Review: mechanisms in creep and anelastic recovery of face-centered cubic alloys

Kun Gao

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Supervisor: Dr.ir. Hans van Dommelen

Eindhoven University of Technology

Department of mechanical engineering
Abstract

In order to understand anelastic recovery behavior of Al-Cu thin films in RF-MEMS, this literature report firstly reviews creep behavior of face-centered cubic (f.c.c.) alloys and corresponding mechanisms including grain boundary sliding, dislocation glide and climb. In addition, the Orowan process, the Friedel process and thermal detachment, which are important in precipitate-strengthened alloys, are also discussed. Then, relations between these mechanisms and the anelastic recovery are investigated. In the second part, some creep models based on the mechanisms in the first part are presented.

The conclusions of this report are as follows: grain boundary sliding due to diffusion is not involved in the anelastic recovery; dislocation glide encumbered by the Orowan stress and the Friedel stress is a possible mechanism in the room-temperature anelastic recovery; the driving force may originate from unbowing of bowed dislocations and dislocation pile-up. At high temperature, dislocation climb may determine creep rate due to active diffusion. Besides climbing, dislocations can also bypass particles by cross-slip, which will occur if internal stress increases, and thermal detachment that appears to be strong for small particles. For modeling the anelastic behavior, the power law is very flexible and it is feasible to include some internal variables for the sake of a stronger physical meaning. In addition, building up direct relations between the strain rate and internal variables is also a good choice.
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Chapter 1 Introduction

RF-MEMS (radio frequency micro-electro-mechanical systems, figure 1) are able to provide radio frequency functionality and can be applied in oscillators, routing networks and other electric devices. Time-dependent mechanical behaviors such as creep are limiting for the reliability of these RF-MEMS devices.

Recently, in order to understand time-dependent behaviors of thin films used in RF-MEMS, a micro-beam of Al-Cu (1 wt.%) alloy with an average grain size of about 20 μm was bent by a micro-clamp (Delhey, 2009). The sample was deflected by approximately 825 nm at room temperature for about 2 days. After unloading, besides an instant elastic recovery, the beam recovered from around -30 nm to -10 nm in two hours (figure 2). This time-dependent phenomenon is referred as anelasticity of metals. It is believed that this anelastic recovery is related with the evolution of the microstructure. However, mechanisms involved in this process are not clear so far.

The Al-Cu (1 wt.%) alloy in the experiment is a face-centered cubic (f.c.c.) alloy, with some small Al-Cu intermetallic precipitates. In addition, the micro-beam sample is a thin structure. This literature study aims to find mechanisms responsible for this anelastic recovery of Al-Cu thin films. Many papers on thin films are associated with in-situ properties such as yield strength (Owusu-Boahen and King, 2001; Wang et al. 2003) or time-dependent behaviors of nanocrystalline materials (Proost et al. 1997; Mohamed, 2002; Haque and Saif, 2003; Tanimoto et al. 2004). Time-dependent behavior of thin films with a grain size of several micrometers is still an open topic. Some experiments focus on samples from several hundred micrometers to millimeters (Behr et al. 1999; Blum and Weckert, 1987; Gibeling and Nix, 1981; Jain and Kumar, 2010; Karthiktyan et al. 1995; Kottada and Chokshi, 2007; Lee et al. 2005; Mathew et al. 2005; Somekawa et al. 2005). The grain sizes of samples in these experiments are in the range of one micrometer to a hundred micrometers. Understanding mechanisms in these experiments can contribute to the study of mechanisms responsible for anelastic recovery of Al-Cu alloys. Hence, this report is not limited to thin films. On the other hand, mechanisms in other time-dependent behavior such as creep or stress relaxation can still be active in the case of anelastic recovery. Study of these mechanisms will be helpful for understanding anelastic recovery.
Therefore, firstly, mechanisms responsible for creep of f.c.c. crystals are investigated. Besides, it is tried to answer the question whether these mechanisms for creep still play an important role in anelastic recovery. In the second part, some creep models that are good references for modeling anelastic recovery are reviewed.
Chapter 2 Mechanisms in creep of crystals

2.1 Grain boundary effects

This section mainly focuses on grain boundary sliding, diffusion and migration. Firstly, mechanisms of grain boundary sliding are presented to make further discussion easier. Thereafter, it shows that grain boundaries affect time-dependent behaviors of crystals, including creep and stress relaxation. In the end, relation between grain boundaries and anelastic recovery is discussed.

2.1.1 Factors that control grain boundary sliding

There are two mechanistically distinct types of grain boundary sliding: Rachinger sliding and Lifshitz sliding (Langdon, 2006).

Rachinger sliding refers to the relative displacement of adjacent grains, where grains retain essentially their original shape. It occurs through the movement of dislocations along boundaries. One example of the process of Rachinger sliding is illustrated in figure 3: the stress concentration at point A leads to intragranular slip in the adjacent grain and dislocations pile up at the first subgrain boundary (point B), when the grain size $d$ is larger than the equilibrium subgrain size $\lambda$ (Langdon, 2006). In fact, mechanisms involving dislocation motion can influence the rate of Rachinger sliding. For example, dislocation climb in grain boundaries could control the rate of Rachinger sliding and dislocation pile-up will obstruct the sliding (Yoshida and Sakuma, 1998; Matsunaga et al. 2009).

\[
\frac{d}{\lambda} > 1
\]

Figure 3 an example of Rachinger sliding by dislocation motion (Langdon, 2006)

Lifshitz sliding occurs by diffusion in a low stress state and it refers to boundary offset due to the stress-directed diffusion of atoms and vacancies in grain boundaries. It is illustrated schematically in figure 4. The vertical tensile force is applied to three adjacent grains and two marker lines $AA'$ and $BB'$ are scribed parallel to the tensile axis. In diffusion creep, due to the applied stress, vacancies diffuse from the transverse to the longitudinal boundaries and equivalently, atoms move reversely. Thus, in figure 4b, the two marker lines remain unchanged in the lower grains but they move closer in the upper grains. During sliding, the grain boundary can be visualized as an extremely viscous thin layer between two grains. The rate equation has a similar form as Newtonian viscous law, in which the viscosity is dependent on the grain size and temperature (Raj and Ashby, 1970; Wei et al. 2007).

Figure 4 three grains with marker lines in Lifshitz sliding: the tensile axis is vertical and the grains are shown (a) before creep and (b) after creep testing (Langdon, 2006)
Moreover, the nominal viscosity in the rate equation is very close to the one in diffusion creep. Hence, it is believed that diffusion flow and Lifshitz sliding are coupled (Raj and Ashby, 1970).

2.1.2 The role of grain boundaries for creep and stress relaxation

In the case of Lifshitz sliding, motion of grain boundaries is related to diffusion. Besides, evidence shows that grain boundaries affect stress relaxation of crystals (Shute and Cohen, 1992; Bruckner and Weihnacht, 1999). Consequently, the discussion consists of two parts: creep and stress relaxation.

Creep

Many experiments show that grain boundaries play an important role in diffusion creep. Langdon (2002) cited the results of various experiments on Mg alloys and summarized that Lifshitz sliding contributes 50%-60% in the deformation of Nabarro-Herring diffusion creep. Moreover, Kottada and Chokshi (2007) tested single-phase Mg-0.7 wt.% Al alloys with an average grain size of 20 μm and found that the contribution of grain boundary sliding in diffusion creep is larger than 60% but the one in dislocation creep is only about 15%. Matsunaga et al. (2009) investigated the role of grain boundaries in the room temperature creep of Zn and found the evidence of grain boundary sliding accommodated by dislocation pile-up. It should be noted that diffusion creep usually occurs at very low stress levels (Langdon, 2002). At high stresses, when dislocation creep is dominant, deformation due to grain boundary sliding is only a small portion of total deformation.

The grain size of samples in above experiments ranges from 10 μm to 1 mm approximately. With the grain size decreasing, the grain boundary becomes a larger component of a grain. Thus, the effect of grain boundaries becomes more important. Yoshida and Sakuma (1998) proposed a model based on grain boundary sliding controlled by dislocation climb and pile-up and it succeeded explaining the dependence of transient time and strain on stress in fine-grained Al₂O₃ (average grain size 0.9μm). Wei et al. (2007) set up a model involving grain boundary diffusion and sliding and claimed that the recoverable creep deformation in nanocrystalline Al and gold films (Rajagopalan et al. 2007) was due to the non-uniform stress distribution resulting from heterogeneous grain boundary diffusion and sliding. In addition, combined with the classical framework of single-crystal plasticity, this model is also used to analyze the strain-rate sensitivity of the mechanical behavior of f.c.c. nanocrystalline materials (Wei et al. 2008).

