Stress relaxation in thin films due to grain boundary diffusion and dislocation glide
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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2010

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):

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Chapter 4

Stress relaxation in thin film/substrate systems by grain boundary diffusion: a discrete dislocation framework

The relaxation of stress in a thin film due to grain boundary diffusion is investigated in terms of a new discrete dislocation framework. Discrete dislocations along grain boundaries (GBs) are nucleated from the free surface and are then driven to ‘climb’ by the Peach-Koehler force, with a mobility that is determined by the grain boundary diffusivity. Application to a planar film/substrate problem with (sub-) micron scale columnar grains shows that the amount of relaxation is dependent on the initial stress and on the grain aspect ratio. For thin columnar grains the relaxation is faster and more effective and the opening displacements along the GB are more uniform, an effect that is not captured by current continuum models. When the initial stress is low and the grain size is small, it is necessary to account for variations in the threshold stress for diffusion among different GBs to achieve realistic results.

Based on Stress relaxation in thin film/substrate systems by grain boundary diffusion: a discrete dislocation framework, Can Ayas and E. van der Giessen, Modelling and Simulation in Materials Science and Engineering, 17, 6, 064007 (2009).
4. Stress relaxation in thin film/substrate systems by grain boundary diffusion

4.1 Introduction

Metallic thin films with thicknesses in the (sub)micrometer range are widely used in MEMS and electronic device technology. The mechanical reliability of these devices is intimately related with size effects in the material properties, especially those governing stress relaxation. In thin film/substrate systems, there are different causes of stress depending on material and on environmental conditions, and they can be found during manufacturing and/or while in service. For example, thermal stresses appear due to the thermal expansion mismatch between film and substrate material as the system undergoes thermal cycling. Intrinsic stress is another type of stress, and is due to the non-equilibrium nature of deposition processes during film growth. Both magnitude and sign of the intrinsic stress depend upon the deposition procedure and the materials involved [3, 5].

Plasticity is a key mechanism for stress relaxation in general. Traditionally it is associated with dislocation glide inside crystallites, but at (sub)micron length scales it is not the only stress relaxation mechanism available. It has been reported in the literature that diffusion of atoms from the surface into the GBs can also act to relax the stress in thin films. Weiss et al. [13], for example, argued by comparing mechanical behavior of capped and uncapped Cu thin films that the relatively low yield point in uncapped films at high temperatures is due to the operation of diffusional creep [5] together with dislocation glide.

In this chapter we study this kind of diffusion along GBs in an initially stressed thin film attached to a stiff substrate. Diffusion is represented through the ‘climb’ motion of discrete GB dislocations in a two-dimensional plane strain situation. Dislocations relax the initial stress by means of material transport from the surface into the boundaries. These dislocations have a Burgers vector that is normal to the plane of GB, thus creating a rotational distortion along the GB plane. For example, in the form of an infinite wall, GB dislocations represent the crystallographic misorientation between neighbouring grains and the boundary has the shape of a linear wedge. However, different dislocation configurations and Burgers vector distributions may result in different GB geometries [11] (see Chapter 3).

In our discrete dislocation model, GB dislocations get nucleated from the surface and move towards to the substrate according to the Peach-Koehler force that arises from a chemical potential gradient along the boundary, while their mobility depends on the diffusion coefficient. The governing equations are presented in some detail in the following section. Subsequently, we use this approach to study the effect of grain size on stress relaxation, with particular emphasis on the final (residual) stress state.

1’GB shape’ denotes the geometry of the extra half planes that have been incorporated into the film due to diffusion.
4.2. Discrete Dislocation Formulation for Diffusion

Gao et al. [5] modelled similar problem by utilizing continuum description of dislocations, but here we develop a method based on discrete dislocations. The approach can be regarded as a discretization of a continuum description, but is at the same time motivated by an atomistic view of diffusion. More specifically, the molecular dynamics study in [2] has revealed snapshots of the GB diffusion process which clearly illustrate that the material diffused into the GB takes the form of distinct extra half planes extending to the surface. This provides definite physical foundation to describing GB diffusion by ‘climb’ of discrete edge dislocations.

In Chapter 3[11] we have investigated size effects in the relaxation of intrinsic stress by dislocation glide. The initially present intrinsic stress was assumed to have resulted from diffusion during film growth and was described by a stack of dislocations along GBs with a characteristic Burgers vector distribution. As a continuation of this, we here study the preceding process, namely the GB diffusion phenomena. The way we have chosen to model the diffusion process is borne out of convenience. The simulation of GB diffusion by dislocation dynamics is similar to that of plasticity by glide dislocations (used, e.g., in [12], [1], [10]). The present framework enables a seamless (future) coupling of GB diffusion and dislocation glide plasticity.

Hartmaier et al. [8, 7] have developed a two-dimensional discrete dislocation model to study the effect of film thickness on coupled dislocation glide and GB diffusion, in which the drag coefficient for climb of is taken to be controlled by a drag coefficient that is 100 times higher than that for glide. In contrast, our analysis is based on the solution of diffusion equation and thus the velocity of GB dislocations are directly tied to GB diffusion coefficient. In fact in Chapter 7[7] we will briefly demonstrate that the time scales of the two mechanisms are much more decoupled than assumed in [8, 7].

4.2 Discrete Dislocation Formulation for Diffusion

For an edge dislocation, glide is the motion confined to the slip plane parallel to its Burgers vector \( \mathbf{b} \); the motion perpendicular to \( \mathbf{b} \) is called climb. The motion of an edge dislocation to represent diffusion along a GB is, by definition, along the GB and hence always perpendicular to the Burgers vector; henceforth we adopt the word ‘climb’ when we refer to the motion of a GB dislocation.

In order to find the governing equations for climb of the discrete GB dislocations, we follow the original idea by Needleman and Rice [9] to consider the energy dissipation during diffusion.

The schematic in figure 4.1(a) illustrates the continuum picture of the problem where the GB is represented by a displacement discontinuity \( \Delta_i = u_i(\Gamma^+) - u_i(\Gamma^-) \) along the
plane $\Gamma$, where $u_i$ is the displacement field. We will require that the dissipation rate according to this description be equal to that in a formulation based on the climb motion of discrete dislocations, as illustrated in figure 4.1(b).

![Figure 4.1](image_url)

**Figure 4.1:** Two energetically equivalent systems; diffusion is described by the opening $\Delta$ along the GB (a) or diffusion is defined by ‘climb’ motion of dislocations (b).

