

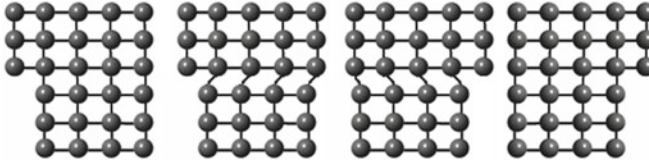
## Chapter 2

# Dislocations

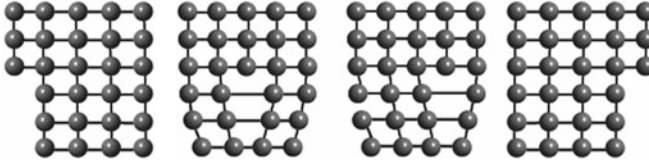
A first attempt to understand how crystals deform was made by Frenkel [1], who posited that under an applied shear stress a crystal undergoes the bulk shear strain illustrated in Fig. 2.1, meaning that the shear stress  $\sigma$  between two crystal planes must vary periodically with the shear displacement strain, i.e.  $\sigma = \sigma_0 \sin(k\epsilon)$ . Requiring Hooke's law  $\sigma = \mu\epsilon$  to hold at small strain, where  $\mu$  is the shear modulus, one obtains a maximum shear strength of  $\sigma_0 \sim \mu/5$  [2]. Unfortunately for this elegant picture, it was already known that the shear stress required to induce plastic deformation was known to be at most  $\mu/10^3$ , going down to  $\mu/10^9$  for ductile metals such as Copper.

After many attempts to explain this discrepancy a solution was proposed independently by Taylor, Orowan and others in 1934 [3]. It was argued that in contrast to the collective planar movement of Frenkel's model, a real crystal *localises* its deformation into linear regions known as *dislocations*. As shown in Fig. 2.2, when the deformation is localised an 'excess' atomic plane can be transferred from one side of a crystal to another without requiring the bulk motion of atoms, which has a much lower energy cost compared to the collective motion required in Frenkel's theory. This was famously analogised by Bragg to the action of moving a carpet by creating a 'ruck' or ripple at one end and then pushing the ruck rather than trying to slide the whole carpet. As with anything that buckles rather than homogeneously deforming, it is energetically cheaper to heavily deform a small amount of material rather than lightly deforming a large amount of material. This phenomena is central to dislocation motion and cannot occur in a harmonic system. The comparative ease of dislocation motion was quantified in a seminal paper by Peierls [4], who showed that a dislocation motion requires a shear stress exponentially smaller than Frenkel's  $\sigma_0$ .

It could be argued that Frenkel's ground-breaking work was an attempt to keep crystal plasticity in the realm of linear response, i.e. bulk deformation must be a 'long-wavelength' excitation requiring the collective motion of all the atoms in the system. It is important to note that this did not work, showing immediately that dislocations are intrinsically non-linear objects unsuited to interpretation by conventional field theories. Furthermore, it is very difficult to construct a continuum field theory that possesses both translational invariance and the ability to sustain static, localised excitations [5], especially in more than one dimension. In contrast, this has been



**Fig. 2.1** A crystal deforming in Frenkel's model



**Fig. 2.2** A crystal deforming by dislocation motion

shown to be a *generic property* of non-linear *discrete* systems [6], which obviously provide a better approximation to a crystal.

These observations strongly imply that dislocations should be treated as non-linear, discrete objects. This is ill suited to the linear continuum of classical elasticity theory, which treat dislocations as line singularities in a vector field of displacements  $\mathbf{u}(x)$  that are regularised either by ad-hoc cut-offs in traditional elasticity [2] or more advanced non-singular methods that suppress singularities through the mapping  $\mathbf{u}(x) \rightarrow \mathbf{u}(x) + \lambda \cdot \nabla \mathbf{u}(x)$  then applying the same linear field theory [7].

