Chapter 2
A Radiation Damage Cascade

To help us understand the nature of the problems that the work in this thesis will address, we now consider the evolution of a typical radiation damage event. This will allow us to highlight where the electrons are expected to play a major role in the evolution of damage and introduce some of the commonly used terminology in the radiation damage field. We will focus our discussion on the concept of a radiation damage *collision cascade* and the various stages in its development. In Fig. 2.1 we give schematic illustrations of these different stages.

2.1 The Early Stages

Our story begins when an energetic particle impinges on some target material (see Fig. 2.1a). This particle, depending on its mass and on its charge, can penetrate a significant distance into the target material before undergoing a collision with an atom of the target. This collision will set the target atom (known as the *primary knock-on atom* or PKA) in motion often with a very high velocity (see Fig. 2.1b). The statistical distribution of the energy of the PKA (its *spectrum*) will vary depending on the target material and on the type of irradiation [1]: a 14 MeV fusion neutron can produce PKAs of up to 1 MeV in iron with half being above 10 keV; the slower neutrons from fission reactors produce PKA energies of up to several hundreds of keV; and the recoiling ^{234}U nucleus from the decay of ^{238}Pu will have an energy of around 100 keV.

2.1.1 Ion Channelling

When a PKA has a kinetic energy $\sim$100 keV it will have a very low cross-section for interaction with other nuclei of the target material and so is able to travel large

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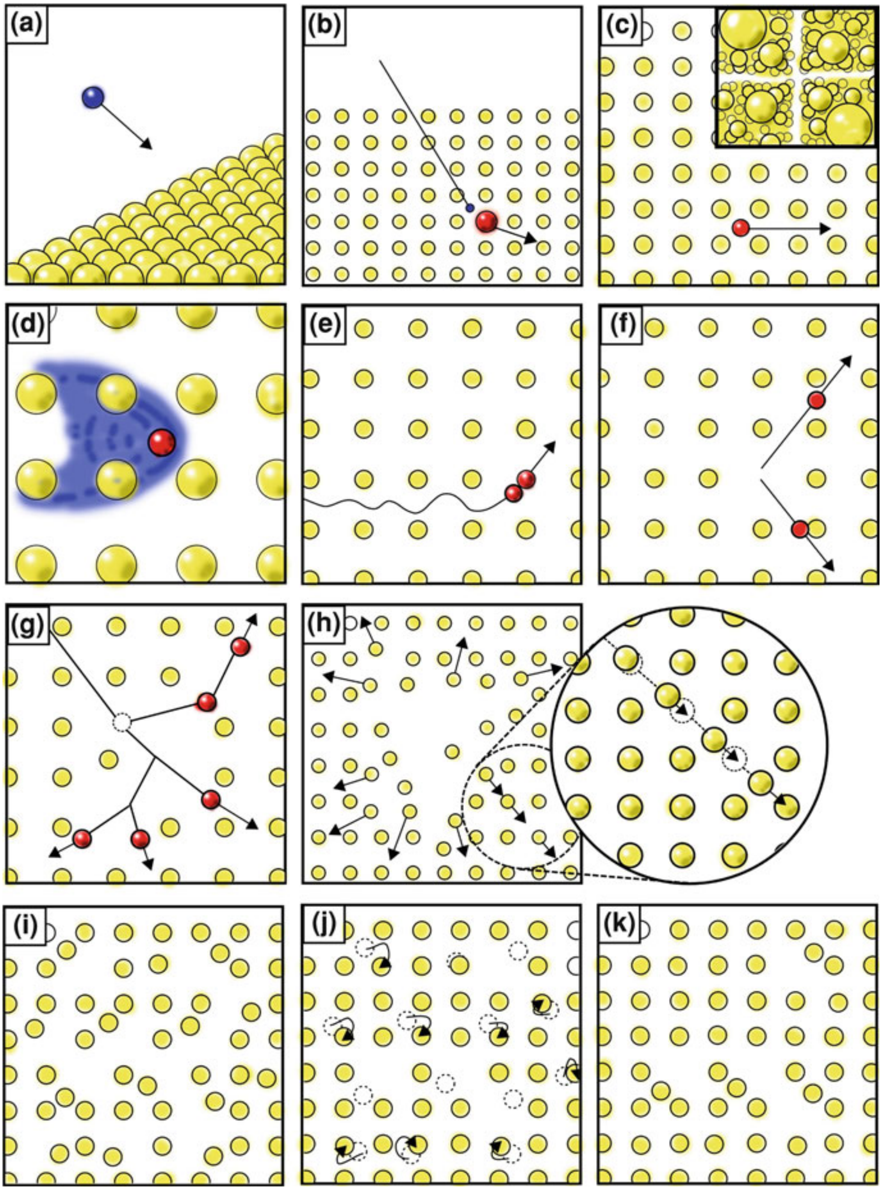

Fig. 2.1 Schematic representations of the stages of evolution of a collision cascade

distances without undergoing a significant collision. This process is known as *channelling* after the open channels in the crystal structure down which such ions move (see Fig. 2.1c) and can be responsible for dramatically changing the damage distribution in crystalline materials. Experiments involving the implantation of

40 keV radioactive ^{125}Xe ions into crystalline tungsten revealed penetration to depths of up to 10^{-6} m for particle beams directed along crystalline axes, compared with a maximum depth in amorphous tungsten of 0.1×10^{-6} m [2].

