Chapter 3

Dislocations and Precipitation Hardening

Dislocations are the principal carriers of plastic deformation in crystalline metals. Without insight in the nucleation and propagation of dislocations, basic concepts of mechanical behavior of crystalline metals cannot be understood. Since their motion is responsible for plastic deformation, the mechanical properties can be controlled by affecting their dynamical behavior. This chapter will present a historical survey of the discovery of the theoretical concept of the dislocation, followed by a section describing the basic properties of dislocations. The largest portion is devoted to the interaction of precipitation with dislocations, because it is the main strengthening mechanism in the alloys examined in this thesis.

3.1 Historic overview

The concept of a lattice dislocation as the crystallographic unit responsible for the deformation of crystalline solids is commonly attributed to three classical papers by Orowan [1], Taylor [2] and Polanyi [3], published in 1934. On the occasion of the 50th anniversary of the dislocation, Nabarro compiled in 1984 a treatise on the ‘pre-history of dislocations’ and the research and thoughts leading eventually to these papers [4]. He points out that in the decades preceding the discovery, several scientists were already remarkably close to postulating this idea.

When a dislocation emerges at a free surface, locally the chemical and mechanical properties may differ from the surrounding matrix. This can be due to lattice distortions, to strain fields associated with dislocations, or due to preferential precipitation or segregation along the dislocation line. When such a surface is etched, the rate at which atoms are removed may increase in the affected region, causing so-called etch pits to occur. These pits have been studied from as early as
the 1850s, without real understanding, but numerous observations and increased knowledge of crystallography converged at the end of the 19th century to a direct link between etch pits and crystallographic disturbances [5]. The first direct observation of decorated dislocations dates back to 1905 when Siedentopf performed microscopy experiments on rock salt [6]. Around the same time calculations were made within elastic continuum models of, what are with hindsight, stress fields around dislocations. Nonetheless, never was the connection made between continuum and atomic models [7-9].

In the 1920s a deadlock was reached, since none of the models was able to explain how a lattice defect could be the cause of crystal plasticity and simultaneously be responsible for the observed hardening of the metal with increased deformation. Another problem was the inconsistency that, if one were to calculate the stress required to displace all atoms on one side of a slip plane, the result would be much higher than the experimentally observed stress required for plastic flow. Furthermore, by such a displacement the lattice would remain perfect, again offering no explanation for strain hardening.

In his 1934 paper, Taylor discards the idea that in a perfect crystal glide is easy and that faults or lattice rotations impede the glide causing hardening. He works out an idea, which starts from the assumption that a perfect crystal can withstand very large stresses and the observed weakness of the crystal is caused by local stress concentrations. Taylor solves the problem of the high stress required to displace all atoms simultaneously by stating:

> It seems that the situation is completely changed when the slipping is considered to occur not simultaneously over all atoms in the slip plane but over a limited region, which is propagated from side to side of the crystal in a finite time.

The paper continues by introducing the dislocation as a unit slip (Fig. 3.1) and by calculating the low stress values required for its movement. Taylor finally shows that this stress increases as the stress fields of multiple dislocations interact, thus explaining strain hardening.

Orowan’s starting point was not a mechanical one, but rather taken from thermodynamics. Starting with the arguments made by Becker [10], namely that slip in crystalline solids is the result of spontaneous fluctuation in the neighborhood of a glide plane extending over a larger number of atoms, Orowan thought of a particular kind of lattice defects that could produce a stress concentration high enough for those fluctuations to occur. The breakthrough came when he realized that these *Fehlstellen* need not be pores or tears in the lattice:
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Diese Fehlstellen brauchen nicht Hohlräume oder Risse zu sein, bei denen der Zusammenhang zwischen den beiden Ufern unterbrochen ist; es genügt z.B., wenn beide Ufer gegeneinander in tangentialer Richtung um eine oder mehrere Gitterteilungen versetzt sind.

He sketches a picture of a piece of material inside the interior of the crystal that has slipped and is separated from the rest of the crystal by a dislocation loop. These loops themselves produce a shear stress on the slip plane that added to the applied stress increases the change of the occurrence of a critical stress fluctuation that will enlarge the region that has slipped. Orowan realized that the transition zone between slipped and unslipped material is identical to the lattice defects described to him by Polanyi during their discussions. After Orowan consulted with Polanyi, the two decide to publish separate papers in the same edition of the Zeitschrift für Physik. Polanyi’s article is by far the shortest of the three. In fact there is only one point made. In reaction to earlier work by Taylor, in which is proposed that little cracks are responsible for the stress concentration necessary for slip, Polanyi writes:

Viel plausibler als die Annahme von spaltformigen Löchern scheint mir die Eventualität zu sein, daß die geringen Schubfestigkeit durch das Vorhandensein einer art Störung verursacht wird, die ich als “Gitterversetzung” bezeichnen möchte.