Despite such conceptual failings the predictions of elasticity theory are valid in the far-field when the deformation induced by dislocations is weak and slowly varying, and these interactions are essential to describe realistic dislocation networks. However, in the current work we focus on accurately coarse graining the stochastic forces acting on thermally fluctuating crystal defects, meaning that we need to be explicitly aware of the non-linear, discrete structure of the dislocation core. This investigation is essentially orthogonal to the valid and important far-field results of elasticity theory. Whilst we will review the topology of dislocation formation and motion, and briefly report initial work on combining the stochastic force with long range elastic interactions, we do not give a review of elasticity theory as there already exist many excellent works on the subject [2, 8, 9].

## 2.1 Topology and Burgers' Vector

Dislocations are defined as *line like* defects in a crystalline material, as distinct from point defects such as impurities, vacancies and self-interstitials atoms or areal defects such as surfaces and grain boundaries. These defects are obviously not

mathematically ideal entities, but their configurational space has topological restrictions which can be identified with the topology of points, lines and planes.

For example, a line of point defects do *not* form a line defect, as this linear cluster of point defects can clearly be continuously transformed to any other cluster of arbitrary shape, losing any topological definition. The topology of a line is defined by Jordan's curve theorem [10] in the plane, which states that a *closed* curve which does not cross itself (either a loop or a line terminating on the boundaries of the containing plane, which may be at infinity) divides a plane into two distinct regions. An open curve can only be contained in the topology of lines if it is considered as the limiting case of an infinitely thin loop. This two-dimensional construction can be translated to three dimensions if we instead consider the continuous family of concave surfaces bounded by a dislocation line [11] as opposed to the division of a plane.

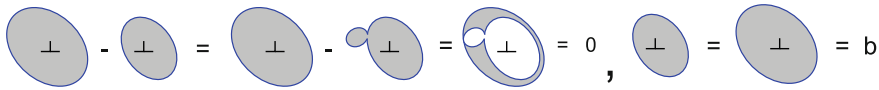
These considerations give our first main topological constraint, namely that for a linear defect to be a dislocation, i.e. to have the topology of a line, it must either form a closed curve or terminate on the boundaries of an areal defect.

For the dislocation to be a structural defect there must be some topologically identifiable structural 'charge' associated with the line, which we will restrict to be rigid translations by a vector  $\mathbf{b}$ .<sup>1</sup> In close analogy with Ampère's law [13], the appropriate operation to extract this 'charge' is any closed path around the line, known as a 'Burgers circuit' after its creator. Starting from an arbitrary atom and taking steps only to nearest neighbours, execute a closed path enclosing one or many dislocation lines, in close analogy to an Ampère circuit. As we know the vectors representing nearest neighbour atomic separations of a perfect crystal, for each step calculate the vectorial difference between the 'ideal' vector and the actual step vector, then sum all of these vectors around the path. In a perfect, dislocation-free crystal this would give identically zero, meaning that dislocations are defined to be linear defects which contribute a non-zero result, giving the total displacement  $\mathbf{b}$  induced by the defect which will be independent of the details of the path taken. This independence is simple to demonstrate by comparing two paths which both enclose the same dislocations. First, if the paths do not overlap, add a closed loop to one path to give overlap with the second path. The two paths now form a set closed loops which do not enclose any dislocation and thus give no contribution to the net displacement (c.f. Fig. 2.3). As these closed loops represent the transformation from one path to the other the path independence is proved.

