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## Stress and dislocations in thin metal layers

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*Document Version*

Publisher's PDF, also known as Version of record

*Publication date:*

2004

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Nicola, L. (2004). *Stress and dislocations in thin metal layers*. [Thesis fully internal (DIV), Groningen]. s.n.

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## Chapter 4

### Relaxation of thermal stress in passivated metal interconnects\*

The reliability of many integrated circuits depends on the failure resistance of metallic interconnects. Typical damage processes that can induce failure in interconnects are void formation and electromigration. These processes are strongly influenced by the stress in the lines that develops as a consequence of the thermal mismatch between the metallic lines and their surroundings. The aluminum and copper alloys used for metallization have coefficients of thermal expansion that differ significantly from that of the silicon substrate to which they are usually bonded. Since the interconnects undergo large temperature excursions during processing, and often during service, their thermo-mechanical response is of interest.

Residual stresses in interconnects have been experimentally determined by X-ray diffraction [1, 2] and by curvature measurements [3, 4, 5]. Experiments have shown that the presence of a passivation layer results in a triaxial stress state in the line [2, 3], a stress state that favors void formation, and that the mechanical behavior of passivated lines strongly depends on their aspect ratio [1, 3]. A disadvantage of most experimental techniques is that they do not measure stress accurately in small geometries. Moreover, they only measure the average stress in the lines and do not capture stress gradients, which can be large in small confined geometries. However, energy-filtered electron diffraction methods [6] and glancing angle X-ray diffraction [7] may offer significant improvement in this regard. Numerical analyses based on conventional continuum constitutive characterizations have been used to predict stress evolution in the lines, with the interconnect mainly treated as an elastic [8, 9, 10] or an elastic-perfectly plastic material [1, 11]. A key

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\*Based on *Relaxation of thermal stress by dislocation motion in passivated metal interconnects*, L. Nicola, E. Van der Giessen, A. Needleman, J. Mater. Res. **19** (2004) 1216 and on *Simulations of dislocation dynamics in aluminum interconnects*, L. Nicola, E. Van der Giessen, A. Needleman, Mat. Res. Soc. Symp. Proc. **731** (2002).

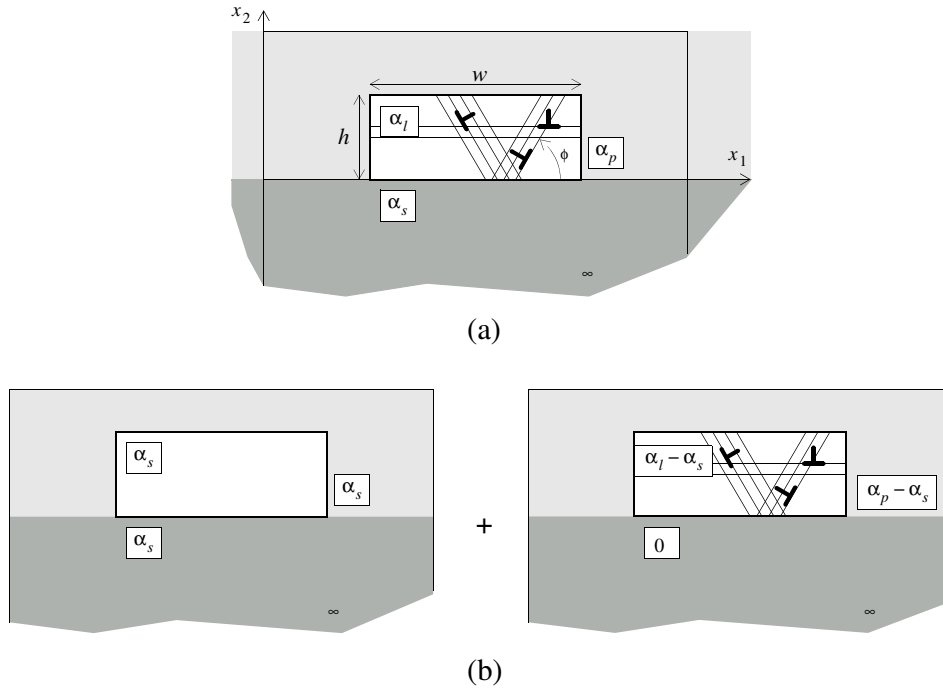
limitation of such approaches is that they cannot account for the size dependence of plastic response in small confined volumes.