The following description of this Versetzung is similar to that of Taylor. Polanyi estimates that the stress necessary to move a dislocation, which has a width of n atomic spacings, is only 1/2n times the shear modulus.

Figure 3.1 Picture taken from the classic article by Taylor explaining how a dislocation can gradually shear the material [2].
After this rather slow start, progress was made rapidly. Shortly after the concept of the dislocation was introduced, theories were proposed on dislocation multiplication, on dislocation dissociation, on dislocations in different crystal structures, on the influence of dislocations on recrystallization and on different hardening mechanisms.

### 3.2 Basic properties of dislocations

Dislocations are present in crystals in three different forms. They can be either of the *edge* type (Fig. 3.2), or of the *screw* type (Fig. 3.3). Finally a dislocation can be mixed i.e. partly edge and partly screw. In all cases the dislocation is a line defect and can be identified by its *Burgers vector*, which is determined by making an atom-by-atom path clockwise around the dislocation line until the starting point is reached again. If this same path is made in a perfect crystal the loop will not close. The Burgers vector is defined as the vector that will close the loop. However, the Burgers vector is not a vector in the usual mathematical sense, because its sign depends on the line sense of the dislocation and thereby on the orientation of the coordinate system. By convention, the direction of the Burgers vector is such that when looking along the dislocation line, hereby defining the positive line sense of the dislocation,
and drawing the Burgers circuit in a clockwise manner, the Burgers vector is that vector that runs from the finish to the start point of the reference circuit in the perfect crystal. This implies that reversing the line sense of the dislocation also reverses the direction of the Burgers vector. Furthermore, dislocations with the same line sense but opposite Burgers vectors are physical opposites and will, when brought together, annihilate and restore perfect order in the crystal.

As can be seen in the figures, the Burgers vector for an edge type dislocation is normal to the line of the dislocation. For a screw type dislocation the Burgers vector is parallel to the dislocation line. It is geometrically impossible for a dislocation line to end suddenly inside the crystal. The line can end either at grain boundaries or free surfaces, branch into other dislocations or form a closed glide loop. Such a loop has a unique Burgers vector and will at two points be a perfect edge type dislocation and at two points a perfect screw type but has mostly a mixed character.

A straightforward analysis of the elastic energy associated with dislocations leads to

![Figure 3.3](image)

(a) Schematic picture of a screw dislocation with Burgers circuit. (b) If the same circuit is drawn in a faultless material a vector QM is needed to close the circuit. For a screw dislocation the Burgers vector is parallel to the dislocation line [11].
the simple but very useful expression:

\[ E_{el} = \alpha \mu b^2 \] (3.1)

with \( \alpha = 0.5 \sim 1.0 \) and \( \mu \) is the shear modulus of the material. \textit{Frank’s rule} is a form of this expression. It states that for it to be energetically favorable for a dislocation \( b_1 \) to split up into two dislocations \( b_2 \) and \( b_3 \), the following has to hold: \((b_2^2 + b_3^2) < b_1^2\).

### 3.2.1 Slip

Dislocation movement can be either conservative or non-conservative, depending on whether or not the volume is preserved. The conservative motion of dislocations is called \textit{glide}; the dislocation moves in the plane that contains both its line and Burgers vector. Non-conservative motion or \textit{climb} occurs when the dislocation moves out of the glide plane. \textit{Slip} is the collective motion of many gliding dislocations and is the most common manifestation of plastic deformation in crystalline materials [11]. Figure 3.4 shows a piece of material that has slipped on a number of distinct planes. Over each of these \textit{slip planes} a large number of

![Figure 3.4](image-url)  

\textit{Figure 3.4  Slip occurring on two slip planes, which have a high-valued Schmid factor \cos \cos [11].}
dislocations have glided. Slip is easiest on the planes with the highest atom density and in these close-packed planes the direction of slip will also be most likely the direction with the highest atom density. In certain cases it is possible for a dislocation to change slip plane. For this *cross slip* to occur, the Burgers vector of the dislocation has to lie in both planes. Only screw dislocation can cross slip, since only for screw dislocations the Burgers vector is parallel to the dislocation line (see Figure 3.6 for an example of cross slip in an fcc crystal).