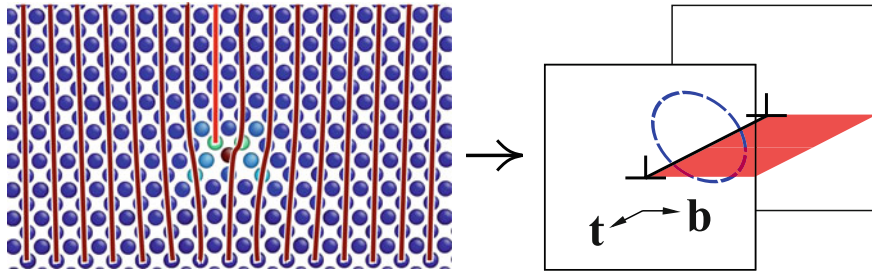
Crucially, if the Burgers vector  $\mathbf{b}$  is not a symmetry operation of the host lattice, an areal stacking fault equal in size to the minimal plane bounded by the dislocation line would develop (the shaded area in Figs. 2.4 and 2.5), meaning that the dislocation becomes a stacking fault and so can no longer be classified as a line defect. This

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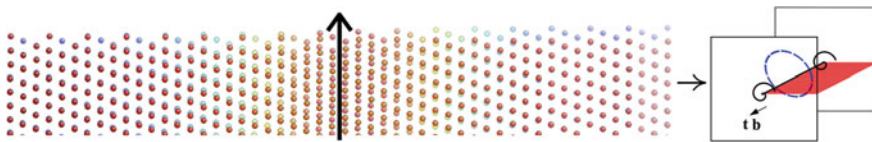
<sup>1</sup>There also exist rotational defects called *disclinations*, but as they can only appear where the violation of bulk translational symmetry induced by this lattice rotation has a controllable energy cost, such as in nanocrystalline metals [12] or liquid crystals [11] we do not consider them here.



**Fig. 2.3** *Left* An  $\langle 100 \rangle (010)$  edge dislocation in Iron. An edge dislocation is formed through the insertion of an additional semi-infinite crystalline plane. *Right* A cartoon of the same edge dislocation line with an example surface bounded by the line and a possible Burgers path, with the line direction  $\mathbf{t}$  and Burgers vector  $\mathbf{b}$  shown



**Fig. 2.4** A demonstration of Burgers path independence. The difference between two paths can always be considered as a closed loop enclosing no defects which cannot therefore contribute to the path integral



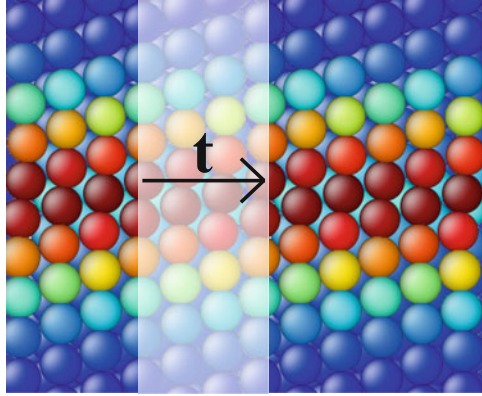
**Fig. 2.5** *Left* A  $(1\bar{1}0)$  plane containing a  $1/2\langle 111 \rangle [1\bar{1}0]$  screw dislocation overlaid on an unfaulted  $(1\bar{1}0)$  plane in Tungsten. We see that the ‘disregistry’ between the two planes eventually becomes equal to  $\mathbf{b}$ . *Right* A cartoon of the same dislocation

leads to the second main topological constraint on dislocations- the ‘Burgers vector’  $\mathbf{b}$  must be a vector of the host lattice.<sup>2</sup>

We now have all the topological elements to build arbitrary dislocations. For straight dislocation lines, the relationship between the line direction  $\mathbf{t}$  and the Burgers vector  $\mathbf{b}$  defines the *character* of a dislocation line; when  $\mathbf{b} \cdot \mathbf{t} = 0$  the dislocation is of ‘edge’ character and the line represents the boundary of an inserted semi-infinite crystallographic plane of normal  $\mathbf{b}$  as illustrated in Fig. 2.3. When  $|\mathbf{b} \wedge \mathbf{t}| = 0$  no additional material is required and we say the line is of ‘screw’ character- the line represents the centre of a spiralling displacement that translates the crystal by  $\mathbf{b}$  around one circuit; an overlay of a plane containing a screw dislocation and a perfect lattice plane is shown in Fig. 2.5.