In the continuum picture the interface separation $\Delta_i$ represents material diffused from the surface in the presence of tractions $T_i$ along $\Gamma$. The dissipation rate during virtual changes (indicated by a superposed $*$) of the separation rate $\dot{\Delta}_i$ is

$$\Theta^* = \int_{\Gamma} T_i \dot{\Delta}_i^* dS$$  \hspace{1cm} (4.1)$$

In a planar situation where all variables of interest are independent of the out-of-plane direction in figure 4.1 the virtual energy dissipation rate per unit depth, $\Pi^*$, becomes

$$\Pi^* = \int_0^h T_i \dot{\Delta}_i^* dx_2$$ \hspace{1cm} (4.2)$$

where $h$ is the length of the GB. Diffusion will cause the GB interface to open in the direction of the GB unit normal $n$, i.e. $\Delta_n = \dot{\Delta}_i n_i = \dot{\Delta}_1$. Since the governing traction component is the normal stress $\sigma_n = n_i \sigma_{ij} n_j = \sigma_{11}$, the dissipation rate can be written as

$$\Pi^* = \int_0^h \sigma_{11} \dot{\Delta}_1^* dx_2 = \int_0^h \sigma_n \dot{\Delta}_n^* dx_2.$$ \hspace{1cm} (4.3)$$

Following [9], we now take conservation of mass into account, written as

$$\dot{\Delta}_n = - \frac{\partial j_i}{\partial x_i}$$ \hspace{1cm} (4.4)$$
4.2. Discrete Dislocation Formulation for Diffusion

in terms of the volumetric flux per unit depth, \( j_i \). Substitution of equation (4.4) into equation (4.3) and integration by parts yields

\[
\Pi^* \left( x_2 \right) = \int_0^h \left[ -\sigma_n \frac{\partial j_i^*}{\partial x_i} \right] \, dx_2 \quad \text{(4.5)}
\]

Fick’s law assigns a linear relation between flux and stress gradient,

\[
j_i = \mathcal{D} \frac{\partial \sigma_n}{\partial x_i} \quad \text{(4.6)}
\]

where \( \mathcal{D} \) can be further expressed as

\[
\mathcal{D} = \frac{D \Omega \delta}{kT} \quad \text{(4.7)}
\]

in terms of the diffusion coefficient \( D \), the thickness of the diffusion layer \( \delta \), Boltzmann’s constant \( k \), temperature \( T \) and the volume of an atom, \( \Omega \). Upon inserting equation (4.6), identifying the non-vanishing component of the flux to be \( j_2 \), and incorporating the zero-flux boundary condition at the film–substrate interface, \( j_2(0) = 0 \), we find that the expression (4.5) for the virtual dissipation rate becomes

\[
\Pi^* = -\sigma_n(h) j_2(h)^* + \frac{1}{\mathcal{D}} \int_0^h j_2^* j_2^* \, dx_2 . \quad \text{(4.8)}
\]

The second boundary condition is flux continuity at the free surface, i.e. the flux at the top of the GB be equal to the flux of atoms migrating from the surface into the GB: \( j_2(h) = j_{s/\text{gb}} \). The driving force for \( j_{s/\text{gb}} \) is the difference between the 11–stress at the top of the GB, \( \sigma_n(h) \) and on the free surface, \( \sigma_s \). The value of \( \sigma_s \) depends on the deposition parameters. If the film does not grow, as assumed for simplicity in this study, then \( \sigma_s = 0 \). In this case surface diffusion will go on as long as \( \sigma_n(h) > 0 \). In the presence of a deposition flux (growing film), \( \sigma_s < 0 \) due to surface atoms experiencing an extra push into the boundaries because of the supersaturation of adatoms \([6]\). In either case the mobility of semi-attached atoms on the surface is higher than that of GB atoms. Therefore material transport at the GB surface junction will limit the rate of entire process.

At this point we consider the diffusion process as represented by the climb motion of dislocations in the GB, see figure 4.11(b), with the aim to find the equivalent of equa-
tion (4.8) in terms of discrete dislocation quantities. In general, the energy that is dissipated during the motion of \( N \) dislocations is

\[
\Theta = - \sum_{I=1}^{N} \oint_{\mathcal{L}(I)} f_i^{(I)} v_i^{(I)} \, dl
\]  

(4.9)

where \( \mathcal{L}(I) \) denotes the dislocation loop, \( v_i^{(I)} \) the velocity and \( f_i^{(I)} \) the Peach-Koehler force on dislocation \( I \). In plane strain, GB dislocations are represented by dipoles of two edge dislocations with opposite signs. To represent diffusion, only the positive dislocation is free to move along the GB, i.e. \( v_i = v_cm_i \) where \( m \) is the in-plane unit tangent of the GB. Consequently, \( f_c \) is the climb component of the Peach-Koehler force, \( f_c = f_im_i \). Accordingly, in two dimensions, the dissipation rate per unit depth during virtual dislocation motions becomes

\[
\Pi^* = \sum_{I=1}^{N} - f_c^{(I)} v_c^{(I)\ast} .
\]  

(4.10)

This is the discrete dislocation equivalent of equation (4.2). In order to confront the right-hand sides of equations (4.8) and (4.10), we proceed with writing the flux in terms of the dislocation climb velocity. The GB opening profile is discretized by distributing edge dislocations along the boundary, whose Burgers vector \( b \) is normal to the GB, as in [11]. In case of a single edge dislocation moving along the GB, the non-vanishing component of the volumetric flux per unit thickness is \( j_2 = v_c b \), with \( v_c \) being the climb velocity of that dislocation. When multiple dislocations are moving on the GB, the flux at any point receives contributions from all the GB dislocation velocities that are moving below that point, i.e.

\[
j_2(x_2) = \sum_{I=1}^{M} v_c^{(I)} b^{(I)} \quad \forall \ I \in [1, M] \text{ for which } s^{(I)} \leq x_2
\]  

(4.11)

where \( s^{(I)} \) is the position of dislocation \( I \) measured along the GB from the film/substrate interface, see figure 4.1(b). The flux at the top of the GB where it meets the free surface, \( j_2(h) \), thus depends on the motion of all the dislocations on that particular GB. Finally, by substituting of equation (4.11) into the right-hand side of (4.8) and equating it to equation (4.10) we find the following equation governing GB diffusion in terms of discrete dislocations:

\[
\sum_{l=1}^{N} f_c^{(I)} v_c^{(I)\ast} = \sigma_s \sum_{I=1}^{N} v_c^{(I)\ast} b^{(I)} - \frac{1}{2} \int_0^h \left[ \left( \sum_{J=1}^{I} v_c^{(J)} b^{(J)} \right) \left( \sum_{K=1}^{I} v_c^{(K)\ast} b^{(K)} \right) \right] \, dx_2 .
\]  

(4.12)
4.3 Formulation of The Problem

In the spirit of the standard principle of virtual work and following [9], we require this equation to hold for all virtual dislocation velocities \( v_{c}^{(I)} \). After discretization of the integral and further simplification (details can be found in Appendix A) this yields a simple linear system of \( N \) equations for the \( N \) velocities \( v_{c}^{(I)} \) in terms of the instantaneous Peach-Koehler forces. The latter are determined by the stress fields of all dislocations and the boundary conditions for the particular problem at hand.