**Slip in face-centered cubic materials**

For a face-centered cubic (fcc) material like aluminum, the most closely packed planes are the \{111\} planes and the most densely packed directions are the \langle110\rangle directions. Here, as in the remainder of this thesis, use is made of the Miller index notation, in which specific planes and directions are indicated by respectively (hkl) and [uvw] and the set of symmetrical equivalent planes and directions by respectively \{hkl\} and \langleuvw\>. In an fcc lattice, there are four \{111\} planes each containing three \langle110\rangle directions. This means that there are twelve different slip systems available for slip. The plane on which slip actually takes place is determined by the direction of the applied stress. Slip takes place on that slip system for which the shear stress resolved on the slip plane in the slip direction is highest. Looking at Figure 3.4, this resolved shear stress can be written as:

\[
\tau = \frac{F}{A} \cos \varphi \cos \lambda
\]

(3.2)

where \(\varphi\) is the angle between the applied force \(F\) and the slip plane normal and \(\lambda\) is the angle between \(F\) and the slip direction. \(A\) is the cross-sectional area over which the force acts. The factor \(\cos \varphi \cos \lambda\) is called the Schmid factor and its size is a measure of the ease or the likelihood of slip on the slip system.

The most common dislocation in fcc structures has a Burgers vector \(b = \frac{1}{2}a \langle110\rangle\) with \(a\) the lattice parameter of the material. Such a dislocation with a Burgers vector equal to a lattice translation vector, is called a perfect dislocation. An fcc lattice consists of an ABCABC stacking of close-packed \{111\} planes. The occurrence of a perfect dislocation will not hamper this stacking. Figure 3.5 shows a ball model of a \{111\} plane, indicating the A, B and C positions [12]. A perfect dislocation will cause the material on one side of the slip plane to be translated by a vector \(b_1\), such that the atoms originally in a B position will glide into another B position. It is however, also possible to make the same translation in two steps. First the atoms glide in the direction of vector \(b_2\) moving the atoms in a B position to a C position followed by a glide \(b_3\) moving them back to a B position and restoring the
normal order. Basically the perfect dislocation splits up or dissociates into two partial dislocations. This can be written as:

\[ \mathbf{b}_1 \rightarrow \mathbf{b}_2 + \mathbf{b}_3 \]

\[ \frac{1}{12} <110> \rightarrow \frac{1}{6} <211> + \frac{1}{6} <12\overline{T}> \]  

(3.3)

These \( \frac{1}{6} <112> \) partial dislocations in fcc crystals are called Shockley partials. According to Frank’s rule their formation is energetically favorable. There is however a repulsive force between the two partials, which can be approximated by:

\[ F = \frac{\mu b^2}{4\pi d} \]

(3.4)

where \( d \) is the spacing between the two Shockley partials. Therefore there will be a tendency for the two partials to separate, creating a region of stacking fault in between them. The normal ABCABC stacking of \{111\} planes will be changed to an ABCACABC stacking, since one B-layer glided into a C-position. Associated with this stacking fault is a stacking fault energy \( \gamma \), which is the force per unit length pulling the two dislocations together. The equilibrium separation is found when the repulsive and attractive forces balance i.e. when \( F = \gamma \) and: 

Figure 3.5  Atomic arrangement on \{111\} planes in an fcc metal indicating the three different positions A, B and C. The vector \( \mathbf{b}_1 \) is a perfect lattice translation, while a translation of the type \( \mathbf{b}_2 \) or \( \mathbf{b}_3 \) will cause a stacking fault [11].
In a gliding dissociated dislocation, the leading partial creates the stacking fault and the trailing partial restores the perfect order on the glide plane. The stacking fault energy varies from one fcc metal to another. For instance, silver has a low stacking fault energy ($\gamma \approx 20 \text{ mJ m}^{-2}$), implying easy dissociation with broad stacking fault ribbons. Aluminum on the other hand has a much higher stacking fault energy ($\gamma \approx 140 \text{ mJ m}^{-2}$). Dissociation is confined to the dislocation core and no partial dislocations are developed.

Cross slip in fcc crystals is possible for perfect dislocations. This is illustrated in Figure 3.6. The figure shows a dislocation loop with Burgers vector $[10\overline{1}]$ slipping in the (111) plane. The Burgers vector lies also in the (111) plane. The screw side of the dislocation loop at $z$ can therefore cross slips onto this plane. The figure also shows double cross slip as at reaching the line CD, the dislocation slips back onto the (111) plane. For the dissociated dislocations, cross slip is not possible since a unique $\frac{1}{6}<112>$ dislocation only lies in one {111} slip plane. The only possibility is for a screw dislocation to form a constriction in the stacking fault, cross slip and subsequently restore the stacking fault. This process requires energy and is unlikely in materials which have low stacking fault energy. Aluminum on the other hand has

\[
d = \frac{\mu b^2}{4\pi\gamma}
\]  

(3.5)

Figure 3.6  Cross slip in an fcc metal. The screw part at $z$ of the dislocation loop with $b=1/2a[\overline{1}01]$ cross slips from the (111) plane onto the (111) plane. In the final picture double cross slip occurs back onto the (111) plane [11].
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high stacking fault energy and cross slip is relatively easy.