In our analyses, plastic deformation in the line is treated as resulting from the collective motion of discrete dislocations which allows stress concentrations and gradients associated with dislocations and dislocation patterns to be captured. Upon cooling from a stress free state, the interconnect is strained by its substrate and by the passivation layer. During thermal loading, the evolution of the stress in the line cross-section and the evolution of the dislocation structure are predicted. Lines with various aspect ratio are analyzed and the results show rather good qualitative agreement with experiments [1, 3] for lines with a small aspect ratio: the larger the aspect ratio, the more elastic the line behavior. The possibility of a size effect is investigated: when the line height or width is sufficiently small (less than  $0.5\mu\text{m}$ ) lines with the same aspect ratio but of different size can exhibit a different response. The influence of slip plane orientation, pitch length and passivation layer thickness on stress evolution are also investigated.

## 4.1 Problem formulation

We consider an infinitely long array of single-crystal lines, perfectly bonded to a semi-infinite substrate and covered by a planar passivation layer (see Fig. 4.1). In the two-dimensional model illustrated in Fig. 4.1 the evolution of the stress field and of the dislocation structure in the cross-section of the lines is studied, assuming plane-strain conditions in the direction along the lines. This configuration is particularly relevant for aluminum lines on a silicon substrate, capped with a silicon-nitride passivation layer. In this type of system, the relatively stiff substrate and passivation layer provide significant constraint on plastic flow in the line in directions perpendicular to the line axis.

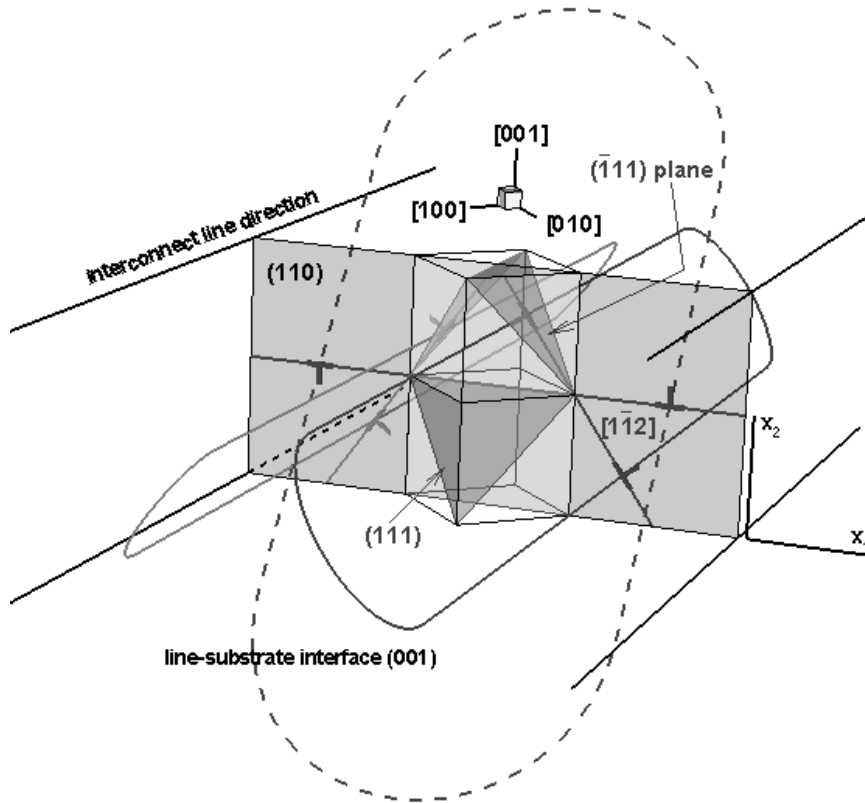
In most calculations, a planar crystal is analyzed that is an idealization of an FCC single crystal orientation with the plane of deformation to be the (110) plane, as illustrated in Fig. 4.2. In this orientation, dislocation loops can form that are extended in the line direction. In the limit of an infinitely long line (which is the plane strain limit), these dislocations are straight and of edge character, [12]. Equal slip along the two face diagonals of the  $(\bar{1}11)$  and  $(1\bar{1}1)$  slip planes is consistent with the  $[110]$  direction being perpendicular to the plane of deformation. Thus, slip on the  $(\bar{1}11)$  plane effectively occurs in the  $[1\bar{1}2]$  direction, while similarly on the  $(1\bar{1}1)$  plane slip effectively occurs in the  $[\bar{1}12]$  direction. Another