Although the formulation relies on the dissipation of energy a generalization can be done based on the free energy consideration given in Appendix B.

4.3 Formulation of The Problem

Here we consider the plane-strain problem of a thin film of infinite width that is perfectly bonded to a very thick elastic substrate, as illustrated in figure 4.2. The film has a thickness \( h \) and comprises columnar grains of width \( d \). The infinitely wide film is modelled by considering a periodic cell of width \( w \) in \( x_1 \) direction. Periodic boundary conditions at the cell edges ensure traction and displacement continuity, while the top surface is traction free.

![Figure 4.2: Illustration of the problem for two grain boundaries. The sources from which the dislocations are nucleated are indicated by open circles.](image)

The Peach-Koehler force on a dislocation in the simulation cell is calculated as

\[
f_{c}^{(I)} = n_{i}^{(I)} \left( \tilde{\sigma}_{ij}^{(I)} + \sum_{J \neq I} \tilde{\sigma}_{ij}^{(J)} \right) b_{j}^{(I)} = b \left( \tilde{\sigma}_{11}^{(I)} + \sum_{J \neq I} \tilde{\sigma}_{11}^{(J)} \right)
\]

(4.13)

where \( n_{i}^{(I)} \) is the unit normal to the GB on which the dislocation \( I \) with Burgers vector \( b_{j}^{(I)} \) resides. The \( \tilde{\sigma}_{ij}^{(I)} \) in equation (4.13) is the singular stress field of dislocation \( I \) and all
its periodic replicas in half–infinite space, as derived by Freund [4], while \( \sigma^{(f)}_{ij} \) represents its non-singular image field necessary to enforce a traction-free top surface (see also [11]). The derivation of the closed-form image stress fields is given in Appendix C. For the configuration shown in figure 4.2, the general definition in the first equality in equation (4.13) simplifies to that in the right-hand side.

At the start of the simulation, the film is in uniform tension while the substrate is under compression and the system is dislocation free. The interface with the substrate is considered to be impenetrable so that dislocations cannot penetrate into the substrate, which thus remains elastic. Dislocations will be nucleated from the sources that are shown in figure 4.2 according to the rule presented subsequently. These sources are situated at a distance \( h_{nuc} \) beneath the surface, which defines the strength of the source, in an indirect manner, as follows. The image force on a dislocation at the position of the source corresponds to a compressive stress. This stress needs to be overcome by the applied stress plus that of all other dislocations in order for a dislocation at that position to move downwards; it is this that becomes our nucleation criterion.

The simulation scheme is as follows: a test dislocation is nucleated from the source if \( \sigma_n \) at the source is tensile. For the current dislocation structure first the Peach-Koehler force on each dislocation is calculated from equation (4.13). After that, equation (4.12) is used to calculate the climb velocities of dislocations. If the test dislocation has a negative velocity (i.e., it moves towards the interface) it is kept, otherwise it is rejected. Subsequently, the dislocation positions are updated for the time step and the cycle is repeated. The time step is taken to be \( 10^{-5} \) s.

The film average stress \( \langle \sigma_{11} \rangle_f \) is calculated by numerically integrating the \( \sigma_{11} \) stress over the cell. A grid of quadrilaterals of 31.25nm x 16.67nm is utilized for this purpose.

4.4 Results & Discussion

We choose the elastic properties of film and substrate to be isotropic and specified by Young’s modulus \( E = 70 \text{GPa} \) and Poisson ratio \( \nu = 0.33 \). From an earlier study [10], we know that the influence of the elastic mismatch between film and substrate in real metal-silicon systems has a negligible effect on the Peach-Koehler forces on the dislocations. The length of the Burgers vector is taken to be \( b = 0.25 \text{nm} \), which is characteristic for FCC materials like Cu and Ag. Beside these properties, the model includes two material parameters specific for the present GB diffusion model: \( h_{nuc} \) which determines the source position and the diffusion parameter \( D \). We have adapted the diffusion coefficient from [6] as \( \delta D = 15 \times 10^2 \exp(-10013/T) \, \mu\text{m}^3/\text{s} \) and, from that, calculated the value of \( D \) for the temperature of the simulation which was chosen to be of 400K. As mentioned in the above, the value of \( h_{nuc} \) sets the source strength. For instance, for \( h_{nuc} = 24b \), the free
4.4. Results & Discussion

surface exerts a compressive stress of around 135MPa to a dislocation at the GB dislocation source which would prevent a dislocation to move in at tensile stresses below this value. In the first subsection, we consider this value of $h_{\text{nuc}}$ for all grain boundaries. Subsequently, we study the effect of variations in $h_{\text{nuc}}$ among neighbouring boundaries.

4.4.1 Constant Nucleation Distance

As long as the nucleation distance is constant a single grain is representative in terms of periodicity and therefore $w = d$ throughout this subsection. Figure 4.3 shows typical stress relaxation curves, in terms of the film average stress $\langle \sigma_{11} \rangle^f$ (normalized with the initial tensile stress $\sigma_0$). Three different levels of initial stress are considered: $\sigma_0 = 250\text{MPa}$, 375MPa and 500MPa (and we recall that the source strength according to the chosen $h_{\text{nuc}}$ value is roughly half of the lowest $\sigma_0$). The thickness of the film is constant, $h = 0.5 \mu\text{m}$, for all simulations while the grain size is varied from $d = h/2$ to $d = 8h$. The average tensile stress is seen to decrease during GB diffusion, until a steady state is attained and diffusion stops. For small grains, faster relaxation is observed owing to the fact that diffusion occurs on many boundaries (per unit area). Not only the relaxation rate but also the effectiveness of relaxation is size dependent: the residual stress after completion of diffusion decreases with decreasing grain size.