Dislocations in other crystal structures

In body-centered cubic (bcc) materials the number of slip systems is less trivial, because slip occurs not only on the most densely packed {110} planes, but also on the {112} and {123} planes. The slip direction is always the close packed <111> direction, with perfect dislocation Burgers vectors of the type \( \frac{1}{2}<111> \). A single <111> direction is shared by no less than three {110}, three {112} and six {123} planes, making cross slip of screw dislocations easy.

The core of a dislocation is the region near the center of the fault in which the displacements become too large for a realistic description by linear elasticity. The strain fields in the cores have to be calculated using computer models in which the atomic displacements are determined by applying appropriate interatomic interaction functions. For screw dislocations in bcc materials, these models predict a non planar core structure, meaning that, when looking along the <111> Burgers vector, the displacements parallel to this line of view do not exhibit a radial symmetry around the dislocation as is the case for fcc materials, but instead, the displacements are concentrated on the three intersecting {110} planes. This complicated strain field changes when an external stress is applied or when the temperature is varied. It can be shown that the non planar core structure is responsible for many experimentally observed characteristics of bcc crystals when deformed, for instance the fact that the mechanical response of bcc crystals is not the same in compression and tension.

Slip on {123} planes is generally only observed at elevated temperatures and will not be discussed further. Still, there remain 24 theoretical slip systems, twelve \{110\}<111> and twelve \{112\}<111>. The choice of slip system is temperature dependent. At low temperatures the \( \frac{1}{2}<111> \) screw dislocation is in its ‘ground state’, its core having a three-fold screw symmetry which will allow slip on \{110\} planes. At elevated temperatures however, the dislocation will enter a metastable ‘excited state’. The core configurations is now such that slip on \{112\} planes is allowed. The temperature at which this first order phase transition occurs for bcc iron is approximately 100K, making the \{112\} planes the dominant slip planes at room temperature [13,14]

In hexagonal close packed (hcp) crystal structures, slip is primarily confined to the basal planes [15]. There are only 3 basal (0002) <11\overline{2}0> slip systems available. Other probable deformation modes are the prismatic \{l\overline{1}00\} <11\overline{2}0> and pyramidal \{l\overline{1}0\} <11\overline{2}0> slip systems but also second-order pyramidal slip
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\{\overline{1}22\} <\overline{1}1\overline{2}3> has been observed in zinc [16,17]. Furthermore deformation twinning is common in hcp metals, with for zinc only the most common \{1\overline{1}T2\} twins active [18]. In general the kind of slip systems active in hcp crystals depends highly on the material, since none of the hcp metals have the ideal close packed c/a ratio, which would be \((8/3)^{1/2} = 1.633\). Due to this difference in directionality of the atomic bonds hcp metals can be very brittle (Be) or quite ductile (Zr, Ti).

3.3 Precipitation hardening

In 1911 Wilm described experiments performed on aluminum alloyed with small amounts of copper, silicon, magnesium or iron, which was quenched from a temperature just below the melting point [19]. He showed that the alloys became harder after being kept for a longer time at room temperature. For this age hardening no plausible explanation existed until Merida et al. in 1920 postulated that age hardening occurs in alloys for which the solid solubility increases with increasing temperature [20]. They argued that the quenching results in the formation of a supersaturated solid solution, from which with time new phases can grow. In the following years the focus of the research was mainly on understanding the mechanisms behind this precipitation and not on the resulting hardening. Even though the discovery of the dislocation as described earlier occurred in 1934, it took until 1940 before an explanation of precipitation hardening in terms of dislocations was given. In that year Mott and Nabarro suggested that the hardening was a consequence of the interaction between dislocations and the misfit strain fields of coherent particles [21]. In 1948, Orowan wrote down his famous equation, which predicts the strength of alloys strengthened by non-deformable particles [22]. In the late 1950s the research on the different mechanisms of precipitation strengthening took solid ground, culminating in more or less quantitative theories in the following decade of coherency strengthening, order strengthening, modulus hardening and stacking fault strengthening, which will be described in the following text for which the excellent review article by Ardell was most helpful [23].