<sup>2</sup>Strictly, this restriction only applies to dislocation in the bulk. On surfaces this restriction does not apply, meaning a different partial dislocations can exist depending on the coincident site lattice [14] of grain boundaries or simply the crystallographic character of a free surface.

**Fig. 2.6** Illustration of a dislocation core ‘unit’ for a  $1/2\langle 111 \rangle(1\bar{1}0)$  edge dislocation in bcc Iron. The atoms are coloured from *blue* to *red* by potential energy. We see the core structure repeats over the line direction lattice vector  $\mathbf{t} = [11\bar{2}]$

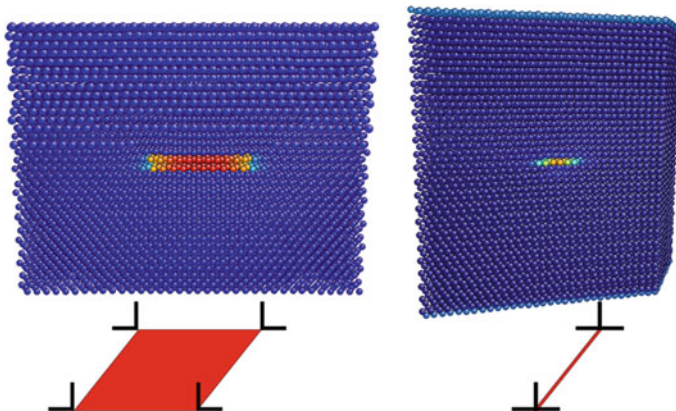


## 2.2 Dislocation Core Structure

We have discussed how the non-linear discrete structure of a crystal localises deformation into dislocations, such that the bulk of the inserted half plane, or spiral deformation, is accommodated in a tight *core* region within which a line co-ordinate may be defined. For a straight line dislocation lying along a lattice vector  $\mathbf{t}$ , the core structure will be periodic with a period of  $\mathbf{t}$  by the discrete translational symmetry of the host crystal, as demonstrated in Fig. 2.6. This naturally leads to a definition of dislocation core ‘units’, a concept which we find very useful to understand the dynamics of dislocation cores. Whilst the picture of a compact core is always appropriate for dislocation formation, in some close packed structures such as face centred cubic metals<sup>3</sup> it can be the case that a compact dislocation can be unstable to core dissociation: an areal stacking fault band bound by two ‘partial’ dislocations where only the total Burgers vector is a lattice vector [2]. As shown in Fig. 2.7, such an arrangement can either be considered as an areal defect or, far from the stacking fault band, a dislocation line.

Such an ambiguity is to be expected as the topological definitions only strictly apply to ideal mathematical entities rather than real localised deformations. Nevertheless, the two restrictions that a dislocation line must be closed and that the (potentially total) Burgers vector must be a lattice vector remain valid as to violate this would induce a stacking fault of a size only determined by the geometry of the line rather than any ‘intrinsic’ energetic considerations that lead to a dissociated core.

<sup>3</sup>Hexagonal close packed and face centred cubic crystal structures assume the optimal packing of spheres, meaning in turn that they maximise inter-planar distances [16], which often leads to very glissile dislocation structures with a low stacking fault energy [15].