Stress relaxation

The results of many experiments indirectly show the existence of such an influence in stress relaxation. Shute and Cohen (1992) calculated the activation energy of residual stress relaxation in Al-2 wt.% Cu thin films on silicon and found that the value of the activation energy was approximate to the one of grain boundary diffusion. Bruckner and Weihnacht (1999) successfully applied a fit function involving two processes, a combined twinning-plus-diffusion process and grain boundary diffusion, in stress relaxation curves of CuNi thin films at temperature higher than 573 K. Moreover, Lee et al. (2005) found that the measured relaxation time was comparable with the value predicted by grain boundary sliding model (Raj and Ashby, 1970) and they concluded that grain boundary sliding was the dominant relaxation mechanism in free-standing Al beams.
2.1.3 Relation with anelastic recovery

When the applied stress is removed, the remaining internal stress will contribute to the strain rate until a new equilibrium is reached. Rachinger sliding is controlled by dislocation motion. The driving force may be due to dislocation motion such as dislocation climb and pile-up in this case. It is more sensible to discuss in the section on dislocation motion.

Generally, grain boundary sliding has a slight influence on anelastic recovery. Raj and Ashby (1970) pointed out that incompatibilities generated by grain boundary sliding could be accommodated by local elastic deformation of crystals themselves. This process is recoverable: when stress is removed, the boundary will slide back under the influence of elastic stress, in which the sliding rate is dependent on the viscosity of the boundary. Nevertheless, the resultant displacement is only about several nanometers. Similarly, Gibeling and Nix (1981) discovered that the anelastic strain of single crystals samples were comparable with those of polycrystalline after a stress reduction during steady creep of f.c.c. metals and grain boundary sliding could not account for anelastic strains greater than the elastic contribution.

In nanocrystalline materials, heterogeneous grain boundary diffusion and sliding resulted in a non-uniform stress distribution that provides a driving force for the plastic strain recovery (Wei et al. 2007). Similarly, through the asymmetry shape of diffraction peaks after unloading, Lonardelli et al. (2009) proposed that the heterogeneity of grain size, which will lead to an inhomogeneous stress distribution, is necessary for recovery. It should be emphasized that these two mechanisms focus on nanocrystalline materials and the plastic recovery in there papers did not occur in samples with an average grain size larger than 180 nm (Rajagopalan et al. 2007).

To summarize, in crystalline materials with an average grain size larger than ~1 μm, grain boundaries will not significantly influence anelastic recovery based on the literature reviewed here.
2.2 Dislocation motion

This section will discuss dislocation motion. In the beginning, some experimental studies that show relations between dislocation motion and creep are discussed. The focus is on analyzing the rate-controlling mechanisms at different stress levels and temperature. The second part of this section focuses on the driving force for dislocation motion during anelastic recovery and the rate-controlling mechanisms.

In many experiments, the strain rate exhibits a power-law dependence on the applied stress. The power-law has various expressions:

\[ \dot{\varepsilon} = A\sigma^n \]  
\[ \dot{\varepsilon} = A \left( \frac{\sigma}{G} \right)^n \exp\left( -\frac{Q}{RT} \right) \]  
\[ \dot{\varepsilon} = A \left( \frac{\sigma - \sigma_{\text{th}}}{G} \right)^n \exp\left( -\frac{Q}{RT} \right) \]

where \( \dot{\varepsilon} \) is the strain rate, \( \sigma \) is the applied stress, \( Q \) is the activation energy, \( G \) is shear modulus of the material, \( T \) is temperature and \( \sigma_{\text{th}} \) is the threshold stress below which the creep rate is negligible.

The stress exponent \( n \) can help to classify mechanisms of creep. For example, for pure aluminum, \( n = 3 \) indicates that dislocation glide may be the dominant mechanism during deformation and \( n = 5 \) refers to dislocation climb. If \( n = 1 \), diffusion creep rather than dislocation creep determines the creep rate. However, this approach to determine mechanisms relies not only on the microstructures of materials but also on experience. Ascertaining mechanisms of creep by the stress exponent is not reliable. Therefore, in the following discussion, besides the stress exponent, other experimental evidences like TEM results and comparisons with theoretical models are supplied.

2.2.1 Dislocation motion and creep

This part will firstly discuss dislocation glide. Dislocation glide is usually accompanied by other mechanisms like dislocation climb. Besides, dislocations may circumvent various obstacles by climb and many evidences show that it is very important at high temperature. Hence, the second topic is dislocation climb. Dislocation cross-slip provides another opportunity to bypass obstacles and accumulated dislocations will result in back stresses that prevent gliding. Thus, after dislocation climb, dislocation cross-slip and pile-up are discussed briefly. In precipitates strengthened alloys, besides bypassing precipitates, dislocations could also shear them. These effects of particles will be studied at the end of this part.

Dislocation glide

Dislocation glide means the propagation of dislocations in slip planes. It is often accompanied by other mechanisms like climb and cross-slip. Generally, dislocation glide itself occurs very easily and
fast; other mechanisms such as dislocation climb and cross-slip have higher energy barriers to overcome and they require more time to complete. However, it should be noted that dislocation glide does control creep rates in some experiments (Mathew et al. 2005). This is due to mechanisms that hinder gliding rather than dislocation glide itself. One example is that, in solid solution alloys, solute atmospheres lock dislocations such that the rate of gliding becomes slower than dislocation climb and cross-slip. In this case, the activation energy for creep is close to that for diffusion of solute atoms.

Yavari et al. (1981) tested Al-5% Mg solid solution samples under double shear conditions at 827 K and found that the stress exponent of the shear strain rate in steady-state creep was 3.1 when the shear stress was larger than 0.5 MPa. By etching a specimen at 3.10 MPa, they discovered that the etch pits were distributed randomly, with no evidence of the preferential alignment of dislocations into subgrain boundaries. Moreover, TEM observation of a sample at 3.45 MPa shown in figure 5 revealed that dislocations were distributed essentially uniformly. According to these evidences, they concluded that dislocation glide controlled deformation at high shear stress. Mathew et al. (2005) did creep tests of Sn-5Sb at 296 to 473 K, for which the material is a solid solution alloy as shown in figure 6, and obtained the stress exponent as 5.0±0.3 and the activation energy as 44.7±3.7 kJ/mol. These values were in good agreement with the low-temperature viscous glide mechanism. If dislocation climb was the dominant mechanism, the activation energy calculated from a theoretical equation was 46 kJ/mol that is close to the experimental energy. However, the corresponding stress exponent equaled to 7, higher than 5. Therefore, the dominant mechanism was dislocation glide. Furthermore, addition of Fe in NiAl was shown to lead to solid solution strengthening by transient compressive test (Wang et al. 2006). The stress exponent of Ni_{40}Fe_{30}Al_{30} at 873 to 1023 K was about 3.4 with an absence of an obvious subgrain structure and they concluded that dislocation glide controlled creep in this case.

**Figure 5** a random distribution of dislocations in a specimen at 3.45 MPa (Yavari et al. 1981)

**Figure 6** initial microstructure of Sn-5Sb, a solid solution alloy (Mathew et al. 2005)

**Dislocation climb**

Dislocation climb refers to an out-of-plane movement for edge dislocations. A large driving force is required to make dislocations move out of the slip plane and this process occurs slowly. Therefore, dislocation climb is usually considered as an important rate-controlling mechanism in creep (Seidman et al. 2002; Jain and Kumar, 2010). The rate of dislocation climb depends on (a) the chemical potential and the mechanical forces due to the chemical potential and the mechanical forces, (b) the mobility of jogs and (c) the rate of
migration of vacancies (Hull and Bacon, 2001). Factors (b) and (c) are directly related with diffusion, which could also alter the chemical potential. Therefore, diffusion probably controls the rate of dislocation climb. Mathew et al. (2005) found the stress exponent of pure tin at 296-423 K was 7.6±0.2 and the activation energy was 60.3±3.8 kJ/mol. They also measured the stress exponent (5.0±0.2) and the activation energy (60.7±6.6) kJ/mol of Sn-3.5Ag alloy where Ag$_3$Sn intermetallic particles were finely distributed in tin matrix. Considering that the temperature investigated was near the melting point of tin (505 K), it was suggested that dislocation climb controlled by lattice diffusion was the rate-controlling mechanism for both two alloys in the range of conditions studied. Somekawa et al. (2005) studied climb-controlled dislocation creep behavior in Mg-Al-Zn alloys. At high temperature, the stress exponent was 5 and the activation energy was close to that for lattice diffusion of Mg, whereas at low temperatures the stress exponent was 7 and the activation energy was close to that for pipe diffusion for all alloys.