3.3.1 The statistics of dislocation-particle interactions

The aim of this section is to describe how the motion of dislocation is influenced by the presence of obstacles in the lattice. It turns out that the critical resolved shear stress \(\tau_c\) at which the dislocation overcomes the obstacles depends on the one hand highly on the nature of the obstacle. Its size, coherency with associated coherency strains, crystal structure and chemical characteristics determine the ease and also the
manner of the passage. On the other hand, the distribution and concentration of obstacles is obviously very relevant. This first part will deal with this latter aspect, for which, according to Nabarro, it is useful to make a distinction between strong obstacles, which only interact when the dislocation is in close contact and diffuse obstacles, which interact with dislocations over a certain distance [24].

Figure 3.7  A dislocation line pinned by obstacles a distance L apart. Under influence of a shear force the dislocation bows out between the obstacles. When this configuration is static, the pinning force $F_m$ is counteracted by the line tension of the dislocation.

Localised obstacles

For localised obstacles, the problem can be treated as the simple force balance drawn in Figure 3.7. The dislocation line is pinned behind the obstacles and bows out between them. In the picture $F_m$ is the maximum force the obstacle can sustain and $\phi_c$ is the critical breaking angle. T is the line tension of the dislocation. The force balance becomes:

$$F_m = 2T \cos(\phi_c / 2)$$  \hspace{1cm} (3.6)

To find a relation between the forces in this expression and the applied shear stress we have to consider that if a piece of dislocation line $dl$ is to be moved a distance $ds$, the crystal above and below the slip plane will be moved by the Burgers vector $b$. This means that the average shear displacement of the crystal by this glide is:

$$\frac{ds \cdot dl}{A} b$$  \hspace{1cm} (3.7)

with $A$ the surface of the slip plane. The work done by the external force $Ar$ is equal to:

$$dW = Ar \frac{ds \cdot dl}{A} b$$  \hspace{1cm} (3.8)
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![Figure 3.8](image)

A schematic view of a piece of dislocation line $dl$, which bows under influence of a shear stress. The line tension $T$ tries to straighten the dislocation. At a curvature $R$ the forces are balanced [11].

Therefore, the glide force on a piece of dislocation of unit length is:

$$ F = \frac{dW}{ds \cdot dl} = \tau b $$

(3.9)

The shear stress can be related to the curvature of the dislocation line by considering a piece of dislocation line as depicted in Figure 3.8. The shear stress acts to maintain the curvature, while the line tension tends to straighten the line. According to Eq. 3.9, the outward force acting on this piece of dislocation is equal to $\tau bd$ this force is balanced by an inward force caused by the line tension of $2T \sin(d\theta/2)$. The balance for small values of $d\theta$ becomes:

$$ Td\theta = \tau bd$$

(3.10)

Since $d\theta = dl / R$, this can be written as:

$$ \tau = \frac{T}{bR} $$

(3.11)

Going back to Figure 3.7, the relationship between obstacle spacing $L$ and curvature $R$ is: $L = 2R \cos(\phi/2)$, which substituted into Eq. 3.11, leads to the following value for the critical resolved shear stress:

$$ \tau_c = \frac{2T}{bL} \cos(\phi / 2) $$

(3.12)

Since the line tension $T$ is just the increase in energy per unit increase in the length of a dislocation line (ignoring angular dependence of dislocation line and Burgers vector), Eq. 3.1 can be used to show that $T = a\mu b^2$ and write down the shear stress in terms of material constants.
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Figure 3.9 To calculate the effective obstacle spacing $L_F$ using Friedel statistics, the area $S_F$ has to be considered, which is swept out by a dislocation after breaking free of one obstacle whilst retaining its critical curvature $R$. This area is assumed to contain exactly one obstacle [23].

The choice of $L$ however is not a trivial one, since it is found to depend on the applied stress. This problem was solved by Friedel by postulating what is now called Friedel statistics [28], although surprisingly it is not a description dealing with statistics. When a pinned dislocation breaks free from an obstacle, the curvature of the dislocation line will remain constant and the dislocation will bow out until it reaches another obstacle. If at the flow stress a steady state flow is reached, on average the area swept by the dislocation after breaking free of an obstacle contains exactly one obstacle. Looking at the geometry shown in Figure 3.9, this means in mathematical terms that:

$$S_F n_s = 1$$

(3.13)

where $S_F$ is area of the large circle segment in Figure 3.9 minus the two smaller segments, all having radius $R$ and $n_s$ is the number of obstacles per unit area on the glide plane. Expressed in the distance between obstacles on the glide plane $L_s = n_s^{-1/2}$, a simple geometric analysis for $L \ll R$ yields:

$$S_F = L_s^2 = \frac{2L_c^3}{3R} - \frac{L_s^3}{6R} = \frac{L_s^3 b \tau_c}{2T}$$

(3.14)

Substituting $L_F$ for $L$ in Eq. 3.12 shows that the effective obstacle spacing is $L_c / (\cos(\phi_c / 2))^{1/2}$ changing expression 3.12 into:

$$\tau_c = \frac{2T}{bL_c} (\cos(\phi_c / 2))^{3/2}$$

(3.15)

For strong obstacles, i.e. when $\phi_c$ approaches zero, this analysis has to be slightly adjusted. Based on computer simulation several expression are proposed, which all increase the effective obstacle distance e.g. [31]:

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\[ \tau_e = 0.8 \frac{2T}{bL_\nu} (\cos(\varphi_e / 2)) \]  \hspace{1cm} (3.16)

Figure 3.10  A dislocation line in a field of diffuse obstacles.