**Figure 4.1** (a) Geometry of the line model. (b) Decomposition of the unit-cell problem into a thermo-elastic problem and a plastic relaxation problem.

deformation possibility is slip in the  $[110]$  direction on the  $(111)$  slip plane. This does not correspond to a dislocation in the  $(110)$  plane (which therefore is dashed in Fig. 4.2), but since symmetry demands equal slip on the  $(\bar{1}\bar{1}1)$  plane, the composition of these is equivalent to slip on the  $(001)$  plane. On the  $(110)$  plane the slip directions are therefore inclined at  $\pm 54.7^\circ$  and  $0^\circ$  with the  $[\bar{1}10]$  direction, which we identify with the  $x_1$  axis.

In our plane strain analyses, we take the angles between slip directions to be near this FCC orientation and use three slip systems with the slip plane orientations:  $\phi^{(1)} = 0^\circ$ ;  $\phi^{(2)} = \phi^{(1)} + 60^\circ$ ;  $\phi^{(3)} = \phi^{(2)} + 60^\circ$ . This corresponds to  $\phi = 60^\circ$  in Fig. 4.1 and we refer to this as the FCC-like orientation.



**Figure 4.2** Schematic of dislocation motion on FCC slip planes when the crystal is oriented with  $[110]$  parallel to the line direction. Because of symmetry and when the line is very long, the slip mode is such that the dislocations can be idealized as three pairs of straight edge dislocations as shown by the  $\perp$  symbols.

#### 4.1.1 Boundary value problem

The analyses are carried out on a single cell of width  $w + 2p$ , where  $w$  is the width of each line and  $2p$  is the spacing (pitch) between lines, Fig. 4.1. In discrete dislocation plasticity, the fields in the line are obtained by coupling the solution of a boundary value problem for the single cell and the analytical solution for the dislocations, treated as line singularities in an infinite elastic medium (for more details see [13]).

The boundary value problem is defined by conditions of equilibrium and com-

patibility and by the constitutive equations:

$$\sigma_{ij,j} = 0; \quad (4.1)$$

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}); \quad (4.2)$$

$$\varepsilon_{ij} = \frac{1+\nu}{E} \left( \sigma_{ij} - \frac{\nu}{1+\nu} \delta_{ij} \sigma_{kk} \right) + \alpha \Delta T \delta_{ij}, \quad (4.3)$$

where  $\sigma_{ij}$  denotes the stresses,  $\varepsilon_{ij}$  the strains,  $u_i$  the displacements,  $\Delta T$  is the temperature difference from the initial stress-free state,  $E$  is Young's modulus and  $\nu$  is Poisson's ratio. The linear coefficient of thermal expansion of the line, the substrate and the passivation layer are denoted by  $\alpha_l$ ,  $\alpha_s$  and  $\alpha_p$ , respectively. Plane strain implies  $\varepsilon_{i3} = 0, i = 1 \dots 3$ .

The problem is decomposed into two parts: an unconstrained thermo-elastic part, denoted by  $( )^{\text{th}}$  and a part that is driven by the thermal expansion mismatch, denoted by  $( )'$  as shown in Fig. 4.1b. Their superposition provides the solution to the problem:

$$u_i = u_i^{\text{th}} + u_i', \quad \varepsilon_{ij} = \varepsilon_{ij}^{\text{th}} + \varepsilon_{ij}', \quad \sigma_{ij} = \sigma_{ij}^{\text{th}} + \sigma_{ij}'. \quad (4.4)$$

The  $( )^{\text{th}}$  part treats the unconstrained thermal expansion of the system line-substrate-passivation layer, under the assumption that all components have the same coefficient of thermal expansion  $\alpha_s$ . The solution is trivial. Since  $\sigma_{ij}^{\text{th}} = 0$  everywhere, dislocations are not involved in the solution of the  $( )^{\text{th}}$  part.