Improvements of diffusion could increase creep rate of climb-controlled dislocation creep. Conversely, when diffusion is blocked, dislocation climb will be inhibited. It will decrease the rate of climb-controlled dislocation creep or make other mechanisms dominant. Sherby and Ruano (2005) proposed a dislocation climb model involving solute atom diffusion for the subgrain boundary. In this model, diffusion of solute atoms makes two single-Burgers vector dislocations come together by climb so that a new double-Burgers vector dislocation forms. Release of the energy from this combination is sufficient to unpin another dislocation from the pile-up. This released dislocation plays a key role that leads to a repetition of the above process and will glide to the subgrain boundary. The model prediction that solute atoms that diffuse more rapidly than Al (matrix) would lead to faster creep rates than pure Al. The results of creep experiments (Sherby and Ruano, 2005) on Al with different solute atoms confirmed this model: alloys with solutes of Bi, Zn, Ge and Cu (Al-0.029% Cu) that show higher diffusion coefficients than that of Al self-diffusion exhibited lower activation energies for creep and faster creep rates. Conversely, alloys with slow diffusive atoms like Fe, Mn, Ti and V showed higher activation energies and slower creep rate. Wang et al. (2006) also confirmed that addition of Fe improved creep resistance and reduced the diffusion coefficient so that creep of Ni$_{50}$Al$_{50}$ was controlled by dislocation climb while dislocation glide determined creep rate of Ni$_{40}$Fe$_{10}$Al$_{50}$.

Temperature definitely influences the activity of diffusion. At high temperature, diffusion of atoms or vacancies becomes more active, which makes dislocation climb occur more easily. Hence, dislocation climb should be more active at high temperature. Kim et al. (2006) found that, the stress exponent for Ni-base superalloy was 4.1 at 1227 K and 5.4 at 1115 K after considering the threshold stress. The activation energies at 1200-1255 K and 1089-1144 K were 237 and 245 kJ/mol respectively, which is consistent with the activation energy for lattice self-diffusion. Besides, they also found that the shape of γ’ particles had slightly changed and many dislocations lay at the γ/γ’ interface and enveloped γ’ particles in steady state creep under 1113 K and 400 MPa, as shown in figure 7. Therefore, the rate-controlling mechanism of creep at high temperature and low stress was dislocation climb.
Dislocation cross-slip

For screw dislocations, they can move from one slip plane to another. This process is referred as cross-slip. Dislocations can also circumvent obstacles by cross-slip when the driving force is large enough. Zhang et al. (2005) compared dislocation configurations in two single-crystal Ni-base superalloys, TMS-75 and TMS-138, during high-temperature low-stress creep (1372 K, 137 MPa). They found that dislocations with Burgers vector $\vec{b} = 1/2[101]$ in TMS-138, which has a larger lattice misfit, were parallel to the (001) plane and stayed in the $\gamma$ channels, which were normal to the [001] tensile axis, after two hours of creep. These characteristics indicated that dislocations moved by cross-slip. The comparison with dislocation configurations of TMS-75 and TMS-138 are shown in figure 8. Due to the larger lattice misfit, internal stress in TMS-138 that was larger than that in TMS-75 supplied a sufficiently large driving force for dislocation motion. This view explained not only the occurrence of dislocation cross-slip in TMS-138, but also the phenomena that TMS-138 had a larger strain in the beginning of creep as shown in figure 8. For the late stage, accumulated interfacial dislocations prevented further deposition so that the strain after 10 hours of creep of TMS-138 was smaller than that of TMS-75 in figure 8.
Dislocation pile-up

Dislocation pile-up will not directly control the rate of creep, since dislocation pile-up affects creep through becoming obstacles of dislocation motion. Although dislocation pile-up is not the rate-controlling mechanism, it does not mean that the effect of dislocation pile-up can be neglected. Jansen and Dunand (1997) studied compressive creep properties of coarse- (the grain size ranged from 1 mm to several centimeters) and fine-grained (the average grain size was 1.3 μm) dispersion-strengthened Al with 25 vol.% submicron Al2O3 dispersoids between 608 K and 773 K. They found that the experimental threshold stresses were significantly higher than predicted with existing models considering a single dislocation interacting with one or more dispersoids. Nevertheless, in their model in which dislocation pile-up contribute to the threshold stress, the numerical threshold stress was close to the experimental value. It should be noted that dislocation climb and cross-lip would help dislocations to escape dislocation pile-up as temperature increases (Jansen and Dunand, 1997; Sherby and Ruano, 2005).

The effects of precipitates

Many experiments show that addition of precipitates increases creep resistance and this effect depends on the strength of both precipitates and matrix (Krajewski et al. 1995; Modlinski et al. 2004, 2005; Karthikeyan et al. 2005). Generally, this strengthening effect is due to precipitates that retard dislocation motion. Precipitates are obstacles for dislocation glide. Consider a dislocation and an array of particles that are impenetrable for the dislocation in figure 9. The dislocation is forced to bow out between particles, since the dislocation is pinned at the particles. When the curvature of the dislocation is large enough, i.e. the characteristic length d is smaller than the obstacle spacing L, the bypass condition is reached (referred as the Orowan process) (Arzt, 1998). Many obstacles such as solute atoms or coherent precipitates are not strong enough to block dislocations. In these cases, dislocations could shear these “weak” obstacles (referred as Friedel process). For example, the observation of a dislocation structure for primary creep in specimen of Ni-base superalloy tested at low temperature and high stress indicated that paired dislocations had sheared γ’ precipitates as shown in figure 10 (Kim et al. 2006).

In precipitation-strengthened materials, yield strength is dependent on particle size: for large particles, the strength is controlled by the Orowan process, while precipitate shearing dominates the
strength of materials with small particles (Arzt, 1998; Seidman et al. 2002). The applied stress plays an important role in creep. Viswannathan et al. (2005) tested Ni-Al superalloys of both coarse and fine γ’ precipitates (Ni₃Al) at 923 K and 790~972 MPa. In samples with fine precipitates, the ½<110> dislocations loop around precipitates at high stress indicating the Orowan mechanism and no obvious pairing of ½{110} dislocations suggested that shearing was not dominant. Whereas in coarse microstructure, isolated faulting, which is not necessarily nucleated on the grain boundary and limited to secondary γ’ particles, dominated the deformation. In creep tests of Ni-Cr-Co superalloy at 1073 K-1148 K, Davies et al. (1992) confirmed that the Orowan loops contributed to a major part of the internal stress formed at low stresses (~150 MPa). While at high stress (~325 MPa), the Orowan loops consisting of partial dislocations surrounding faulted γ’ particles were formed by shearing particles as shown in figure 11. Noting that the size of γ’ particles in Davies et al.’s paper (~40 nm) is smaller than the size of fine microstructure in Viswannathan et al.’s paper (50~100 nm) and that the materials in two papers are different, the conclusions in these two papers are not contrary.

At high temperature, dislocations may also bypass obstacles through climb, cross-slip and detachment. Since climb and cross-slip have been discussed above, the following will focus on detachment in this part. Experiments showed that there is an attractive interaction between particles and dislocations (Herrick et al. 1988). This interaction is due to thermal detachment (Arzt, 1998; Arzt et al. 2001; Behr et al. 1999). Rosler et al. (1992) discussed the threshold stress of creep of dispersion-strengthened aluminum alloys with various dispersoid types (Al₄C₃, Al₂O₃ and MgO). They found that the threshold stresses predicted by a dislocation climb model were much smaller than the one obtained from experiments and that climb of dislocations over particles of low volume fraction was rapid. However, the thermal detachment model was in good agreement with the experiments.