Diffuse obstacles

When the obstacles exert attractive or repulsive forces on the dislocation line, for instance as a result of misfit strain fields, the situation may change drastically as illustrated in Figure 3.10. Here the dislocation line is not pinned behind the obstacles but instead follows a contour of minimum interaction energy. This arrangement requires a different approach, which has first been developed by Mott [29]. A useful parameter following from the work of Mott and others is \( \eta_0 \) defined as:

\[ \eta_0 = \frac{\omega}{L_\nu} (\cos(\varphi_e / 2))^{1/2} \]  \hspace{1cm} (3.17)

where \( \omega \) is the distance over which the force acts. The prediction is made that when \( \eta_0 \gg 1 \), i.e. in case the forces are felt everywhere between the obstacles, Mott statistics has to be applied and in the limit \( \eta_0 \ll 1 \), Friedel statistics accurately describes the interaction. When solute atoms are the predominant barriers to mobile dislocations, as has been shown in earlier in situ pulsed nuclear magnetic resonance (NMR) experiments, the mean jump distance can be predicted by Mott-Nabarro’s model of weakly interacting diffuse forces between Mg solutes and dislocations in Al rather than by Friedel statistics [25,26,27]. The details and consequences of Mott statistics can be found in literature [29,23].

3.3.2 Precipitation hardening mechanisms

There are several ways in which a precipitate can impede the motion of a dislocation and thereby strengthen the material. These include chemical strengthening, stacking fault strengthening, modulus hardening, coherency strengthening and order strengthening. For most of these hardening mechanisms quite accurate theories exist, which will be shortly described in the following sections. The type of hardening depends highly on the type of precipitate. For some alloys just one of the
aforementioned mechanisms is active but in most cases several of them play a 
significant part in determining the size of the critical resolved shear stress. Upon 
aging, not only the size of the precipitates may change. For many alloys, the Al-Cu 
system being the most extensively studied, other characteristics as for instance the 
shape, chemical composition and coherency changes dramatically with aging time. 
Since the size of the precipitates will be relevant in the following sections, it is 
useful to give the relation between \( L_s \), the average particle radius \( \langle r \rangle \), the average 
planar particle radius \( \langle r_p \rangle \) and the volume fraction \( f \) [23]:

\[
L_s = \left( \frac{32}{3\pi f} \right)^{1/2} \langle r_p \rangle = \left( \frac{2\pi}{3f} \right)^{1/2} \langle r \rangle 
\]  

(3.18)

Bypassing or cutting

When the critical bending angle \( \phi_c \) is larger than zero, the dislocation will pass the 
obstacles by cutting. This shearing mechanism itself creates some resisting forces 
which will be described later.

For very strong impenetrable precipitates for which \( \phi_c = 0 \), the dislocation has to 
bypass the obstacle. The most common bypass mechanism is the so-called Orowan 
mechanism which is sketched in Figure 3.11. The two segments of the dislocation 
line at either end of the precipitate attract and finally this constriction leads to the

![Figure 3.11](image)

Figure 3.11  The Orowan mechanism. (a) The obstacle is strong enough for the dislocation bow completely around it. The parts of dislocation line constrict until (b) the dislocation has passed the obstacles leaving dislocation loops around the particle [11].
advancement of the dislocation line and a dislocation loop around the particle. The critical shear stress is given by Eq. 3.16. Making the substitution $T = \frac{\mu b^2}{2}$ and adding some factors to correct for the nature of the dislocation and the finite particle size, the final version of the Orowan equation becomes [30]:

$$
\tau_c = \frac{0.84 \mu b}{2\pi(1-\nu)^{\frac{3}{2}} L} \frac{\ln(\Lambda / r_0)}{L - 2\langle r_c \rangle}
$$

(3.19)

In this expression $\nu$ is Poisson’s ratio and $\Lambda$ and $r_0$ are the outer and inner cut-off distances used to calculate the line energy of the dislocation.