To gain a better understanding of the phenomena, we start out by investigating the dislocation distributions along the GBs. In figure 4.4 the steady-state distributions are shown after relaxation from $\sigma_0 = 500\text{MPa}$, together with the induced GB opening $\Delta(x_2)$. In order to quantify the shape of the GB opening profile, we introduce the following measure:

$$\xi = \frac{1}{\Delta(h)h} \int_0^h \Delta(x_2)dx_2. \quad (4.14)$$

A triangular opening corresponds to $\xi = \frac{1}{2}$, while the larger $\xi$, i.e. the closer to 1, the more uniform the GB opening is. As seen in figure 4.4 the GB opening profile for large grains is more V-shaped, with $\xi$ being significantly smaller than 1. When grains become columnar the opening becomes more U-shaped ($\xi$ increases), tending towards the opening profile of a single super dislocation at the root of the GB. This shape change is mainly due to the fact that the amount of diffused material per GB decreases as the grains become more columnar. The shift from a V to U–shape with decreasing $d$ is also observed for the other $\sigma_0$ values (as can be seen later in figure 4.5(a)). Moreover, for a fixed grain size, the GB opening becomes slightly more U–shaped with decreasing $\sigma_0$ (see figure 4.5(a)), for the same reason that less diffusion is necessary for relaxation from a lower $\sigma_0$. Finally in figure 4.4 the closed-form approximation of the continuum solution according to [5] is superimposed. Excellent agreement is found between the
4. Stress relaxation in thin film/substrate systems by grain boundary diffusion

Figure 4.3: Development of film average stress (normalized by the initial stress $\sigma_0$) with time for different grain sizes for a film with $h = 0.5 \, \mu m$. The dashed lines represent the closed-form approximation of the continuum solution from [5]. The shape parameter $\xi$ is defined in equation (4.14).

Figure 4.4: GB opening profiles for different grain sizes after full relaxation from an initial stress value of 500MPa. The dashed lines represent the closed-form approximation of the continuum solution from [5]. The shape parameter $\xi$ is defined in equation (4.14).
4.4. Results & Discussion

continuum and the present discrete dislocation solution for the case with \( d = 1 \, \mu m \). The agreement for the other cases is somewhat less.

In order to elaborate on the difference between two models further, the GB displacement profiles according to the continuum model for \( d = 1 \, \mu m \) and for \( d = 0.5 \, \mu m \) are illustrated once again in figure 4.6. Gao et al. \cite{5} reported that the GB shape can be approximated by the mode I crack face displacement

\[ \Delta(x_2) = \Delta(h) \sqrt{1 - \left(1 - \frac{x_2}{h}\right)^2}. \]  

(4.15)

From equation (4.14) this functional form corresponds to a universal GB shape parameter of \( \xi = 0.79 \). Recall that the perfect agreement with the discrete dislocation model was found in figure 4.4(b) for \( d = 1 \, \mu m \) for which \( \xi = 0.78 \). However, \( \xi \) is a function of \( d \) in the discrete framework, and so does the extent of the agreement between the two models as seen in figure 4.4.

This deviation stems from a fundamental difference between two models: in the discrete dislocation model the Burgers vector is finite whereas the continuum solution is based on a smeared-out distribution of a possibly infinitesimal Burgers vector. This distribution is governed by the Burgers vector density \( \rho_b(x_2) \) which dictates the opening along the GB as follows

\[ \Delta(x_2) = \int_0^{x_2} \rho_b(\eta) d\eta. \]  

(4.16)

The density \( \rho_b(x_2) \) can be calculated by simple differentiation of equation (4.15) with

Figure 4.5: GB shape parameter \( \xi \) for different \( d \) and \( \sigma_0 \) values (a). Dislocation density at the steady state for different grain sizes (b).
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Figure 4.6: Burgers vector density $\rho(x_2)$ (solid lines) and GB opening profiles (dashed lines) for $d = 1 \mu m$ and $d = 0.5 \mu m$ in the continuum framework [5].

respect to $x_2$, leading to

$$
\rho_b(x_2) = \Delta(h) \frac{1 - x_2/h}{h\sqrt{1 - (1 - x_2/h)^2}}
$$

(4.17)

which is also plotted in figure 4.6. On the contrary, when dislocations are discrete entities, $\rho_b(x_2)$ is represented by a series of delta peaks. However the same normalization described in equation (4.16) still holds.

Thus, the GB shape according to the continuum solution is virtually independent of the grain size, whereas the shape change is quite significant in the discrete dislocation prediction. It is not trivial, however, why the GB dislocation distribution and therefore the opening profile depends on the amount of diffused material because it is the outcome of the concurrent processes of stress relaxation and stress-driven diffusion. The key in this competition is the development of back stresses on the source as well as among dislocations. In the beginning of the process, dislocations migrate easily towards the interface, where the first one is blocked and creates a back stress on the source. As the density of dislocations increases towards the GB root, the back stress increases, thus inhibiting nucleation of new dislocations and their subsequent propagation to the film/substrate interface. Hence when the amount of diffused material increases, the GB shape will become more V-shaped due to the enhancement of the dislocation pile-up. Indeed figure 4.4 reveals that the pile-up for $d = 2 \mu m$ is highly densely packed while it is rather sparse for smaller $d$ values.
In addition to this, a more uniform stress distribution results inside smaller grains, see figure 4.7. Higher average stress levels persist in large grains due to the long-range stress field of edge dislocations. The $\sim 1/x_1$-decay of the compressive $11$–stress field of a single dislocation leaves a significant part of each grain where the initial tensile stress is not relaxed. In small grains, on the other hand, the dislocation fields overlap effectively to leave almost uniformly relaxed grains, as seen in figure 4.7c.

![Figure 4.7](image)

**Figure 4.7**: Distribution of $\sigma_{11}$ (and superimposed dislocation distribution) when the steady state has been reached for an initial stress of 500MPa; (a) $d = 2\, \mu m$, (b) $d = 1\, \mu m$, (c) $d = 0.25\, \mu m$.

Whereas the tensile $11$–stress is partially relaxed with formation of the diffusion wedge, a non-zero shear stress $\sigma_{12}$ develops out of the initial uniform tensile state prior to diffusion where this stress component vanishes. The distribution of $\sigma_{12}$ is given in figure 4.8 for different grain sizes. Its value is especially high near the film/substrate interface just beside the GBs for $d = 2\, \mu m$ (see figure 4.8(a)). This stress field can be responsible for the dislocation activity in horizontal slip planes as considered in [8, 7]. However the effectivity of this mechanism is bounded by the GB spacing since both the area of high shear stresses and the available slip distance shrink as the grain size decreases.

An overview of the grain size and stress dependence of relaxation is provided by figure 4.9. For large grains, i.e. small $h/d$, there is no effect of initial stress; this only
4. Stress relaxation in thin film/substrate systems by grain boundary diffusion

Figure 4.8: Distribution of $\sigma_{12}$ (and superimposed dislocation distribution) when the steady state has been reached for an initial stress of 500MPa; (a) $d = 2\,\mu m$, (b) $d = 1\,\mu m$, (c) $d = 0.25\,\mu m$. Occurs above $h/d > 0.5$. For the highest initial stress level, $\sigma_0 = 500\,\text{MPa}$, the smaller the grain size $d$, the more efficient relaxation is. When the initial stress is lower, $\sigma_0 = 375\,\text{MPa}$, there is a weaker dependence on $d$ in the range $h/d > 0.5$, while for $\sigma_0 = 250\,\text{MPa}$ we find a somewhat surprising increase in residual stress above $h/d = 1$.