Figure 11 a schematic representation of shearing of γ’ particles at high stress. An Orowan loop is formed by a dislocation with Burgers vector BA (a-c). A new dislocation of Burgers vector CA reacts with the loop, shearing the particle and leaving it with a loop of a partial dislocation and a super-lattice stacking fault (c-g) (Davies et al. 1992)

Generally, thermal detachment happens more easily for small particles than large particles. Compared with climb, thermal detachment takes more time and is likely to be the rate-controlling mechanism. Behr et al. (1999) recorded in-situ creep tests of oxide-dispersion strengthened alloys at 1273 K as shown in figure 10. In figure 12a, dislocations approached particles from the right side and only touched the larger particle. In contrast, dislocations were attached strongly to the smaller
particle. A second pair of dislocations arrived while the first pair of partial dislocations were still attached the small particles in figure 12b. After about 3 s, the leading partial dislocation detached from the particle and almost instantly reduces its radius of curvature and line length and the arrival of further dislocations finally leads to detachment of the second partial of the first superdislocation. In the video, dislocations are not significantly slowed down while climbing across the particle and this showed that dislocation climb happened in a time interval shorter than the time between two video frames. It indicated that the rate-limiting step was detachment from the backside of particles and not the climb step across particles.

Figure 12 images taken from a TV sequence recorded during in-situ deformation of Ni$_3$Al (Behr et al. 1999)

2.2.2 Dislocation motion and anelastic recovery

When samples are loaded, various internal stresses will arise in order to accommodate the incompatibilities generated during deformation and recover to the original state. In crystalline materials, internal stresses contain the stresses that retard dislocation motion and the non-uniform stress from inhomogeneous strain. Back stresses retarding dislocations may come from solute drag, barriers of climb and cross-slip, and dislocation pile-up. In precipitates-strengthened alloys, it may also contain interactions of dislocations and precipitates such as bowed dislocations, the Orowan loops, the Friedel stress and attractive force between particles and dislocations. After applied stress is removed, a part of internal stresses may change their roles from retarding to driving dislocation motion, as is the case of dislocation pile-up, unbowing of bowed dislocations (Gibeling and Nix, 1981). In the study of anelastic recovery after a stress reduction in creep tests, Gibeling and Nix (1981) pointed that unbowing of bowed dislocations was insufficient to account for the relatively large reverse strain that was several times larger than the elastic strain and dislocation pile-up contributed to the recoverable strain of the order of the elastic strain. In addition, inhomogeneous strain, which is related to lattice dislocations, grain-boundary defects and intracrystalline gradients, will result in a non-uniform stress that can also supply a driving force for anelastic recovery (Lonardelli et al. 2009). Savage et al. (2002) observed room-temperature creep recovery in titanium alloys, which refers to a significant increase in the observed creep rates upon reloading after a period of unload, and they found that intense pile-up of a/2[110] dislocations were on both (101) primary slip plane and (211) cross slip plane. They also proposed that a significant stress concentration within α phase due to dislocation pile-up was a prerequisite for the recovery. It should be noted that
titanium alloys were h.c.p. not f.c.c., whereas the micro-beam in the anelastic recovery experiment (Delhey, 2009) is aluminum alloy (f.c.c.). Moreover, the recovery in Savage et al.’s paper was manifested as a significant increase in the observed creep rates upon reloading after a period of unload and it is different from the anelastic recovery that refers to a deformation recovery after unloading. Therefore, dislocation pile-up may not be necessary for anelastic recovery, whereas it cannot be neglected.

Blum and Wecker (1987) discussed events followed a stress reduction during a tensile creep test for Al-Mg alloys. In this paper, a stress reduction caused the following events: (a) a contraction due to lattice elasticity; (b) a contraction due to unbowing of bowed dislocation segments which are not free to glide; (c) reduction in the velocities of thermally activated glide of mobile dislocations and subgrain boundary migration. The reaction (a) is time-independent since elasticity is controlled by the stress. Strictly speaking, unbowing of bowed dislocation still belongs to dislocation glide. Considering that dislocation glide is a fast process, unbowing of dislocations also responses very fast. Gibeling and Nix (1981) indicated that the unbowing in pure metals might occur at a rate in the $10^3 \text{ s}^{-1}$ and $10^6 \text{ s}^{-1}$ range. Therefore, the possible rate-controlling mechanisms of anelastic recovery are the mechanisms that retard dislocation glide, that is, the Orowan process and the Friedel process. When the applied stress has been removed, the driving forces for dislocation climb, cross-slip and thermal detachment are significantly reduced. These mechanisms are difficult to occur and control the rate of recovery. At high temperature or in cases where internal stress is large enough, they are still possible to become the rate-controlling mechanisms. Nes (1994) reviewed models on the recovery of mechanical properties during annealing. These models were based on dislocation density and the recovery of flow stress can be obtained by considering the time-dependent growth of a dislocation network. It was demonstrated that, when the growth of the dislocation network was controlled by dislocation climb or cross-slip, the decay of dislocation density could be described by a power law; however, thermally activated glide would result in a logarithmic decay in dislocation density.

To conclude, bowed dislocations and dislocation pile-ups are the possible sources of the driving force. The possible rate-controlling mechanism at low temperature is dislocation glide encumbered by the Orowan process and the Friedel process. At high temperature, the possibilities of dislocation climb, cross-slip and thermal detachment increase.
Chapter 3 Models of creep

This chapter will focus on various models of creep. Firstly, models for grain boundary sliding are discussed: two models for Lifshitz sliding related with diffusion are described in detail; the part on Rachinger sliding is discussed briefly. Afterwards, according to the rate-controlling mechanisms, dislocation motion models are classified into three parts: dislocation glide and climb, dislocation cross-slip and precipitate-strengthening effects.

Models on grain boundary sliding

Mechanisms involved in grain boundary sliding have been discussed in chapter 2. For Lifshitz sliding, it is feasible to apply chemical potential to describe diffusion. For example, Raj and Ashby (1970) studied steady state sliding with diffusion accommodation for 2D conditions. An illustration of the steady state sliding is shown in figure 13. The original grain boundary is presented as a solid line in figure 13. In time Δt, the sliding translates the upper half crystal from the solid line to the dashed line and the average velocity is denoted as \( \bar{U} \).

In the steady state, where a chemical equilibrium is reached, the chemical potential \( \mu(x, y) \) will satisfy the Laplace equation

\[
\Delta \mu(x, y) = 0
\]

(4)

On the grain boundary, the chemical potential is dependent on the normal stress acting on the grain boundary

\[
\mu = \mu_0 - \sigma_n \Omega
\]

(5)

where \( \mu_0 \) is the chemical potential in the stress-free reference state and \( \Omega \) is the atomic volume. The normal stress \( \sigma_n \) can be obtained through a mechanical equilibrium.

\[
\int_{-\lambda/2}^{\lambda/2} \sigma_n dx = \tau_0 \lambda
\]

(6)
where \( \tau_a \) is the applied shear stress and \( \lambda \) is the wave length in figure 13. This normal stress can be obtained by a Fourier series

\[
\sigma_n = -\frac{\tau \lambda}{\pi} \sum_{n=1}^{\infty} \alpha_n \sin \frac{2\pi n}{\lambda} \gamma_n y
\]  

(7)

The \( \alpha_n \) are numerical constants to be determined and the meaning of \( h \) is shown in figure 13. It still requires the continuity equation involving displacement \( \dot{U} \Delta t \) and the volume diffusion flux that depends on the gradient of the chemical potential. Then the steady state diffusion-controlled sliding rate is given by

\[
\dot{U} = \frac{2 \tau \Omega}{\pi k_B T} \frac{\lambda}{h^2} D_v \left[ \sum_{n=1}^{\infty} \left( \frac{1}{n} + \frac{\pi \delta}{\lambda} \frac{D_B}{D_v} \right) \frac{1}{h^2} \right]^{-1}
\]  

(8)

With \( k_B \) Boltzmann’s constant, \( T \) the temperature, \( D_v \) the bulk self-diffusion coefficient, \( D_B \) the coefficient for boundary diffusion and \( \delta \) the thickness of grain boundary that measures the area across which the boundary flux passes.

For polycrystalline materials, grain boundaries can be idealized as an array of hexagons as shown in figure 14. There are two modes of sliding shown with heavy lines in figure 14. These two modes are orthogonal, so that the net strain rate \( \dot{\gamma} \) is the sum of the strain rates contributed by each mode. A good estimate of the sliding rate at a boundary with an obvious basic periodicity is given by approximating the shape by a sine wave of the same periodicity and amplitude. Then, the series in equation (8) has only one term \( n = 1 \) and the shear strain rate of a polycrystalline material can be derived by

\[
\dot{\gamma} = \frac{2}{d} \frac{\tau_a \Omega}{k_B T} \frac{1}{a^2} \left[ D_v + \frac{\pi \delta}{\lambda} D_B \right]
\]  

(9)

where \( d \) is the length of the grain and it equals with \( 2h \) as shown in figure 14. This model can be extended to a 3D case in which the boundary contains a periodic array of cube-shape particles with a size of \( a \). The derivation for a 3D problem can be found in Raj and Ashby, 1970. The approximated solution is given by

\[
\dot{U} = 1.6 \frac{\tau_a \Omega}{k_B T} \frac{\lambda^2}{a^2} \left[ D_v + \frac{\delta}{a} D_B \right]
\]  

(10)

where \( \delta \) is the thickness of the interface.