In the  $( )'$  part of the problem, the thermal expansion coefficients of the substrate and passivation layers are taken to be  $\alpha_s = \alpha_p = 0$  and that of the line is  $\alpha = \alpha_l - \alpha_s$ . The  $( )'$  part is subject to the following boundary conditions on the cell:

- stress-free surface

$$\sigma'_{12}(x_1, h_p) = \sigma'_{22}(x_1, h_p) = 0; \quad (4.5)$$

- periodicity conditions

$$u'_i(0, x_2) = u'_i(w + 2p, x_2). \quad (4.6)$$

When dislocations are present, the solution to the ( )' part is obtained by decomposing the fields as

$$u'_i = \hat{u}_i + \tilde{u}_i, \quad \varepsilon'_{ij} = \hat{\varepsilon}_{ij} + \tilde{\varepsilon}_{ij}, \quad \sigma'_{ij} = \hat{\sigma}_{ij} + \tilde{\sigma}_{ij}, \quad (4.7)$$

where the ( $\tilde{\quad}$ )-fields are the fields associated to the dislocations treated as individual dislocations in an infinite medium. The ( $\tilde{\quad}$ )-fields are given by the sum of the long-range fields of each dislocation in the cell (including their replicas in the periodic cells),

$$\tilde{u}_i = \sum_I u_i^{(I)}, \quad \tilde{\varepsilon}_{ij} = \sum_I \varepsilon_{ij}^{(I)}, \quad \tilde{\sigma}_{ij} = \sum_I \sigma_{ij}^{(I)}, \quad (4.8)$$

where the superscript ( $I$ ) denotes the  $I$ th dislocation. The ( $\tilde{\quad}$ )-fields are singular at the positions of the dislocations, and satisfy the standard equations of linear elasticity outside the dislocation core region. The ( $\hat{\quad}$ )-fields in (4.7) are the image fields which correct the ( $\tilde{\quad}$ )-fields in order to satisfy the boundary conditions (4.5) and (4.6) on the unit cell, cf. [13].

#### 4.1.2 Rules for dislocation motion

The calculations make use of the same three rules used in the previous study on thin films presented in chapter 2:

- nucleation of a dipole from a point source occurs when the Peach-Koehler force on the source is larger than the nucleation strength  $\tau_{\text{nuc}}b$  during a time span  $t_{\text{nuc}} = 10$  ns. Such a point source is a two-dimensional representation of a Frank-Read source;
- dislocation glide is drag controlled: the velocity of a dislocation is proportional to the Peach-Koehler force acting on it through the drag coefficient  $B = 10^{-4}$ MPa,  $v^{(I)} = B^{-1}f^{(I)}$ ;
- annihilation of a dipole occurs when the dislocations approach each other within the annihilation distance  $L_e = 6b$ .

The Peach-Koehler force on dislocation  $I$  is given by

$$f^{(I)} = m_i^{(I)} \left( \hat{\sigma}_{ij} + \sum_{J \neq I} \sigma_{ij}^{(J)} \right) b_j^{(I)},$$

with  $m_i^{(I)}$  the slip plane normal and  $b_i^{(I)}$  the Burgers vector of dislocation  $I$ .

To accurately resolve dislocation-dislocation interactions, a small time step  $\Delta t = 0.05\text{ns}$  is needed. Therefore, to limit the computing time, the cooling rate is taken to be  $\dot{T} = 40 \times 10^6\text{K/s}$  which is much faster than experimental cooling rates.

## 4.2 Results and Discussion

We analyze the evolution of thermal stress in the line section while the temperature is decreased by 200K from a stress free and dislocation free state. The stress in the line arises from the thermal mismatch between the line, the substrate and the passivation layer. We take the thermal expansion coefficient of the line to be representative of aluminum,  $\alpha_l = 23.2 \times 10^{-6}/\text{K}$ , and use a value representative of silicon,  $\alpha_s = 4.2 \times 10^{-6}/\text{K}$ , for the substrate. In practice, aluminum lines on silicon substrates are usually passivated by silicon-nitride, which has a coefficient of thermal expansion that is very close to that of silicon; hence, in our calculations we take  $\alpha_p = 4.2 \times 10^{-6}/\text{K}$ . Moreover, for the lines, the elastic properties for aluminum are specified by  $E = 70\text{GPa}$  and  $\nu = 0.3$ . As in our previous analysis [15] of thin films, differences in elastic properties are neglected, so that the same elastic constants are used for the substrate and passivation layers.