For the interpretation of the curves given in figure 4.9 identifying a simple equation with few parameters for the relaxation is insightful. When GB diffusion inserts material along the GB corresponding to an average strain $\langle \varepsilon_{11} \rangle_f$, the average film stress becomes

$$\langle \sigma_{11} \rangle_f = \sigma_0 - \bar{E} \langle \varepsilon_{11} \rangle_f$$

where $\bar{E} = E/(1 - \nu^2)$ is the plane strain elastic modulus. When relating this induced strain to the GB opening caused by a distribution of dislocations with Burgers magnitude $b$, we find

$$\langle \sigma_{11} \rangle_f = \sigma_0 - \bar{E} \frac{1}{bd} \int_0^h \Delta(x_2) dx_2$$

$$= \sigma_0 - \bar{E} \xi \rho_{\text{disl}} bh$$ \hfill (4.18)

where $\rho_{\text{disl}}$ is the dislocation density. From the equation above, since the elastic constants and the Burgers vector are material constants, the residual stress level is seen to depend
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on $\xi$, $\rho_{\text{disl}}$, $h$ and $\sigma_0$. For the three values of $\sigma_0$ investigated, we can now explain the trends in figure 4.9 as follows.

Figure 4.5 shows the dependence of the shape parameter $\xi$ and the GB dislocation density on $h/d$. The opening is more U-shaped, i.e. $\xi$ closer to 1, for larger $h/d$, see figure 4.5(a), so that equation (4.18) predicts that the residual stress decreases with $h/d$ (at constant dislocation density). Indeed, this is what is found in figure 4.9 for $\sigma_0 = 500\text{MPa}$.

However, dislocation density is not independent of grain size, as seen in figure 4.5(b). For the case with $\sigma_0 = 500\text{MPa}$, $\rho_{\text{disl}}$ increases with $h/d$ when the grains are relatively large, simply due to the increase in the number of nucleation events (per unit film area). Yet, this levels off at higher $h/d$ when dislocation interaction effects tend to suppress nucleation. Apparently, the increase in $\xi$ overcompensates the decrease in $\rho_{\text{disl}}$ when then their product determines the efficiency of relaxation. The behavior under a somewhat lower initial stress, $\sigma_0 = 375\text{MPa}$, is similar, but now the critical value for $d$ where $\rho_{\text{disl}}$ levels off, shifts to $2 \mu m$. This is consistent with the observation in figure 4.9 that relaxation loses efficiency for small grain sizes.

For the smallest initial stress considered, $\sigma_0 = 250\text{MPa}$, there is even an increase in the average residual stress at the small $d$ end in figure 4.9. However this is an artifact of our model. When the initial stress is low (i.e. not significantly higher than the image stress at the source) and the grain size is rather small, the number of dislocations per GB

Figure 4.9: Steady-state film average stress normalized with the initial stress as a function of grain size (with $h = 0.5 \mu m$) for different values of $\sigma_0$. 

[Diagram showing the normalized steady-state film average stress as a function of grain size ($h/d$) for different values of $\sigma_0$.]
becomes very small. Under these circumstances, nucleation of a single dislocation becomes overwhelmingly important for the average residual stress, and hence relaxation becomes very sensitive to the value of $h_{nuc}$. The nucleation of one dislocation more per GB can strongly alter the amount of residual stress.

In order to demonstrate this sensitivity of relaxation to the number of dislocations and also some other features we consider two simple ideal relaxed GB configurations. In the first one, called the perfect–V case, the GB opening profile is assumed to be a linear wedge ($\xi = 0.5$) where the dislocations are equally spaced along the GB. This spacing is determined for each $\sigma_0$ and $h/d$ by computing the stress at the source for a successively increasing number of dislocations. A tensile stress at the source indicates that more dislocations could nucleate; once the source stress changes sign, the final relaxed stress is assumed to have been attained. The resulting film average stress is reported in figure 4.10(a). The other extreme is the perfect–U case, where all dislocations are merged into one super dislocation at the GB root, giving $\xi = 1$. The number of dislocations is determined by first computing the real-valued ‘number’ of dislocations, $n^*$, such that the stress state at the source be exactly zero. Then upper bound and lower bound film average stresses are calculated for a super-dislocation at the root which has a Burgers vector of $B = \text{int}[n^*]b$ and $B = \text{int}[n^*](b+1)$, respectively (the function $\text{int}[x]$ truncates the decimal part of $x$ and makes it integer). The lower and upper bound values are plotted as a function of $h/d$ in figure 4.10(b). Reality, as reported in figure 4.9, is somewhere in between the these two idealized cases. Although the amount of relaxation is significantly underestimated by the perfect–V case, figure 4.10(a), it does pick-up the steep drop in residual stress for large $d$. The reason is that the actual values of $\xi$ (see figure 4.5(a)) are not so different from 0.5 for large $d$. As the grain size decreases, $\xi$ approaches 1 similar to the perfect–U idealization. Indeed, although the relaxed stress is again too high, the dependence on $h/d$ above values of around 1 in figure 4.10(b), is qualitatively similar to the computed behavior in figure 4.9 at least for the higher initial stress levels. However, there is a relatively big difference between lower and upper bound for the lowest stress, $\sigma_0 = 250\text{MPa}$ in the range of small grain size. In that situation, apparently, the nucleation of one more dislocation has a big impact on relaxation. Due to the periodicity of the problem along $x_1$, a single nucleation event corresponds, in effect, to nucleation on many GBs per unit area. Although, at a certain stage during relaxation, the stress is relatively high it may not be not enough to overcome simultaneous nucleation on all closely spaced GBs. Careful analysis of the numerical simulations for figure 4.9 reveal that it is this feature that is responsible for the increase in residual stress with $h/d$ for $\sigma_0 = 250\text{MPa}$ (black curve).
4.4. Results & Discussion

Figure 4.10: Two simple idealizations for the GB shape and the respective average relaxed stress values, for perfect V–shape (a), for perfect U–shape (b) where two data sets for each $\sigma_0$ represents the upper and lower bound solutions.

4.4.2 Fluctuating Nucleation Distance

The sensitivity to the nucleation of a single dislocation in small grain films under low initial stress is intimately tied to the fact that all GBs were equal: dislocations nucleated on all GBs at the same moment. This synchronicity can be avoided by assuming that the nucleation distances $h_{\text{nuc}}$ on different GBs are not identical. Physically this is to be expected, in fact, since the atomic structure of different GBs will vary in a systematic manner as a function of misorientation across the GB, and also stochastically even for the same misorientation. To mimic this, we now modify the problem so that a periodic cell contains a number of grains with GB sources whose position on different GBs, $h_{\text{nuc}}^{(f)}$, fluctuates about a mean distance of $\bar{h}_{\text{nuc}}$, as illustrated in figure 4.11. The distribution of distances is chosen to be Gaussian with a mean value equal to that used previously, i.e. $\bar{h}_{\text{nuc}} = 24b$, and with a standard deviation of 20% of $\bar{h}_{\text{nuc}}$.