This model supplies an analytical solution of the rate of sliding. The simplification of grain boundaries and particles limits the usage in a more complex problem. The biggest disadvantage of this model is that it ignores the microstructure evolution of diffusion creep. However, the idea of describing grain boundary sliding is still accepted (Lee and Morris, 2010).
It is also possible to use a Newtonian viscous law to describe grain boundary sliding. Wei et al. (2007) proposed such a model associated with grain boundary sliding and diffusion. A representative grain boundary $\Gamma$ is shown in figure 15 and there is an atomic flux $j$ through the boundary. The displacements of atoms at the grain boundary are given by $u^+$ and $u^-$ respectively. The stress along the boundary can be decomposed as two parts: the shear stress along the boundary $\tau$ and the normal stress perpendicular to the boundary $\sigma_n$. At a point $x$ along the grain boundary as shown in figure 15, for grain boundary sliding,

$$\eta \frac{\partial u_s}{\partial t} = \tau,$$

where $u_s = (\bar{u}^+ - \bar{u}^-) \cdot \bar{m}$ is the relative sliding displacement across the grain boundary and $\eta$ is the viscosity. For grain boundary diffusion, the required chemical potential is dependent on the normal traction $\sigma_n$ and it is given by equation (5). Since only the derivative of the chemical potential takes an effect in this model, the reference potential is taken as zero. The atomic flux is given by

$$j = \frac{\delta D}{k_B T \Omega} \frac{\partial \mu}{\partial x}$$

According to mass conservation,

$$\frac{\partial u_n}{\partial t} = -\frac{\partial (\Omega j)}{\partial x}$$

with $u_n = (\bar{u}^+ - \bar{u}^-) \cdot \bar{n}$ the width of new material being inserted at $x$ by grain boundary diffusion. One can calculate the displacement of the grain boundary by solving equation (11) and (13). This model can be coupled with the classical framework of rate-dependent single-crystal plasticity that will be applied in the grain interior. It was shown that the coupled model succeeded in simulating the strain-rate sensitivity behavior and matched well with experiment data (Wei et al. 2008).
For Rachinger sliding, Langdon proposed an equation based on a power law

\[
\dot{\varepsilon}_{\text{gb}} = A'' D_G b \left( \frac{b}{d} \right) \left( \frac{\sigma}{G} \right)^3
\]

where \( A'' \) is a dimensionless constant, \( D_j \) is the diffusion coefficient, \( b \) is the length of Burgers vector and \( G \) is the shear modulus. This equation is in good agreement with the experimental observations (Langdon, 2006; Kottada and Chokshi, 2007). However, it is a phenomenological equation and cannot help to understand the physical processes during deformation. Models based on dislocation motion should have a more rigid physical meaning to describe Rachinger sliding, which is related to dislocation motion like dislocation glide and climb.

**Models for dislocation glide and climb**

In creep models, the essential equation is the expression of the strain rate. The power law, connecting the strain-rate with the stress directly, is an example that is widely employed. A usual format of the power law is given by equation (3). In fact, the expression of the threshold stress, the activation energy and the coefficient \( A' \) are adjustable. As a result, the power law can easily be coupled with different mechanisms (Yavari et al. 1981; Mathew et al. 2005; Seidman et al. 2002; Somekawa et al. 2005; Kim et al. 2006).

There are other approaches related to the strain rate besides the power law. It is feasible to assume that the strain rate is dependent on internal variables like dislocation density, the velocity of glide and climb. The Orowan equation is a well-known example. Based on the Orowan equation, Blum et al. (2002) proposed such a model in which dislocation glide was considered as the rate-controlling mechanism. The shear strain rate is given by

\[
\dot{\gamma} = b \rho_{\text{mob}} v_g
\]

where \( \rho_{\text{mob}} \) is the density of mobile dislocations, \( v_g \) is the average glide velocity. There are two types of dislocations in this model: single dislocations \( \rho_{\text{sgl}} \) and dislocations in dipole configurations \( \rho_{\text{dip}} \). The mobile dislocation density consists of a fraction of the single dislocations:

\[
\rho_{\text{mob}} = f_{\text{mob}} \rho_{\text{sgl}}
\]

There are two terms needed to be determined in equation (15): the dislocation density and the glide velocity. Single dislocations are generated during deformation. When two single dislocations with opposite signs get closer than a certain value \( d_{\text{dip}} = \frac{1}{8\pi(1-v)} \frac{Gb}{\tau} \), they will be stuck in a dipole configuration, which means the annihilation of single dislocations and the generation of dipoles; if two dislocations come too close (<\( d_{\text{spon}} \), they will annihilate spontaneously without producing the dipole. For dipoles, the annihilation consists of spontaneous annihilation and thermally activated dissolution due to climb or cross-slip. Based on the above process, the generation rate of single dislocations is given by
\[ \dot{\rho}_{sgl} = \frac{\gamma}{b\Lambda} \]  

where \( \Lambda \) is called the mean free path, representing the total distance by which a dislocation glides during its life. The annihilation rate of single dislocations is

\[ \dot{\rho}^{-}_{sgl} = 4d_{spon} \left( \frac{\dot{\gamma}}{b} \right) \frac{2\rho_{sgl}}{n_{g}} \]  

with \( n_{g} \) the number of active slip systems. Thus, the evolution of the density of single dislocations is described as

\[ \dot{\rho}_{sgl} = \dot{\rho}^{+}_{sgl} - \dot{\rho}^{-}_{sgl} = \frac{\dot{\gamma}}{b} - 4d_{spon} \left( \frac{\dot{\gamma}}{b} \right) \frac{2\rho_{sgl}}{n_{g}} \]  

The spontaneous annihilation rate of single dislocations is

\[ \dot{\rho}^{-}_{sgl,spon} = \frac{d_{spon}}{d_{dip}} \dot{\rho}^{-}_{sgl} \]  

Thus, the evolution of the density of dipoles is given by

\[ \dot{\rho}_{dip} = (\dot{\rho}^{+}_{sgl} - \dot{\rho}^{-}_{sgl,spon}) - \dot{\rho}^{-}_{dip} = \left( 1 - \frac{d_{spon}}{d_{dip}} \right) 4d_{spon} \left( \frac{\dot{\gamma}}{b} \right) \frac{2\rho_{sgl}}{n_{g}} - \frac{2\rho_{dip}v_{c}}{d_{dip} - d_{spon}} \]  

where \( v_{c} \) is the velocity of dipole dislocations that move in the direction perpendicular to the slip plane. It is expressed in terms of climb of edge dislocations:

\[
\begin{align*}
 v_{c} &= \frac{D\Omega\sigma_{c}}{bk_{\mu}T} \\
 \sigma_{c} + \frac{v_{c}}{B} &= \frac{Gb}{2\pi(1-v)} \frac{2}{d_{spon} + d_{dip}}
\end{align*}
\]

where \( \Omega \) is the atomic volume and \( D \) is the coefficient of self-diffusion.

On the other hand, the gliding velocity can be phenomenologically expressed as

\[ v_{g} = B\sigma_{eff}^{m} \]  

Here, the effective stress \( \sigma_{eff} = \sigma - c\alpha Gb\sqrt{\rho_{sgl} + c_{dip}\rho_{dip}} \) (\( c \) is a numerical factor, \( \alpha \) is the dislocation interaction constant and \( c_{dip} \) is a weighting factor). It should be noticed that the coefficient \( B \) is used for simplicity. In fact, this coefficient has various complex forms under different conditions, for example, in solid solution alloys,
By solving equation (19), (21)-(23), the dislocation density can be obtained. The evolution of dislocation density reflects the microstructure evolution. The numerical result showed that this model could reproduce some important features of creep (Blum et al. 2002): the power law for steady-state deformation and its breakdown at high stress; the distinction between climb-controlled creep in pure metals and glide-controlled creep in solid solution alloys. However, this model neglects the heterogeneity of the microstructure during deformation. There are some large discrepancies between numerical results and experiments. Therefore, Blum replenished this model by considering the existence of subgrains (Blum and Eisenlohr, 2009).