Because the rapidly moving channelling ion interacts only fleetingly with the surrounding ions it loses energy predominantly to the electrons of the target material (see Fig. 2.1d) and so the rate of energy transfer into the electrons is a significant issue. We investigate the influence of electrons on ion channelling in Chap. 10. Experimental analysis of irradiated samples, particularly of insulators, often reveals *tracks* of damage surrounding the paths traversed by channelling ions. This damage to the lattice must be mediated by the electrons and several mechanisms have been proposed. One possibility is that some electrons in the channelling ion's path become so excited that they are ballistically ejected from the track region, which then experiences a build up of spatial charge. The coulombic repulsion between the charged ions is then thought to be responsible for the damage and this model is referred to as the *coulomb explosion model*. Alternatively, the passage of the channelling ion might serve to rapidly heat the electrons. The transfer of this heat energy into the ions in the track region would then be responsible for generating the damage. This is the *thermal spike model*. A third possibility is suggested by some of our work (see Chap. 9): the excitation of the electrons implies a weakening of the bonding forces in the track region such that the surrounding material is placed under an implied strain and the resulting outward pressure may be directly responsible for the damage.

2.1.2 Sub-cascade Branching

Eventually our channelling ion will either slow to the point that its cross-section for inter-ionic interaction becomes significant or it will encounter a defect in the channel. At this point it will undergo a collision with another ion (see Fig. 2.1e). Depending on the energies of the two ions emerging from the collision it may be possible for them both to continue to penetrate a significant distance into the target material, in which case we have sub-cascade branching (see Fig. 2.1f) or no further channelling will occur and the next stage of cascade evolution will begin.

The phenomenon of sub-cascade branching is important for anyone engaged in simulating collision cascades. Any ion moving with a kinetic energy greater than $\sim$10 keV will tend to impart enough energy to its collision partner to form a sub-cascade. Hence, the behaviour of a collision cascade arising from a high energy PKA will look very much like a set of several lower energy cascades. Provided a simulator can reach length-scales large enough to contain cascades of up to 10 keV, they can claim to be able to capture much of the physics of collision cascades up to much higher energies. (Though not all: phenomena arising from the overlap of the effects of several sub-cascades will not be captured, of course.)

2.2 The Displacement Phase

Once the kinetic energies of our moving ions (either a PKA or an ion in a sub-cascade) get below ~ 10 keV then their interactions with surrounding ions will be strong, collisions will be frequent and the *displacement phase* of the cascade begins. Over the course of 1–10 ps the majority of ions in a region of 10–100 nm in size will be displaced from their equilibrium lattice sites by a series of collisions forming a *displacement spike* (see Fig. 2.1g).

The predominant mode of energy loss from a given moving ion during the displacement phase will be to other ions, but the electrons will still have an important role to play in the dynamics. At this stage of the cascade the initial excess of energy imparted by the incoming radiation is still predominantly contained within the ionic system and so there is a net energy flow from ions to electrons. Thus the electronic system tends to damp the ionic motion and if this damping is strong the evolution of a cascade can be curtailed and the damage produced can be reduced. Understanding the precise nature of the damping is an open problem, which we address in Chap. 11. As the cascade progresses the electrons become increasingly excited. In Chap. 8 we investigate what form these excitations might take and in Chap. 9 we consider how their accumulation might affect the motion of the ions.

During the displacement phase we often see the formation of *replacement collision sequences* (RCS) in which a series of collisions takes place along a close-packed line of ions (see Fig. 2.1h). Each ion replaces the next along the close-packed line until sufficient energy has been lost (to the surrounding atoms and to the electrons) that the sequence is terminated and an interstitial defect atom results. The RCS is an important mechanism for carrying defects large distances from the centre of a cascade and we consider the possibility that their formation might be affected by electronic excitations in Chap. 9.

2.3 The Thermal Spike

After the displacement phase there follows a brief *relaxation phase* during which the cascade energy is rapidly shared amongst all the ions in the cascade region forming a hot (and potentially molten) region sometimes referred to as a *thermal spike*. At this stage an initial defect distribution will be evident, with many interstitial atoms and vacancies (see Fig. 2.1i).

There is then a *cooling* phase, lasting several hundred picoseconds, during which the thermal spike gradually grows and cools and many of the interstitial and vacancy defects recombine (see Fig. 2.1j) and a final damage distribution is established (see Fig. 2.1k). This process of *recovery* takes place in a region of the target material in which the ions will be interacting with excited electrons. The rate at which energy exchange between the ionic and electronic subsystems takes place can have a significant impact on the final damage distribution. The presence of a hot electronic system, acting as a heat bath in contact with the ionic system, can help to anneal defects and reduce the amount of residual damage. Conversely, a rapid transfer of energy from the ions to the electrons might quench in a higher defect population. There is still much to discover about the role played by electrons during the cooling phase and there are many open questions about the so-called *electron-phonon coupling* (discussed in Sect. 3.3). However, the time-scale of the cooling phase lies beyond the reach of our semi-classical simulations and so we will have little to say about such matters here.

References

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