In this approach, we first need to determine the size $w$ of the periodic cell corresponding to a statistically meaningful sampling of source positions. A small number of grains in the cell will give rise to a large scatter in the relaxation results for different realizations with different random $h_{\text{nuc}}^{(f)}$ values. Therefore a convergence study has been carried out by changing the width $w$ of the periodic cell and monitoring the average steady-state residual stress for five realizations for each $w$. The results of this study for $\sigma_0 = 250\text{MPa}$ and $d = 0.25\ \mu\text{m}$ in figure 4.12 indicate that the mean value of the residual stress has converged for a cell width of $w = 8d$. For the other $d$ and $\sigma_0$ values used in this investigation, the scatter in the results will be less due to a weaker dependence on
Figure 4.11: Schematic of the fluctuation of dislocation source positions on different GBs about the mean value $h_{nuc}$.

Figure 4.12: Dependence of steady-state relaxed stress on width $w$ of the periodic cell when the nucleation distances follow a Gaussian distribution with mean value $h_{nuc} = 24b$ and a standard deviation of 20%. Each fulldiamond is the result of a single realization of source positions, while the black line passes through their mean. The error bars denotes the standard deviation from the average.

Thus, the results presented in figure 4.14 are the mean values of five realizations of a periodic cell containing eight grains. When we compare this figure with figure 4.9 for constant $h_{nuc}$ we see that the results for the highest initial stresses, $\sigma_0 = 375$MPa
4.5 Conclusions

We have studied the relaxation of stress in a thin film bonded to a substrate with a discrete dislocation model, in which the diffusive transport of material from the surface into the GB is represented by dislocation nucleation and ‘climb’. Our key findings are:

and $\sigma_0 = 500\text{MPa}$, are the same and that the unexpected increase for $\sigma_0 = 250\text{MPa}$ has disappeared. When the error bars are taken into account it can be concluded that also for $\sigma_0 = 250\text{MPa}$ relaxation reaches a plateau with decreasing grain size, just like for the higher initial stresses. The reason is that since the dislocation distributions along the various GBs are no longer identical, the effect of one extra nucleation event on a GB is averaged out. This is illustrated for two realizations in figure 4.13: it can be seen that the number dislocations on the various GBs and their positions vary in accordance to their respective $h_{\text{nuc}}$ values. The figure also reveals that slightly different GB distributions are capable of yielding varying steady state $\langle \sigma_{11} \rangle_f$ values when $h/d$ is small.

All computations reported so far were carried out for a constant film thickness of $h = 0.5 \mu\text{m}$, and $h/d$ was varied by considering different grain sizes. It bears emphasis however that the results do not depend only on the ratio $h/d$ since there are two other length scales in the problem — $b$ and $h_{\text{nuc}}$—, hence a total of three dimensionless size parameters. Yet, since the nucleation distance is kept constant, with $h_{\text{nuc}}/h \ll 1$ and the Burgers vector constant throughout the calculations, $h/d$ remains the governing parameter. For verification, figure 4.14 also shows results (dashed lines) where the grain size was kept constant at $d = 0.5 \mu\text{m}$ and the film thickness $h$ was varied. As expected there is no difference within the spread of the results.

Figure 4.13: Distribution of $\sigma_{11}$ (and superimposed dislocation distribution) in a $d = 0.25 \mu\text{m}$ film after relaxation from $\sigma_0 = 250\text{MPa}$ in case of fluctuating nucleation distances. Two different realizations are plotted in (a) and (b).
Figure 4.14: Steady-state film average stress as a function of $h/d$ predicted by the model with random nucleation distances with mean value $\bar{n}_{\text{nuc}} = 24b$. Each data point is the average over five realizations. Solid lines are for a film thickness of $h = 0.5 \mu m$ and varying grain size $d$ (as in figure 4.9 for a uniform distance), while the dashed are for a constant grain size $d = 0.5 \mu m$ and varying $h$.

- GB diffusion operates faster and is more effective when the grain aspect ratio $h/d$ is high (slender columnar grains). However this effect saturates at a critical aspect ratio, the value of which depends on the initial stress $\sigma_0$.
- The GB shape is rather uniform ($\xi \sim 1$) when the grains are slender, and becomes more V-like when the grains are wider. This GB shape dependence is absent in a continuum model [5], as it is owing to the finite Burgers vector.
- For slender columnar grains under low initial stress, a variation of the source strengths at different GBs about a mean value causes diffusion in different GBs to initiate at different stress levels. The amount of stress relaxation thus increases due to the presence of weak GBs.

The model presented is limited by the fact that diffusion is decoupled from dislocation glide. Coupling of these two within the same discrete dislocation framework is the focus of current research.
4.5. Conclusions

Appendix A

To convert equation (4.12) into the set of linear equations for dislocation velocities in equation (4.21) we start out by simplifying it to

\[
\sum_{I=1}^{N}\left(\sigma_{s} - \frac{f_c^{(I)}}{b^{(I)}}\right)v_c^{(I)}b^{(I)}(I) = \frac{1}{\Omega} \int_{0}^{h} \left[ \left( \sum_{J=1}^{I} v_c^{(J)}b^{(J)} \right) \left( \sum_{K=1}^{I} v_c^{(K)}b^{(K)} \right) \right] dx_2
\]

The next step is to introduce an approximation for the integral on the right-hand side on the basis of the value of the integrand at the dislocation positions, giving

\[
\sum_{I=1}^{N}\left(\sigma_{s} - \frac{f_c^{(I)}}{b^{(I)}}\right)v_c^{(I)}b^{(I)} \approx \frac{1}{\Omega} \sum_{I=1}^{N} \left( \sum_{J=1}^{I} v_c^{(J)}b^{(J)} \right) \left( \sum_{K=1}^{I} v_c^{(K)}b^{(K)} \right) \Delta s^{(I)}
\]

(4.19)

where \(\Delta s^{(I)}\) is the distance between the dislocations with index \(I\) and \(I + 1\). The right-hand side of equation (4.19) can be reorganized to write the multiplication of sums as consecutive ones which gives

\[
\sum_{I=1}^{N}\left(\sigma_{s} - \frac{f_c^{(I)}}{b^{(I)}}\right)v_c^{(I)}b^{(I)} = \frac{1}{\Omega} \sum_{I=1}^{N} \sum_{J=1}^{N} \sum_{K=1}^{J} v_c^{(I)}b^{(I)}v_c^{(K)}b^{(K)} \Delta s^{(J)}
\]