**Fig. 2.7** Comparison of dislocation cores. *Left* a disassociated  $1/2\langle 110 \rangle (\bar{1}12)$  edge dislocation in fcc Nickel. The wide stacking fault can clearly be seen, though a line picture emerges far from the core. *Right* the compact core of a  $1/2\langle 111 \rangle (\bar{1}10)$  edge dislocation in bcc Iron. As bcc metals have no metastable stacking faults dislocation cores never disassociate [15]

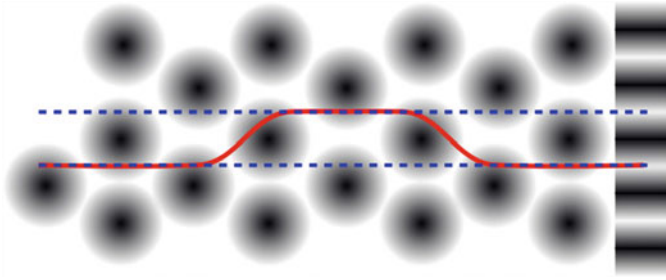
### 2.3 Dislocation Motion and the Kink Mechanism

As mentioned above, when  $\mathbf{t}$ ,  $\mathbf{b}$  are not aligned the dislocation requires the addition of material to the host crystal proportional to  $M|\mathbf{b} \wedge \mathbf{t}|$ , where  $\mathbf{b}$ ,  $\mathbf{t}$  are lattice vectors and  $L$  is the shortest distance from the dislocation line to the boundary of the crystal. As the dislocation line itself can be thought of as the boundary of this additional material, if the dislocation line moves out of the plane defined by  $\mathbf{b} \wedge \mathbf{t}$ ,  $M$  will change, meaning that material will have to be added or removed. Such non-conservative motion is known as *climb* motion and is typically facilitated by the biased diffusion of vacancies to the dislocation core [17]. Whilst such a motion is certainly dependent on stochastic thermal forces to drive vacancies over their large migration barriers, these barriers are very large meaning that climb motion is extremely slow (and consequently atomistic simulation becomes extremely expensive). In this thesis we focus on *glide* motion, where dislocation motion is restricted to the *glide plane* of normal  $\mathbf{t} \wedge \mathbf{b}$ . As glide motion is conservative it occurs much more readily and is the dominant form of dislocation mediated deformation under typical mechanical conditions. Such is the predominance of glide motion, dislocations are typically characterised by their Burgers vector and glide plane in the form

$$\langle \text{Burgers Vector} \rangle \{ \text{Glide Plane} \} \text{ Character, i.e. } \langle 100 \rangle \{ 010 \} \text{ Edge.}$$

Glide planes are normally low index lattice planes, as these have the greatest atomic density hence a larger interplanar separation [16]. However, although dislocation glide is a conservative process, the discrete structure of a crystal breaks any continuous translational symmetry, meaning minimum energy configurations will only





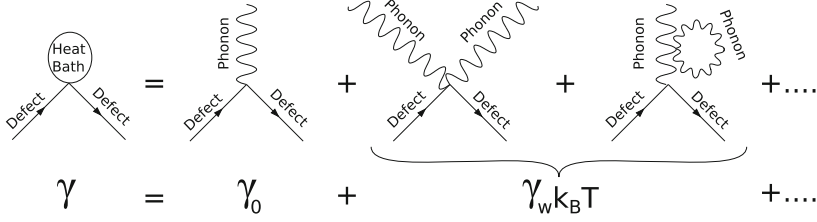
**Fig. 2.8** A cartoon of the kink mechanism. The background gradient illustrates the variation of dislocation core energy due to the discrete structure, which when aggregated into motion perpendicular to the bulk line direction gives a one dimension periodic function known as the Peierls barrier, as illustrated in the right hand strip. The *red line* illustrates the typical kink pair configuration a dislocation line takes to migrate through the periodic landscape. This occurs because the barrier for rigid migration scales linearly with the line length, whilst the kink pair energy is length independent

by invariant after rigid translation by a lattice vector. In between these positions the energy varies periodically under rigid translation. This energy barrier to dislocation motion is called the Peierls barrier and is a rate limiting process in transition metals such as Iron and Tungsten, where the highly directional bonding accentuates this discreteness effect. To see the influence of the Peierls barrier, consider an infinitely long straight dislocation sitting in a minimum energy position. It is clear that the magnitude of the energy barrier to rigid motion will scale linearly with the dislocation line length (the Peierls barrier is defined by unit length) implying that an infinitely long dislocation line has an infinitely large barrier between adjacent minimum energy positions. Nevertheless, the dislocation can still migrate through the a process known as the kink mechanism.

