E_1}\right)}.$$

This can be put in a more convenient form if we introduce the Bohr radius a_0 (0·53 Å) as our scale of distance and the Rydberg energy E_R (13.6 eV) as our scale of energy.

For
$$a_0 = \frac{\hbar^2}{m_0 e^2},$$

where m_0 and e are the mass and charge of the electron and

$$E_R = \frac{e^2}{2a_0},$$

hence
$$\hbar = a_0 \sqrt{(2 m_0 E_R)}$$

and
$$\lambda\!\!\!^{-} = a_0 \sqrt{\left(\frac{4 E_R m_0}{E_1 M_1}\right)}.$$

Then the criteria become:

(1)
$$E_1 \gg E_1^* \tag{4.12}$$

with
$$E_1^* = 4 E_R \frac{m_0}{M_1} \left(\frac{a_0}{a}\right)^2.$$

(2)
$$\phi^2 E_1 \gg E_1^*. \tag{4.13}$$

Since ϕ is always either less than unity, or at the worst, of the same order as unity, the second criterion is sufficient for both. It is clear from (4.13) that in glancing collisions, involving small values of ϕ, the requirement for large E_1 becomes more stringent. Further consideration is given to this point in §4.3.

For charged particles incident on atoms it will be shown in the §4.2.1 that $(a_0/a)^2 \doteq (Z_1 Z_2)^{\frac{1}{3}}$. In nuclear collisions $a \sim 10^{-13}$ cm.

Table 9 shows values of E_1^* for various cases with Li and U atoms chosen as extreme cases of light and heavy metals.

It is plain to see that for charged particles with mass at least as great as the proton's, classical collision approximations are valid in the energy range of interest in radiation damage. Although the electron is charged and has an a value comparable to that of the proton, its mass is very small, and collisions must fall into the quantum category. Further, because its energy must be of the order of $m_0 c^2$ (= 0·51 MeV) to be of interest in radiation damage, collisions must be treated by *relativistic* quantum mechanics. Equation (4.8) is not valid in this case and $\hat{E}_1$ and E_q have to be calculated using (4.56) to give $\hat{E}_2$. The neutron, because of the short range of nuclear forces, always requires the use of quantum mechanics to describe its collisions.

4.2. Interatomic Forces

4.2.1. *Theoretical.* This section deals with the most fundamental question in the book, for until one knows the forces between pairs of atoms one cannot give detailed consideration to the collision problems in the primary event, nor to the calculation of defect properties. We are interested both in the forces between unlike atoms, or ions and atoms; and in the forces between like atoms. Suppose we have two atoms with mass ratios M_1 and M_2, nuclear charges $Z_1 e$ and $Z_2 e$ respectively, their nuclei separated by a distance r. The force is best described by a potential energy $V(r)$ which arises from many-body interactions involving the electrons and the nuclei. Even in the simplest cases $V(r)$ has never been determined exactly but some simple considerations show that it must be dominated by two distinct contributions in the range of separations that we are interested in.

There are two useful reference points in the scale of separation: the Bohr radius of the hydrogen atom, a_0 = 0·53 Å, which gives a rough idea of the position of the atomic electron shells; and D, the spacing between neighbouring atoms in the crystal (typically 2·5 Å). When $r \gg D$ the electrons populate the energy levels of the individual atoms and it follows from the Pauli Exclusion Principle that there is a maximum number that can occupy any set of levels. The lowest levels corresponding to the inner closed shells will all be occupied