Requiring this virtual dissipation condition to hold for all virtual velocities, we find the following expression for the motion of dislocations:

\[
\sum_{I=1}^{N}\left(\sigma_{s} - \frac{f_c^{(I)}}{b^{(I)}}\right) = \frac{1}{\Omega} \sum_{I=1}^{N} \sum_{J=1}^{N} \sum_{K=1}^{J} v_c^{(K)}b^{(K)} \Delta s^{(J)}
\]

(4.20)

This can be written in matrix notation as

\[
\begin{bmatrix}
\sigma_{s} - \frac{f_c^{(1)}}{b^{(1)}} \\
\sigma_{s} - \frac{f_c^{(2)}}{b^{(2)}} \\
\vdots \\
\sigma_{s} - \frac{f_c^{(N)}}{b^{(N)}}
\end{bmatrix}
= \frac{1}{\Omega} \begin{bmatrix}
\sum_{M=1}^{N} \Delta s^{(M)} & \sum_{M=2}^{N} \Delta s^{(M)} & \ldots & \sum_{M=N}^{N} \Delta s^{(M)} \\
\sum_{M=2}^{N} \Delta s^{(M)} & \sum_{M=2}^{N} \Delta s^{(M)} & \ldots & \sum_{M=N}^{N} \Delta s^{(M)} \\
\vdots & \vdots & \ddots & \vdots \\
\sum_{M=N}^{N} \Delta s^{(M)} & \sum_{M=N}^{N} \Delta s^{(M)} & \ldots & \sum_{M=N}^{N} \Delta s^{(M)}
\end{bmatrix}
\begin{bmatrix}
v_c^{(1)}b^{(1)} \\
v_c^{(2)}b^{(2)} \\
\vdots \\
v_c^{(N)}b^{(N)}
\end{bmatrix}
\]

\[
\begin{bmatrix}
f^{(2)}_c - \frac{f^{(1)}_c}{b^{(1)}} \\
f^{(3)}_c - \frac{f^{(2)}_c}{b^{(2)}} \\
\vdots \\
f^{(N)}_c - \frac{f^{(N-1)}_c}{b^{(N-1)}}
\end{bmatrix}
= \frac{1}{\Omega} \begin{bmatrix}
\Delta s^{(1)} & 0 & \ldots & 0 \\
\Delta s^{(2)} & \Delta s^{(2)} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
\Delta s^{(N)} & \Delta s^{(N)} & \ldots & \Delta s^{(N)}
\end{bmatrix}
\begin{bmatrix}
v_c^{(1)}b^{(1)} \\
v_c^{(2)}b^{(2)} \\
\vdots \\
v_c^{(N)}b^{(N)}
\end{bmatrix}
\]

(4.21)

Upon Gauss-Jordan elimination this can be written in the convenient form
which allows for direct backward substitution of the unknown $v_c^{(1)}$s.

**Appendix B**

The internal energy $U$ of a continuum can be given as internal energy density $e$ integrated over its volume $V$,

$$U = \int_V e \, dV. \tag{4.22}$$

First law of thermodynamics in terms of a power balance dictates

$$\dot{U} = \int_{\partial V} t \cdot \dot{u} \, dA - \int_{\partial V} \dot{q} \cdot n \, dA \tag{4.23}$$

where $\partial V$ is the surface of the body under consideration. The first integral on the right hand side is the external power supplied where $t$ and $u$ are traction and displacement vectors. The second integral on the right hand side is the heat flux $q$ through the surfaces of the body having a unit normal vector $n$. Superimposed dot denotes rate of change of a quantity in time. The free energy is the quantity defined in thermodynamics as

$$\Phi = U - TS, \tag{4.24}$$

where $T$ is the temperature and $S$ is the entropy. The rate of change of free energy denoted by $\dot{\Phi}$ is simply

$$\dot{\Phi} = \dot{U} - \dot{T}S - T\dot{S}. \tag{4.25}$$

We assume temperature $T$ to be constant and uniform so that the second term on the right hand of side equation (4.25) cancels out. Plugging in the rate of change of entropy (either produced $\zeta_s$, or transported via heat flux) will yield

$$\int_V \dot{\phi} \, dV = \int_{\partial V} t \cdot \dot{u} \, dA - \int_{\partial V} \dot{q} \cdot n \, dA - T \left( \int_V \dot{\zeta}_s \, dV - \int_{\partial V} \frac{\dot{q}}{T} \cdot n \, dA \right). \tag{4.26}$$

Since we assume uniform temperature across the body, $T$ in the last integral can be taken out and the expression simplifies into

$$\int_V \dot{\phi} \, dV = \int_{\partial V} t \cdot \dot{u} \, dA - \int_{\partial V} \dot{\zeta}_s T \, dA. \tag{4.27}$$

Our assumption of $T$ being constant and uniform can be justified due to the fact that diffusion is a slow process, for instance when compared with dislocation glide.

For an irreversible process entropy gets produced within the material. This is equivalent to the part of the energy which is lost in the energetic sense and hence dissipated.
Now the second integral on the right hand side becomes nothing but the definition of dissipation. Denoting the rate of dissipation per unit volume with $\theta$ will give

$$\int_V \dot{\phi} \, dV = \int_{\partial V} t \cdot \dot{u} \, dA + \int_V \theta \, dV \quad (4.28)$$

For the specific problem that is solved in this chapter where all the surfaces are traction free, dissipation is equal to the rate of change of free energy since the first integral on the right hand side vanishes. However for the general case diffusion is governed by the rate of change of free energy. In the discrete dislocation framework the dissipation rate or for the problem considered here equivalently the rate of change of free energy is given as

$$\int_V \dot{\phi} \, dV = - \sum_{l=1}^N \int_{g(l)} f^{(l)}_i v_i^{(l)} \, dl \quad (4.29)$$

**Appendix C**

In this appendix we derive the image stress fields due to the traction-free surface for a dislocation in half-infinite space. Freund [4] has given the closed form expression for the stress fields of a dislocation both in infinite space, $\Sigma_{ij}$, and in half-infinite space, $\sigma_{ij}$ (see figure 4.15) in terms of functions of the complex variable $\zeta = x_1 + ix_2$. The stress fields in infinite space (no boundaries) read as follows:

$$\frac{1}{2}(\Sigma_{11} + \Sigma_{22}) = 2\Re(\Phi'(\zeta)) \quad (4.30)$$

$$\frac{1}{2}(\Sigma_{22} - \Sigma_{11}) + i\Sigma_{12} = \zeta \Phi''(\zeta) + \Psi'(\zeta) \quad (4.31)$$

where

$$\Phi'(\zeta) = \frac{\mu}{4\pi(1-\nu)} \left( \frac{ib}{\zeta + ih} \right) \quad (4.32)$$

$$\Psi'(\zeta) = \frac{\mu}{4\pi(1-\nu)} \left( -\frac{i\tilde{b}}{\zeta + ih} + \frac{bh}{(\zeta + ih)^2} \right) \quad (4.33)$$

are functions of the elastic constants (shear modulus $\mu$ and Poisson ratio $\nu$), and the Burgers vector $b = b_1 + ib_2$; $h$ is the distance between the dislocation and the origin of the coordinate system and $\zeta$ the coordinate of any point on the complex plane.