Similar to dislocation glide in the Orowan equation, relationship between the strain rate and the dislocation climb in climb-controlled creep could be expressed as follows. Yoshida and Sakuma (1998) proposed a model based on grain boundary sliding accommodated by dislocation climb. In the model, grain boundary sliding is assumed to occur by dislocation glide in grain boundaries as shown in figure 16. The creep is controlled by dislocation climb and dislocation pile-up resulting in a back stress to reduce the creep rate. The shear strain rate also depends on the number of boundaries per unit volume $M$

$$\dot{\gamma} = b \Gamma M \dot{s}$$

(25)

where $\Gamma$ is the area swept by a dislocation during glide along the grain boundary. The climb frequency $\dot{s}[1/s]$ is written as

$$\dot{s} = Nb\kappa = N \frac{D_b}{k_bT} \frac{8q\pi\Omega}{d\ln(L/b)} (\tau - \tau_b)$$

(26)

where $N$ is the length of grain boundary dislocations in an area, $\kappa$ is climb velocity of dislocations, $D_b$ is the diffusion coefficient, $q$ is a converting factor from normal stress to shear stress, $\Omega$ is the vacancy volume and $L$ is the distance from the dislocation to the region where the vacancy flow is in equilibrium. Notice that the grain has a hexagon shape and it is assumed that $\Gamma = \pi d^2 / 4$ and $M = 6 / (\pi d^3)$. Besides, for simplicity, the length of grain boundary dislocations in an area is assumed as $N \sim 2\pi(1-v)\tau / (Gb)$. By substituting of equation (26) into equation (25)

$$\dot{\gamma} = A(\tau - \tau_b)\tau$$

(27)

with $A$ is the product of other coefficients.
In this model, the back stress is assumed to be originated from dislocation pile-up. Yoshida et al. (1998) calculated the total work done by internal stress (an integration of the elastic stress) of a pile-up of edge dislocations in the grain boundary and the back stress is estimated by

\[ \tau_b \sim \frac{nGb}{\pi(1-v)d} \ln \frac{d}{2nab} \]  

(28)

Where \( a \) is a proportionality factor larger than 1 and \( n \) is the number of grain boundary dislocations that annihilates by dislocation climb. Thus, the evolution rate of this number

\[ \dot{n} = \rho v \alpha - n \kappa \]  

(29)

Here, \( \rho \) is dislocation density on a grain boundary, \( v \) is the glide velocity of a dislocation and \( \alpha \) is a material constant. According to the Orowan expression for the shear strain rate \( \dot{\gamma} = \rho b v \), equation (29) can be rewritten by substitution of equation (28),

\[ \dot{\tau}_b = H \dot{\gamma} - \kappa \tau_b \]  

(30)

The combination of equation (27) and (30) gives an analytical expression of the shear strain rate, which yields a time dependent strain of the form

\[ \varepsilon = a_1 t + a_2 (1 - \exp(-a_3 t)) \]  

(31)

The first term in equation (31) represents the steady-state creep strain and the second term is the transient creep strain. This model could describe transient creep in constant stress creep tests at high temperature when dislocation climb is the rate-controlling mechanism.

**Models for dislocation cross-slip**

Dislocation cross-slip could occur at a high stress level. Since cross-slip refers to the movement from a slip plane to another one, it is feasible to study cross-slip by considering a discrete dislocation configuration. For example, Wang et al. (2007, 2008) employed a parametric dislocation dynamic method to study the role of cross-slip. The dislocation loops are modeled as discrete curved segments. Along dislocation loops, the equilibrium is given by
\[
\oint_c (f(t) - Bv(t) - ma(t)) d\Gamma = 0
\]  

(32)

where \( f \) is the total force acting on the dislocation, \( v \) is dislocation velocity, \( B \) is the dislocation drag coefficient, \( m \) is the effective mass for a moving dislocation and \( a \) is the acceleration. For each dislocation loop, the probability of a cross-slip event in the discrete time step \( \delta t \) is defined as:

\[
P \left\{ \begin{array}{ll}
\frac{L}{L_0} \frac{\delta t}{\delta t_0} \exp \left[ - \frac{V(\tau_0 - \tau_{cs})}{kT} \right] , & \tau_{cs} < \tau_0 \\
1 , & \tau_{cs} > \tau_0
\end{array} \right.
\]

(33)

At each time step, probabilities for cross-slip of all screw segments are calculated and each probability is compared with a different randomly generated number between 0 and 1. If this probability is larger than the random number, cross-slip is activated for this dislocation loop. Otherwise, cross-slip is disregarded.

This model is feasible to study the effect of cross-slip and can be applied to explain the slip band formation in high rate deformation of single f.c.c. crystals (Wang et al. 2007, 2008). However, because dislocations are considered as discrete, it makes numerical computation very expensive, especially in the late stage when the number of cross-slip events accumulates with increasing deformation. In addition, it is much more complex in polycrystalline materials where the direction of cross-slip may be different among grains and in cases that are coupled with other mechanisms like dislocation climb.

Another approach to model cross-slip is employing empirical potentials. For example, Lu et al. (2004) proposed a semi-discrete variational Peierls-Nabarro model (SVPN). Consider a screw dislocation sited at the intersection of the primary (plane \( \text{I} \)) and cross-slip plane (plane \( \text{II} \)) as shown in figure 17. The screw dislocation can glide in \( X \) direction at plane \( \text{I} \) and in \( X' \) direction at plane \( \text{II} \). Both planes are discretized as many nodal points. The corresponding dislocation densities of plane \( \text{I} \) \( \rho^I(x) \) and plane \( \text{II} \) \( \rho^{\text{II}}(x') \) with respect to nodal distances from the intersection are also shown in figure 17.

Figure 17 a schematic of dislocation cross-slip (Lu et al. 2004). A screw dislocation sited at the intersection of two planes (left); the corresponding dislocation densities (right)
The total potential energy of the dislocation $U_{\text{tot}}$ contains three parts: the energy associated with the dislocation spreading on plane $I$ ($U_I$), the energy when the dislocation glides on plane $II$ ($U_{II}$) and the elastic interaction energy between dislocation densities on planes $I$ and $II$ ($\tilde{U}$).

$$U_{\text{tot}} = U_I + U_{II} + \tilde{U}$$

(34)

The expressions of these energies are given by

$$
\begin{align*}
U_n &= \sum_{i,j} \frac{1}{2} \chi_{ij} \left[ K_e \left[ \rho^e(i) \rho^e(j) + \rho^n(i) \rho^n(j) \right] + K_s \rho^n(i) \rho^n(j) \right] \\
&+ \Delta \chi \gamma_5 \left( f^e(i), f^n(i), f^n(i) \right) - \sum_{i,j} \frac{\chi^n(i) - \chi^n(i-1)^2}{2} \rho^n(i) \chi^n_i \\
&+ K b^2 \ln L, \quad n = I, II \\
\tilde{U} &= -\sum_{i,j} K_e \rho^e(i) \rho^e(j) A_{ij} - \sum_{i,j} K_s \left[ \rho^n(i) \rho^n(j) + \rho^l(i) \rho^l(j) \right] A_{ij} \\
&- \sum_{i,j} K_s \left[ \rho^l(i) \rho^l(j) B_{ij} + \rho^l(i) \rho^l(j) C_{ij} - \rho^l(i) \rho^l(j) D_{ij} - \rho^l(i) \rho^l(j) D_{ij} \right]
\end{align*}
$$

(35)

Here, $f_{e}^{I}\left(i\right)$, $f_{n}^{I}\left(i\right)$ and $f_{s}^{I}\left(i\right)$ represent the edge, vertical and screw component of the general dislocation misfit vector at $i$-th nodal point in plane $I$ ($II$); $x^{I}\left(i\right)$ is the coordinate of $i$-th nodal point along $X(X')$ direction. The corresponding component of dislocation density is defined as

$$
\rho^n_m(i) = \frac{f^n_m(i) - f^n_m(i-1)}{x^n(i) - x^n(i-1)}, m = 1, 2, 3; n = I, II
$$

(36)

The projected dislocation density $\rho^p(i)$ is the projection of the density $\rho^n(i)$ from plane $II$ onto plane $I$. $\tau_i^{I}\left(i\right)$ is the external stress component. Other coefficients are the weighing factors and can be found in Lu et al. 2004. The model starts by inputting an initial configuration $f^I$ and the external stress. The equilibrium configuration is determined from the minimum of the total energy with respect to dislocation densities. When cross-slip occurs, dislocation density will decrease in plane $I$ and it will increase in plane $II$. Therefore, the peak of dislocation density in plane $II$ shows the occurrence of cross-slip. The disadvantage of this model is that it cannot show the dynamic process of cross-slip.