The kink mechanism can be pictured in direct analogy to a first order phase transition, with the initial and final configurations as two phases. Rather than a homogeneous change of state, a small region of the new phases is nucleated, then grows through the motion of domain walls. The domain walls are short segments known as kinks. A more physical picture of the kink mechanism is given in Fig. 2.8; we shall explain the kink mechanism in more detail when investigating the atomistic simulation of dislocations.

## 2.4 Dislocations and Phonon Scattering Theory

All treatments of dissipative defect forces have employed scattering theory to describe the interaction between dislocations and thermal vibrations [2, 18, 19]. As we take an entirely independent approach in this thesis we will only summarise the qualitative results. Indeed, one disadvantage of scattering theory predictions is even under drastic assumptions of dislocation core structures the resulting expressions involve



**Fig. 2.9** A diagrammatic picture of phonon scattering. The dislocations and phonons are assumed to be well defined entities which only interact through scattering processes which may be systematically evaluated. Higher order processes contribute terms of higher order in temperature. The linear and quadratic dispersion relations mean the first order term vanishes for subsonic defect speeds. The second process represents a simple ‘in-out’ scattering and represents the well-known ‘Phonon Wind’ mechanism

complicated integrals meaning quantitative predictions are sensitive to regularisation techniques such as infra-red/ultraviolet cut-offs or gradient approximations [20] required by all continuum linear field theories [21].

Scattering theories assume that dislocations and phonons are canonical objects which are non-interacting to quadratic order, meaning each have well defined energy and momenta. One then perturbs this harmonic system with higher order terms giving an expression for  $\gamma$  which is evaluated in a series of scattering events. A cartoon diagrammatic representation is shown in Fig. 2.9. Given that we expect the phonon number to be proportional to temperature, it is not surprising that higher order scattering events lead to higher order temperature dependence in  $\gamma$ . However, given the simulation evidence we only consider the zeroth and first order terms  $\gamma_0$  and  $\gamma_w k_B T$ .

As dislocations and phonons are assumed to be canonical in this scattering approach each diagram is dependent on the phase space available for the scattering process they represent. This means the temperature independent term  $\gamma_0$  is reliant on a one-body absorption or emission, whilst  $\gamma_w k_B T$  includes more typical ‘in-out’ process. Selection rules for these terms can be derived when noting that we are concerned only with subsonic dislocations moving much slower than the wave speed. Taking a linear phonon dispersion relation  $\hbar\omega_{\text{ph}} = \hbar ck$  where  $c$  is the wave speed (it turns out that more complicated dispersion relations do not qualitatively affect the results) and a quadratic dislocation dispersion  $\hbar\omega_{\text{dis}} = (\hbar K)^2/2m$ , we obtain the balance

$$\hbar ck + (\hbar K)^2/2m = (\hbar K + \hbar k)^2/2m \Rightarrow c \simeq \hbar K/m. \quad (2.1)$$

But we know that the dislocation speed is subsonic, i.e.  $\hbar K/m \ll c$ , meaning that the above balance cannot be met in the subsonic regime. This is universally invoked in all scattering approaches to conclude that

$$\gamma_0 = 0. \quad (2.2)$$



We will show, through the analysis of extensive atomistic simulations by ourselves and many other researchers that this conclusion is false. This qualitative failure is a manifestation of the erroneous canonisation present in all scattering theories. The main result of this thesis is an entirely new approach that solves these shortcomings. For higher order processes the phase space is not so restrictive and so continuum theories in general predict that

$$\gamma \simeq \gamma_w k_B T, \quad (2.3)$$

with the second term in Fig. 2.9 being the dominant contribution.

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