Chemical strengthening

The shearing of a precipitate creates two new ledges of precipitate-matrix interface. The formation of this new surface with interfacial energy $\gamma_s$ produces a resisting force such that [31]:

$$
\tau_{sc} = \left( \frac{6\gamma_s b f}{\pi T} \right)^{1/2} \langle r \rangle^{-1}
$$

(3.20)

This expression predicts that for a constant volume fraction the critical shear stress decreases when the particle size increases, which is in contrast with experimental observation. It is therefore believed that chemical hardening does not play an important role in the strengthening of aged alloys.

Stacking fault strengthening

When the stacking fault energies of the matrix and the precipitate differ, the spacing between the partial dislocations will vary between the two phases causing an increase in the flow stress. Different relationships between the size of the precipitates and the separation of partial dislocations in the matrix and in the precipitate require separate analyses. Several of these scenarios have been worked out by Hirsch and Kelly [32] and later by Gerold and Hartman [33]. In its simplest form the expected relationship between the flow stress and the difference in stacking fault energies $\Delta \gamma$ is given by:

$$
\tau_{sc} = \left( \frac{\Delta \gamma}{b} \right)^{1/2} \left( \frac{3\pi^2 f \langle r \rangle}{32 T} \right)^{1/2}
$$

(3.21)

where the assumption is made that $2\langle r_c \rangle$ is smaller than the width of the stacking fault ribbon in the matrix.
Modulus Hardening

Assuming the shear modulus $\mu$ of the precipitate is not equal to that of the matrix, the elastic energy of a dislocation will change when it enters a particle. The force associated with this change in energy has been studied by, among others, Melander and Persson [34] and Nembach [35]. Their results are slightly different. Nembach argues that the force can be expressed as:

$$F_m = C_0 \Delta \mu b^2 \left( \frac{\langle r \rangle}{b} \right)^m$$  \hspace{1cm} (3.22)

Here, $\Delta \mu$ is the shear modulus difference between precipitate and matrix and $C_0$ and $m$ are constants equal to 0.05 and 0.85 respectively. Substituting this force in Eq. 3.15 and utilizing Eq. 3.6 and Eq. 3.18 yields the following expression for the increase in shear stress by modulus hardening:

$$\tau_{\mu \mu} = 0.0055 \left( \frac{f}{T} \right)^{1/2} \Delta \mu^{3/2} b \left( \frac{\langle r \rangle}{b} \right)^{3/2}$$  \hspace{1cm} (3.23)

Unfortunately, it is very difficult to create experimental conditions, in which the different theories can be validated.

Coherency hardening

In most cases the atomic spacing in the precipitate will differ from that in the matrix. In other words the particle does not fit exactly in, or is not coherent with, its surroundings. This misfit gives rise to strain fields which will interact with the dislocations and may impede their motion. This is the earliest source of hardening recognized but in the same time it is also the least accurately described quantitatively. Most models consider solely the case of the straight edge dislocation interacting with the strain fields around a completely spherical precipitate [31,36,37]. The results for the increase in resolved shear stress are of the form:

$$\tau_{\epsilon \epsilon} = \chi(\epsilon \mu)^{1/2} \left( \frac{\langle r \rangle fb}{T} \right)^{1/2}$$  \hspace{1cm} (3.24)

where $\chi$ is a constant between 2 and 3 depending on the theory followed and $\epsilon$ is the misfit parameter defined as:
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\[ \varepsilon = \frac{1}{3} \delta \left( \frac{1 + \nu}{1 - \nu} \right) \approx \frac{2}{3} \delta \]

(3.25)

where \( \delta \) is the classical misfit parameter, relating the lattice parameter of the matrix \( a \) with that of the precipitate \( a_p \):

\[ \delta = \frac{a_p - a}{a} \]

(3.26)

Ardell compares these theories to experimental data on different copper alloys and concludes that Eq. 3.24 overestimates the hardening due to coherency strain possibly due to the fact that they ignore screw dislocations and consider only straight dislocations i.e. weak obstacles [23].

Order strengthening

When a perfect dislocation (\( b = \frac{1}{2} a <110> \) in fcc materials) shears an ordered precipitate, an antiphase boundary (APB) may be created with a specific APB energy \( \gamma_{APB} \). This energy per unit area on the slip plane is equal to the force per unit length opposing the motion of the dislocation entering the precipitate. In the simplest analysis this force is therefore equal to:

\[ F_w = 2 \gamma_{APB} \langle r_c \rangle \]

(3.27)

Using Eq. 3.6 and Eq. 3.15 leads to the expression [31]:

\[ \tau_{\alpha O} = \frac{\gamma_{APB}}{b} \left( \frac{3 \pi^2 \gamma_{APB} f(r)}{32 T} \right)^{1/2} \]

(3.28)

For strong obstacles of course, Eq. 3.16 should be used instead.