**Models for precipitate-strengthening alloys**

Due to the difference of the microstructure, models for precipitate-strengthening alloys mainly focus on the interaction between particles and dislocations. It is still feasible to adjust the expression of the power law so that the strain rate is associated with not only the applied stress but also the particle size. For example, based on the power law, Dutta (2003) studied creep with coarsening particles and assumed that the rate-controlling process is climbing over the second-phase particles. The strain rate may be expressed as
\[ \dot{\varepsilon} = A \left( \frac{G b}{k_B T} \right) \left( \frac{\lambda^2}{d_p} \right) \left( \frac{\sigma b}{G} \right)^\alpha D_{eff} \]  
(37)

where \( \dot{\varepsilon} \) is the quasi steady-state creep rate, \( \lambda \) is the interparticle spacing, \( d_p \) is the particle size and \( D_{eff} \) is the effective self-diffusivity. In order to make equation (37) applicable over a larger range of stresses, it could be rewritten as

\[ \dot{\varepsilon} = A \left( \frac{G b}{k_B T} \right) \left( \frac{\lambda^2}{d_p} \right) \sinh \left( \frac{\alpha \sigma b}{G} \right)^\alpha D_{eff} \]  
(38)

By assuming that the microstructure contains a uniform distribution of particles for a fixed-volume fraction, the parameter \( \lambda^2 / d_p \) is dependent on the particle radius \( r \)

\[ \frac{\lambda^2}{d_p} = A_2 r \]  
(39)

where \( A_2 \) is depended on the geometry and the alloy-phase constitution. By substituting equation (39) into (38),

\[ \dot{\varepsilon} = A \left( \frac{G b}{k_B T} \right) r \sinh \left( \frac{\alpha \sigma b}{G} \right)^\alpha D_{eff} \]  
(40)

During the deformation, coarsening of particles occurs, that is, the radius of the particle is variable with time. The evolution follows from

\[ 3r^2 \frac{dr}{dt} = B \gamma V_m C_0 D_{sol} \exp \left( \frac{\sigma N \Omega}{k_B T} \right) \left[ 1 + N \dot{\varepsilon} (1 - e^{-\tau r_r}) \right] \]  
(41)

Equation (40) and (41) describe the dynamic second-phase particle coarsening during creep of alloys with a microstructure of finely dispersed intermetallics in a soft matrix.

Relations like equation (15) and (25) can also be adjusted. For example, Marquis and Dunand (2002) proposed a model, in which dislocation climb is the rate-controlling mechanism, for creep of precipitation-strengthened alloys with coherent particles (Marquis and Dunand, 2002). This model well reproduced the general shape of stress-strain rate curves of creep tests of Al-0.3wt.%Sc alloys at 573 K. In this model, for simplicity, particles are assumed as cylinders with diameter and height both equal to \( 2r \) as shown in figure 18. The segment AB is placed at a point where the glide forces due to modulus mismatch \( F_g^m \) and lattice mismatch \( F_g^l \) are balanced by the applied force.

\[ \tau b \frac{\lambda}{2} + F_g^m + F_g^l = 0 \]  
(42)
The sources of the glide force and the climb force are: (a) the elastic interaction due to the modulus mismatch effect

\[
[F_g^\mu, F_c^\mu] = -r \left[ \frac{\partial E}{\partial y}, \frac{\partial E}{\partial z} \right]
\]

where \( E \) is the interaction energy for a unit length of dislocation and it is derived based on the assumption of an infinitely long cylindrical particle interacting with a straight edge dislocation (Marquis and Dunand, 2002); (b) the elastic interaction from the constrained lattice parameter mismatch \( \varepsilon \) between the coherent particle and the matrix

\[
[F_g^\varepsilon, F_c^\varepsilon] = \frac{Gb\varepsilon r^4}{(y^2 + z_0^2)^{5/2}} [3yz_0, -2y^2 + z_0^2]
\]

Figure 18 the geometry of the climb model, showing an edge dislocation with segment CD in the glide plane and segment AC climbing over a cylinder particle (Marquis and Dunand, 2002)

Then, the chemical potential at the particle interface corresponding to the driving force for adding vacancies to the dislocation segment is written as

\[
\mu_{ABD} = \mu_{AB} = \left[ \frac{Gb^2}{2} \left( \frac{\delta l}{\delta y} \right)_{BD} - (F_g^\mu + F_g^\varepsilon) - (F_c^\mu + F_c^\varepsilon) \right] \left[ \frac{1}{a_v} \frac{dA_{AB}}{dy} \right]
\]

where \( dA_{AB} \) is the change in area below dislocation line AB. It can simulate diffusion flow during climb in order to obtain the dislocation climb bypassing time

\[
t_c = \int \left[ \frac{\pi D_r r}{k_B T} \left[ \mu_{ABD}(x_0, z_0) \right] \right]^{-1} dy
\]

where \( D_r \) is the self-diffusion coefficient. The glide time between particles is assumed negligible as compared to the climb time \( t_c \). Thus, the strain rate of creep is given by

\[
\dot{\varepsilon} = \rho b \frac{1}{1 - \tau / \tau_{cr}} \frac{\dot{\lambda}}{t_c}
\]
A correction factor \((1 - \frac{\tau}{\tau_{Or}^*})^{-1}\) is required to account for the fact that some particles are bypassed instantaneously by the Orowan looping mechanism (Marquis and Dunand, 2002). The effective Orowan stress is obtained as follows: calculate the dislocation velocity \(\lambda / \tau\) as a function of the normalized applied stress \(\tau / \tau_{Or}^*\) for different glide plane heights; then obtain a new curve by taking an average on the stress at constant velocity over several heights; from this new curve, the average distance between repulsive obstacles could be obtained as \(2\lambda\). The Orowan stress is given by

\[
\tau_{Or}^* = \frac{Gb}{2\lambda}
\]  

(48)

In precipitate-strengthening alloys, dislocations could also bypass the particle by thermal detachment process. The detachment stress is given as

\[
\sigma_d = \sqrt{1 - k^2} \sigma_o
\]  

(49)

where \(\sigma_o\) is the Orowan stress and \(k\) is a parameter describing the relaxation of the dislocation strain field near the particle-matrix interface; such a relaxation results in a desired attractive interaction (Arzt et al. 2001). In addition, the following rate equation for detachment-controlled creep is derived:

\[
\dot{\varepsilon} = \dot{\varepsilon}_0 \exp \left[ \frac{Gb^2 r}{k_o T} (1 - k)^{3/2} \left(1 - \frac{\sigma}{\sigma_d}\right)^{3/2} \right]
\]  

(50)

where \(r\) is the particle radius and \(\dot{\varepsilon}_0\) is a reference strain rate containing diffusivity, dislocation density and the particle spacing. Equation (50) has been proved successfully in several dispersion-strengthened alloys, whereas less applicable for polycrystalline materials that show complicating features (Arzt et al. 2001). The most difficult problem in equation (50) is to determine the parameter \(k\). Rosler et al. (1992) once proposed a method that attempts to find an approximation solution of equation (50) to determine this parameter \(k\). However, it is too empirical. Therefore, a theoretical approach to determine \(k\) remains to be studied.

The effect of dislocation pile-up in Yoshida and Sakuma’s model (1998) was attributed to elastic stress generated by dislocation. For alloys with particles, dislocations can also pile-up in the interface between particles and matrix. Models related to dislocation pile-up should consider the stress from these dislocations near the interface. For example, in Dunand and Jansen’s model (1997), a single pile-up of dislocations forms at dispersoids when the number of mobile matrix dislocations of length per dispersoid is larger than unity. The ratio of the number of dislocations and the number of dispersoids per unit volume is expressed by

\[
N = (1 - f) \rho L^2
\]  

(51)
where $f$ is the volume fraction of the dispersoids, $\rho$ is the density of mobile dislocation and it could be expressed as $\rho = \left( \frac{\sigma}{\alpha G b} \right)^2$ with $\sigma$ is the applied stress and $\alpha$ is a constant factor, $L$ is the center to center spacing of spherical dispersoids arranged on a cubic lattice:

$$L = d \left( \frac{\pi}{6f} \right)^{1/3}$$

(52)

where $d$ is the diameter of dispersoids.