For the half-infinite space solution, the traction-free surface is taken to coincide with the real axis of the coordinate system. The stress fields are given as

$$\sigma_{22} - i\sigma_{12} = \phi'(\zeta) - \phi'(\bar{\zeta}) + (\zeta - \bar{\zeta})\phi''(\zeta) \quad (4.34)$$
**Figure 4.15:** Dislocation with an arbitrary Burgers vector in an infinite space (a), in half–infinite space(b).

\[
\sigma_{11} + i\sigma_{12} = \varphi'(\zeta) + \varphi'(\bar{\zeta}) - (\zeta - \bar{\zeta})\varphi''(\zeta) + 2\varphi'(\zeta) \tag{4.35}
\]

where

\[
\varphi'(\zeta) = \frac{\mu}{4\pi(1-\nu)} \left( \frac{ib}{\zeta + ih} - \frac{i\bar{b}(\zeta + ih)}{(\zeta - ih)^2} - \frac{i(b - \bar{b})}{\zeta - ih} \right) \tag{4.36}
\]

Now the image stress due to the free surface —denoted by \(\tilde{\cdot}\)— is the difference between the infinite space field and the half-infinite space field, i.e.,

\[
\tilde{\sigma}_{22} - i\tilde{\sigma}_{12} = \sigma_{22} - i\sigma_{12} - (\Sigma_{22} - i\Sigma_{12}) \tag{4.37}
\]

\[
\tilde{\sigma}_{11} + i\tilde{\sigma}_{12} = \sigma_{11} + i\sigma_{12} - (\Sigma_{11} + i\Sigma_{12}) \tag{4.38}
\]

The term between parentheses in equation (4.37) can be found by summing equation (4.30) and the conjugate of equation (4.31), while that in equation (4.38) can be calculated by subtracting the conjugate of equation (4.31) from equation (4.30). With the aid of the equality \(2\Re(\Phi'(\zeta)) = \Phi'(\zeta) + \overline{\Phi'(\bar{\zeta})}\), equation (4.37) can be further written as

\[
\tilde{\sigma}_{22} - i\tilde{\sigma}_{12} = \varphi' - \varphi'(\bar{\zeta}) + (\zeta - \bar{\zeta})\varphi''(\zeta) - (\zeta\overline{\Phi''(\zeta)}) + \overline{\Phi'(\bar{\zeta})} + \Phi'(\zeta) + \overline{\Phi'(\bar{\zeta})} \tag{4.39}
\]
4.5. Conclusions

Expanding all terms in the above expression we find

\[
\tilde{\sigma}_{22} - i\tilde{\sigma}_{12} = \frac{\mu}{4\pi(1 - \nu)} \left[ \left( \frac{ib}{\zeta + ih} - \frac{i(b - \bar{b})}{(\zeta - ih)^2} - \frac{i(b - \bar{b})}{\zeta - ih} \right) \right.
\]

\[
- \left( \frac{ib}{\zeta + ih} - \frac{i(b - \bar{b})}{(\zeta - ih)^2} - \frac{i(b - \bar{b})}{\zeta - ih} \right)
\]

\[
+ (\zeta - \bar{\zeta}) \left( \frac{i\bar{b}}{(\zeta - ih)^2} - \frac{2ib(\zeta - ih)}{(\zeta + ih)^3} - \frac{i(b - 2\bar{b})}{(\zeta + ih)^2} \right)
\]

\[
- \zeta \frac{i\bar{b}}{(\zeta - ih)^2} \left( \frac{-ib}{\bar{\zeta} - ih} + \frac{\bar{b}h}{(\zeta - ih)^2} - \frac{ib}{\bar{\zeta} + ih} + \frac{i\bar{b}}{\zeta - ih} \right), \quad (4.40)
\]

or, after simplification,

\[
\tilde{\sigma}_{22} - i\tilde{\sigma}_{12} = \frac{\mu}{4\pi(1 - \nu)} \left[ \frac{-i\bar{b}(\zeta + ih)}{(\zeta - ih)^2} - \frac{i(b - \bar{b})}{\zeta - ih} \right] + \left( \zeta - \bar{\zeta} \right) \left( \frac{-2ib(\zeta - ih)}{(\zeta + ih)^3} - \frac{i(b - 2\bar{b})}{(\zeta + ih)^2} \right) \quad (4.41)
\]

This result can be put into a more compact form by introducing the function

\[
\varphi'(\zeta) = \varphi'(\zeta) - \Phi'(\zeta) = \frac{\mu}{4\pi(1 - \nu)} \left( \frac{-i\bar{b}(\zeta + ih)}{(\zeta - ih)^2} - \frac{i(b - \bar{b})}{\zeta - ih} \right) \quad (4.42)
\]

similar to the ones defined above, so that equation (4.41) simplifies to

\[
\tilde{\sigma}_{22} - i\tilde{\sigma}_{12} = \varphi'(\zeta) - \Phi'(\zeta) + (\zeta - \bar{\zeta})\varphi''(\zeta). \quad (4.43)
\]

Application of the same procedure to equation (4.38) gives the complementary equation for the image stress field description,

\[
\tilde{\sigma}_{11} + i\tilde{\sigma}_{12} = \varphi'(\zeta) + \Phi'(\zeta) + (\zeta - \bar{\zeta})\varphi''(\zeta) + 2\varphi'(\zeta) \quad (4.44)
\]

The results above are for a single dislocation in (half-) infinite space, while in this chapter we use a periodic distribution. The stress field for a periodic array of dislocations can be obtained by using superposition. If the spacing between dislocations in the \(x_1\) direction is \(w\), then contributions from dislocations at \(x_1 = nw, x_2 = -ih\) should be summed over all integer values of \(n\). According to Freund [4], this yields (the superscript label \(\pi\) indicates that these functions apply to a periodic distribution)

\[
\Phi'(\zeta)^{\pi} = \frac{\mu}{4(1 - \nu)w} \left[ ib \cot \left( \frac{\pi(\zeta + ih)}{w} \right) \right] \quad (4.45)
\]

\[
\varphi'(\zeta)^{\pi} = \frac{\mu}{4(1 - \nu)w} \left[ -ib \cot \left( \frac{\pi(\zeta - ih)}{w} \right) + \frac{2\pi\bar{b}h}{w} \csc^2 \left( \frac{\pi(\zeta - ih)}{w} \right) \right] \quad (4.46)
\]