Dislocations in a material with ordered precipitates are often found to travel in pairs, the second dislocation removing the disorder left behind by the first. If order hardening is a dominant strengthening mechanism, the resistance experienced by the second dislocation when shearing a precipitate can be very low, resulting in a straight dislocation line. To calculate the total effect of both dislocations the following force balances, in which the terminology of Figure 3.12 is utilized, have to be considered [38]:
for the leading dislocation:  \( \tau_{\infty} + \frac{\mu b}{2\pi(1-\nu)} l = \frac{\gamma}{b} \left( \frac{d_1}{L_1} \right) \)  

for the trailing dislocation:  \( \frac{\mu b}{2\pi(1-\nu)} l = \tau_{\infty} + \frac{\gamma}{b} \left( \frac{d_2}{L_2} \right) \) 

leading to:

\[
2\tau_{\infty}b = \gamma_{\text{APB}} \left( \frac{d_1}{L_1} - \frac{d_2}{L_2} \right) 
\]

If we consider the second dislocation to be perfectly straight \( d_2 / L_2 \) becomes equal to \( f \) and the first dislocation will bow out between the obstacles following Friedel’s hardening model: \( d_1 / L_1 = 2\langle r \rangle / L_F \) resulting in:

\[
\tau_{\infty} = \frac{\gamma_{\text{APB}}}{2b} \left[ \frac{3\pi^2\gamma_{\text{APB}}f\langle r \rangle}{32T} \right]^{1/2} - f 
\]

Equation 3.29 finally, can be used to calculate the distance 1 between the two dislocations.
Figure 3.13  *Al-rich end of the binary aluminum-copper phase diagram. The solubility of copper in aluminum increases with increasing temperature, enabling age hardening.*

### Age hardening

As stated in the beginning of this section, age hardening occurs in alloys for which the solubility of the alloying element in the matrix material increases with increasing temperature. Such occurs in the aluminum-copper system for which the aluminum-rich side of the phase diagram is shown in Figure 3.13. When an Al-2at.%Cu alloy is kept at a temperature of 550 °C, all the copper atoms will eventually dissolve in the aluminum. On slowly cooling down this stable solid solution, Al$_2$Cu precipitates will be formed starting at a temperature of around 500 °C. When room temperature is reached, the system will contain very large Al$_2$Cu precipitates in thermal equilibrium with the aluminum matrix. However, if the solid solution is quenched very rapidly from 550 °C to room temperature, there will not be sufficient time for precipitation and a super saturated solid solution is obtained.

Since the solubility of copper in aluminum at room temperature is very low, there is a driving force for the nucleation of Al$_2$Cu precipitates. When sufficient thermal energy is put into the system, for instance by annealing at 150 °C, precipitates will nucleate. If this process is allowed to continue long enough, eventually the equilibrium configuration is reached. In the aluminum-copper system, as in many other alloys, this transition from a solid solution to the equilibrium precipitated state, occurs via the formation of a number of metastable phases, for which a lower
thermodynamical threshold exists. They may differ from the equilibrium phase in e.g. composition, coherency and shape.
In the early stages of aging, the yield stress will increase rapidly through the nucleation of many small precipitates, which act as obstacles for dislocation motion as described in the previous section. As the precipitates grow, initially the yield stress will continue to increase, since for a constant volume fraction, all strengthening mechanisms, with the exception of chemical hardening, predict a higher critical resolved shear stress when the precipitate radius increases. Precipitates cannot grow indefinitely without losing their coherency. After reaching a specific size, depending on the misfit, they become at first semi-coherent, i.e. the misfit strains are relieved by the formation of a dislocation at the precipitate-matrix interface. Eventually the precipitate becomes completely incoherent with its surroundings causing the misfit strains to become very small. The hardening due to coherency strengthening disappears. Furthermore, when their size increases, the obstacles might become too strong to be sheared by the dislocations and the Orowan bypassing mechanism (Fig. 3.11) takes over. According to Eq. 3.19 further aging will cause the yield stress to drop steadily. A typical hardening curve therefore might look like the one sketched in Figure 3.14. In the underaging regime, the yield stress increases with increasing precipitate size. Either due to coherency loss or due to Orowan looping, a peak strength is reached, after which overaging sets in and the material softens.

Figure 3.14 Yield stress versus aging time. Initially the yield stress increases since shearing of the precipitates becomes increasingly difficult when they grow. Due to the Orowan mechanism and coherency loss, a peak strength is reached. Prolonged aging will cause the yield stress to drop.
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CHAPTER 3