Then, positions of dislocations of a single pile-up are required. In the beginning, only 2D case is considered and positions of these dislocations are denoted as $(x_i, y_i)$. As shown in figure 19, a repeating unit cell with $(N+1)$ parallel, coplanar edge dislocations arranges in a pile-up. It consist of $(N-1)$ mobile dislocations bound by two immobile dislocation at $x_0 = 0$ and $x_N = L$. Under the influence of the applied shear stress $\tau_a$, the equilibrium positions $x_i (i = 1, \cdots, N-1)$ of the $(N-1)$ mobile dislocations are given by the force equilibrium condition:

$$\sum_{j=0}^{N} \tau(x_i - x_j; 0) - \tau_a = 0$$

(53)

where the shear stress $\tau(x, y)$ at point $(x, y)$ owing to the stress field of an edge dislocation at the origin is

$$\tau(x, y) = \frac{Gb}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$

(54)

Solving the system of $(N-1)$ non-linear equations leads to the equilibrium positions of these dislocations in an isolated pile-up. A simple approximate solution for this problem is also applied in Dunand and Jansen, 1997.

![Figure 19 2D view of pile-up configuration (Dunand and Jansen, 1997)](image)

Once the x-coordinates are obtained, their height are determined by
In this model, thermal detachment from dispersoids is taken as the rate-controlling mechanism for creep. If the detachment occurs at the origin, dislocation pile-up from \( x_{(N-1)} \) to \( x_1 \) exerts the stress:

\[
\tau_b = \sum_{i=1}^{N-1} \tau(L-x_i, y_i) \quad (56)
\]

By symmetry, dislocation pile-up from \( x_{(N-1)} \) to \( x_1 \) exerts the stress

\[
\tau_f = \sum_{i=1}^{N-1} \tau(-x_i, y_i) \quad (57)
\]

Along the z-axis, dislocation line is separated into two regions as shown in figure 20. The dispersoid region with a line length fraction \( 1 - (L-d)/(PL) \), with \( P \) the number of dispersoids; the interdispersoid region with a line length fraction \( (L-d)/(PL) \). The net pile-up back stress should be

\[
\tau_p = \frac{L-d}{PL} (\tau_b^p + \tau_f^p) + \left(1 - \frac{L-d}{PL}\right) (\tau_b^p + \tau_f^p) \quad (58)
\]

The threshold stress contains the back stress from dislocation pile-up. It should be noted that it is assumed that dispersoids do not affect the elastic stress field of dislocations and the number of dislocations in the grain boundary is much smaller than the one of dislocations near dispersoids.

There are other approaches to model precipitate-strengthening alloys. For example, it is possible to simulate the dynamics of isolated dislocation lines and loops. Chen et al. (2010) proposed such a model: a dislocation is represented by the intersection of two curved surface functions, \( \phi(\vec{r}, t) \) and \( \psi(\vec{r}, t) \).
\[
\begin{align*}
\phi(\vec{r}, t) &= 0 \\
\psi(\vec{r}, t) &= 0 
\end{align*}
\] (59)

The motion of a dislocation could be described by the time evolution of curved surfaces

\[
\begin{align*}
\phi_t + \vec{v} \cdot \nabla \phi &= 0 \\
\psi_t + \vec{v} \cdot \nabla \psi &= 0 
\end{align*}
\] (60)

The dislocation velocities \( \vec{v} \) are linearly proportional to the local force on the dislocation line.

\[
\vec{v} = M \cdot \vec{f}
\] (61)

where \( M \) is the mobility tensor and \( \vec{f} \) is the Peach-Koehler force on the dislocation. The mobility tensor for a pure edge dislocation contains the glide and climb components

\[
M = \begin{cases} 
m_x (I - \vec{n} \otimes \vec{n}) + m_y \vec{n} \otimes \vec{n}, \text{nonscrew} \\
m_z I, \text{screw} \end{cases}
\] (62)

In this equation, \( I \) is the unit tensor and \( \vec{n} \) is the slip plane normal vector. The Peach-Koehler force per unit length is given by

\[
\vec{f} = (\sigma + \sigma_y + \sigma_m) \cdot (\vec{b} \times \vec{\psi})
\] (63)

with \( \sigma \) and \( \sigma_y \) denote the applied stress and the self-stress. The stress due to the misfit particles

\[
\sigma_m = \frac{2G\varepsilon R^3}{r^5} (r^2 I - 3\vec{r} \otimes \vec{r}) \Theta(r - R) - 4G\varepsilon I \Theta(R - r)
\] (64)

where \( r \) denotes the distance from the point to the particle center, \( \varepsilon = \varepsilon_0 \frac{1 + \nu}{3(1 - \nu)} \) and \( \Theta \) is a step function with \( \Theta(x) = 1, x > 0 \) and \( \Theta(x) = 0, x \leq 0 \). This model is suitable for the study of mechanisms in creep, whereas it is difficult to implement in the engineering field since the simulation of large quantities of dislocations is very expensive.

**Summary**

The power law is very flexible and it can be coupled with various mechanisms like grain boundary sliding, dislocation glide, climb and the effects of precipitates. A direct employment is to choose the approximate parameters to fit the experiment data. In creep models, it is feasible to change the expressions of the threshold stress and the activation energy by adding some internal variables like dislocation density and the internal stress so that the model has a stronger physical meaning. For example, in Arzt’s model (1998), the activation energy is related to the thermal detachment stress so that it can simulate thermal detachment process. Another example is Dutta’s model (2003) that adds the particle diameter into the expression of the power law. Since internal variables do not appear explicitly in the power law, it is an indirect method to build up the relation between the
microstructure (internal variables) and the macroscopic behavior (the strain rate). It is also possible to build up a direct relation between the strain rate and the internal variables in creep models. This approach directly relates the microstructure and macroscopic deformation such as Blum’s model (2002) and Marquis’s model (2002). However, this method is not appropriate in complex cases, in which two or more mechanisms are active.

Moreover, the force due to dislocation pile-up is calculated as the integration of elastic stress of dislocations pile-up. In calculation, number of dislocations or dislocation density is required. Cross-slip seems to make the modeling more complex: using discrete dislocation dynamic to simulate cross-slip requires much computation time; the problem of the method on the minimum potential energy is the difficulty in calculating the total energy when multi-slip planes are active or in polycrystalline materials.

Atomistic simulations can also be used to model dislocation motion. However, this method is more feasible in studying mechanisms in nanocrystalline materials. It is very expensive to apply in engineering field.
Chapter 4 Conclusion

In order to understand mechanisms responsible for anelastic recovery of Al-Cu thin films in RF-MEMS, this report firstly reviewed creep behavior of crystalline materials (mainly f.c.c. alloys) and mechanisms including grain boundary sliding, dislocation glide, climb, cross-slip and the effects of precipitates. Then, the relations with the mechanisms and the anelastic recovery are discussed. In the second part, some creep models based on these mechanisms are involved for reference. The conclusions are as follows:

In crystalline materials with average grain sizes of several micrometers, despite that grain boundary is important in diffusion creep, it seems not to control the anelastic recovery. Grain boundary takes an effect by retarding dislocation motion.

In dislocation creep, dislocation glide is likely to be the rate-controlling mechanism in solid solution alloys due to solute drag and in precipitate-strengthened alloys where the Orowan stress for strong precipitates or the Friedel stress for weak precipitates encumber gliding. This is a possible rate-controlling mechanism for room-temperature anelastic recovery, in which the driving force may be unbowing of bowed dislocations and dislocation pile-up. At high temperature, when diffusion of atoms and vacancies is active, dislocation climb probably determines the creep rate. Meanwhile, dislocations can also bypass particles by cross-slip which will occur more easily if internal stress increases, and thermal detachment that appears to be strong for small particle size.

For modeling creep behavior, the power law is very flexible and it is feasible to change expressions of the threshold stress and the activation energy by adding some internal variables like dislocation density and internal stress for the purpose of a stronger physical meaning. Besides, building up a direct relation between the strain rate and internal variables is also a good choice. It is also possible to combine two approaches to simulate complex cases where two or more mechanisms are active.

Based on the above discussion, in order to model the room-temperature anelastic recovery of Al-Cu thin film in RF-MEMS, it should firstly consider dislocation glide hindered by the Orowan stress and the Friedel stress due to precipitates. A feasible approach is to add these stresses into the threshold stress in the power law. Since the recovery occurs at room temperature, dislocation climb, cross-slip and thermal detachment may be inactive and this hypothesis still requires experiments to prove. If these mechanisms are active or cannot be neglected, it is possible to add the energy barriers of climb and cross-slip into the activation energy in the power law. Besides, building a direct relation between the strain rate and the climb frequency can also be operable.
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