As in our thin film study [15], Frank-Read sources are placed at random positions on the slip planes. The source density in all simulations is  $\rho_{\text{nuc}} = 60/\mu\text{m}^2$ . Hence, only some of the slip planes in the line are potentially active. The source strength is taken to be  $\tau_{\text{nuc}} = 25\text{MPa}$ . The interfaces with substrate and passivation layer are modeled as impenetrable. Sources are not placed closer to these interfaces than the nucleation distance  $L_{\text{nuc}}$ : when a dipole is generated, both dislocations must be contained in the line. This implies that there is a zone of thickness  $L_{\text{nuc}} \sin\phi$  around the line edges that is source free, independent of the line size.

The finite element mesh used to solve for the ( $\hat{\cdot}$ ) fields is based on bilinear displacement four-node rectangular elements. A refined mesh is used inside the line, specially around the line corners. The mesh is gradually coarsened in the substrate with the mesh spacing increasing with distance from the line. The number of elements and degrees of freedom depend on the line size, with the meshes used consisting of from 48 to 252 elements inside the line.



### 4.2.1 Shape effects

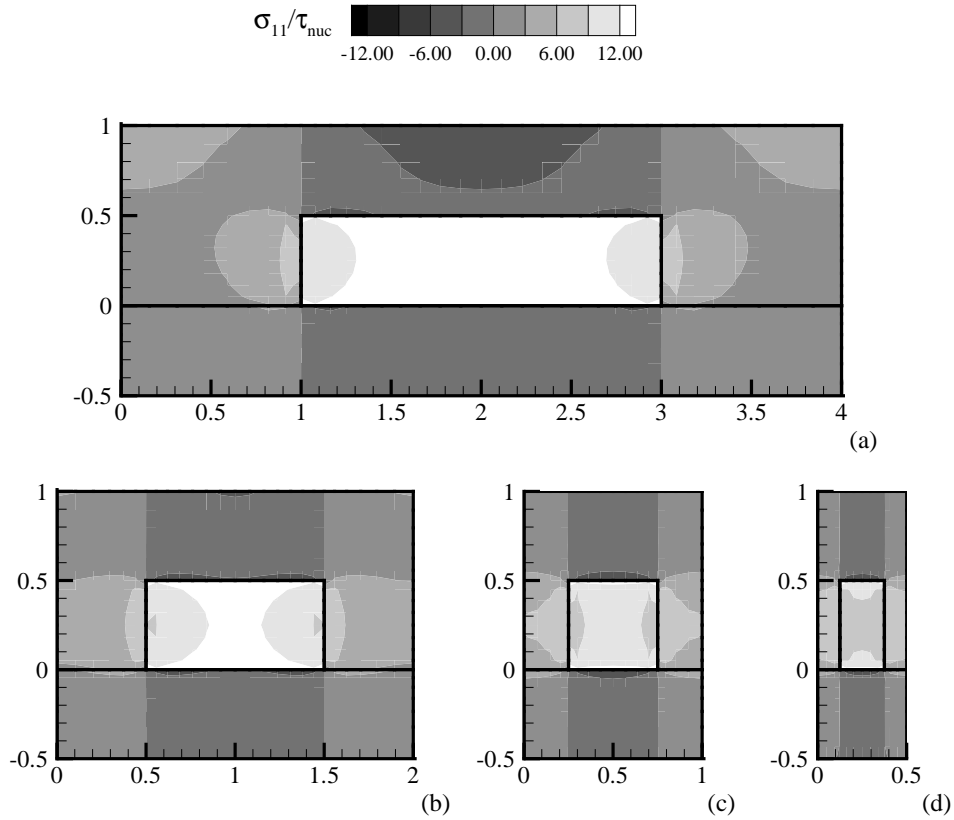
All simulations start from a stress and dislocation-free state. As the temperature is decreased, an inhomogeneous stress state develops in the line, with the stress distribution and magnitude depending on the geometry of the line and of the passivation layer. The characteristics of the elastic stress field are key for the relaxation behavior. Therefore, we first present elastic simulations for four lines with various aspect ratios  $h/w$ . We take the line height to be constant,  $h = 0.5\mu\text{m}$ , and the line width to vary between  $w = 0.25$  and  $w = 2\mu\text{m}$ , so that the aspect ratio ranges from  $h/w = 0.25$  to  $h/w = 2$  (see Fig. 4.1). In order to keep the line area fraction the same for the four lines, the ratio of passivation layer thickness to line height and the ratio of pitch  $2p$  to line width  $w$  are fixed at  $h_p/h = 2$  and  $2p/w = 1$ , respectively.

Figure 4.3 shows the distribution of  $\sigma_{11}$ , the stress parallel to the line-substrate interface, in the four lines after cooling by 200K.

The line with  $h/w = 0.25$  (Fig. 4.3a) is in a high, rather homogeneous tensile state with edge effects near the interfaces with the passivation layer. As  $h/w$  increases, Figs. 4.3b–d, the stress state changes such that  $\sigma_{11}$  in the core of the line is lower. High concentrations of stress are found close to the interface with the substrate and close to the top interface with the passivation layer. The compressive stress in the substrate is very small due to the large size of the substrate. The passivation layer, on average, is in tension between lines, especially for the taller lines. Above the line, the passivation layer is on average in compression.

The effect of dislocation glide on stress evolution is investigated for the same line geometries. The initial response of the line is elastic. The  $\sigma_{11}$  field has the distribution shown in Fig. 4.3 which then, along with the slip plane orientation, determines which source is subjected to the highest resolved shear stress. When the Peach-Koehler force on one of the sources attains the nucleation strength during a period  $t_{\text{nuc}}$ , the first dipole is nucleated. After nucleation, dislocations move apart on their slip plane, and relax the stress in the line. If they do not meet other dislocations on their path, they glide until they reach the impenetrable interfaces. More dislocations are nucleated and as the dislocation density increases, junctions between crossing dislocations form. These junctions may act as obstacles for other dislocations, but may also trigger dislocation nucleation from nearby sources. The stress field in the lines evolves due to continued cooling and to the nucleation and motion of dislocations.

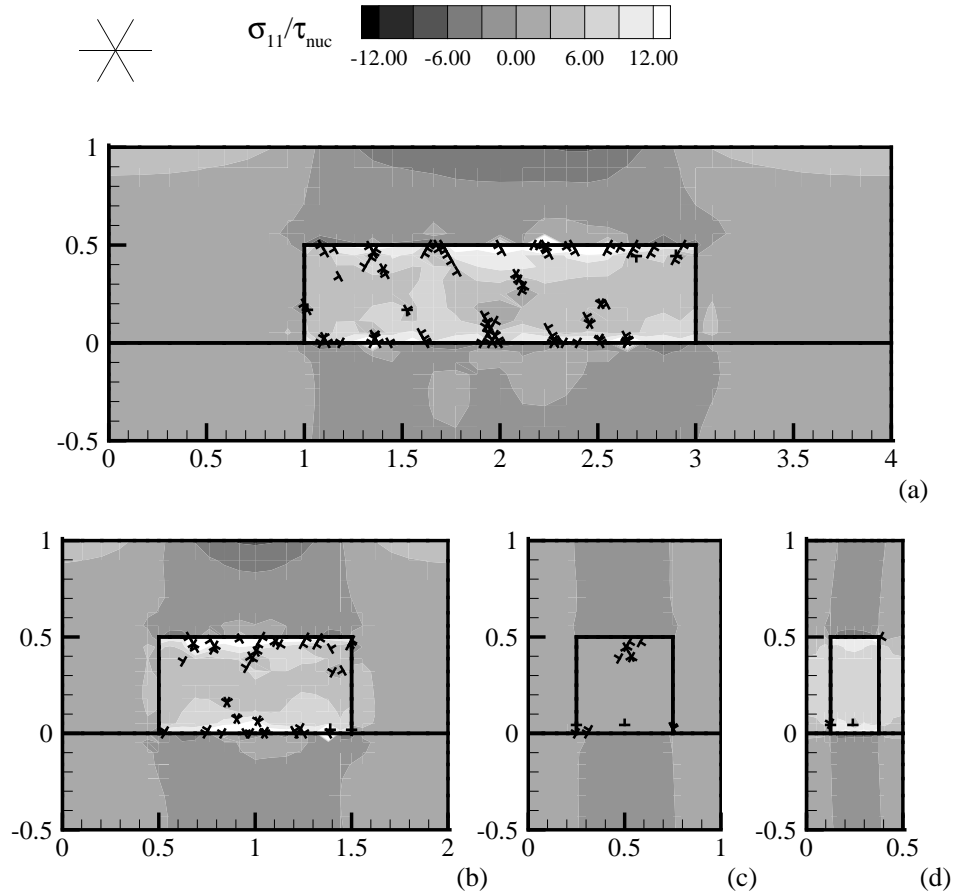
Figure 4.4 shows the stress field  $\sigma_{11}$  in the lines at final temperature (400K),



**Figure 4.3** The elastic stress state. Contours of  $\sigma_{11}$ , normalized by the nucleation strength  $\tau_{\text{nuc}}$  for four lines of height  $h = 0.5 \mu\text{m}$  with various aspect ratios: (a)  $h/w = 0.25$ , (b)  $h/w = 0.5$ , (c)  $h/w = 1$  and (d)  $h/w = 2$ .

with the corresponding dislocation distribution superimposed. Many dislocations have nucleated in the lines with aspect ratio  $h/w < 1$  (see Figs. 4.4a and 4.4b) and have piled up at the top and at the bottom of the lines. Some dislocations have met other dislocations crossing their slip planes and have formed junctions in the cores of the lines. The dislocation activity in the lines with  $h/w = 1$  and  $h/w = 2$  is rather limited (see Fig. 4.4c and 4.4d). In the narrow line with aspect ratio  $h/w = 2$  (Fig. 4.4d) only two dipoles have nucleated; the motion of these two dipoles does not significantly affect the stress field inside the line, as can be seen by comparing Fig. 4.4d with Fig. 4.3d.

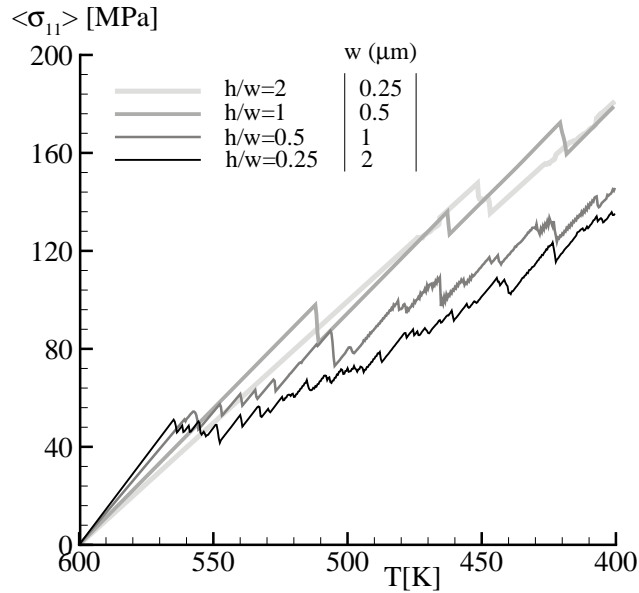
Figure 4.5 shows the evolution of the average stress in the line,  $\langle \sigma_{11} \rangle$ , during



**Figure 4.4** Relaxed state at final temperature. Contours of  $\sigma_{11}$ , normalized by the nucleation strength  $\tau_{nuc}$ , and dislocation distribution for four lines of height  $h = 0.5\mu\text{m}$  with various aspect ratios: (a)  $h/w = 0.25$ , (b)  $h/w = 0.5$ , (c)  $h/w = 1$  and (d)  $h/w = 2$ .

cooling. The stress-temperature curves for the four lines considered differ mainly in the elastic slope and in the onset of plasticity (dislocation activity starts earlier in lines with smaller aspect ratios). In lines with  $h/w < 1$  the stress at yield is  $\sigma_{11}^y \simeq 50\text{MPa}$  for the parameters used in the calculations. The first dislocation nucleation is immediately followed by many other nucleation events, so that relaxation is very effective until  $T \simeq 540\text{K}$ , especially in the line with  $h/w = 0.25$ . Then, when the back stress associated with dislocation pile-ups formed at the

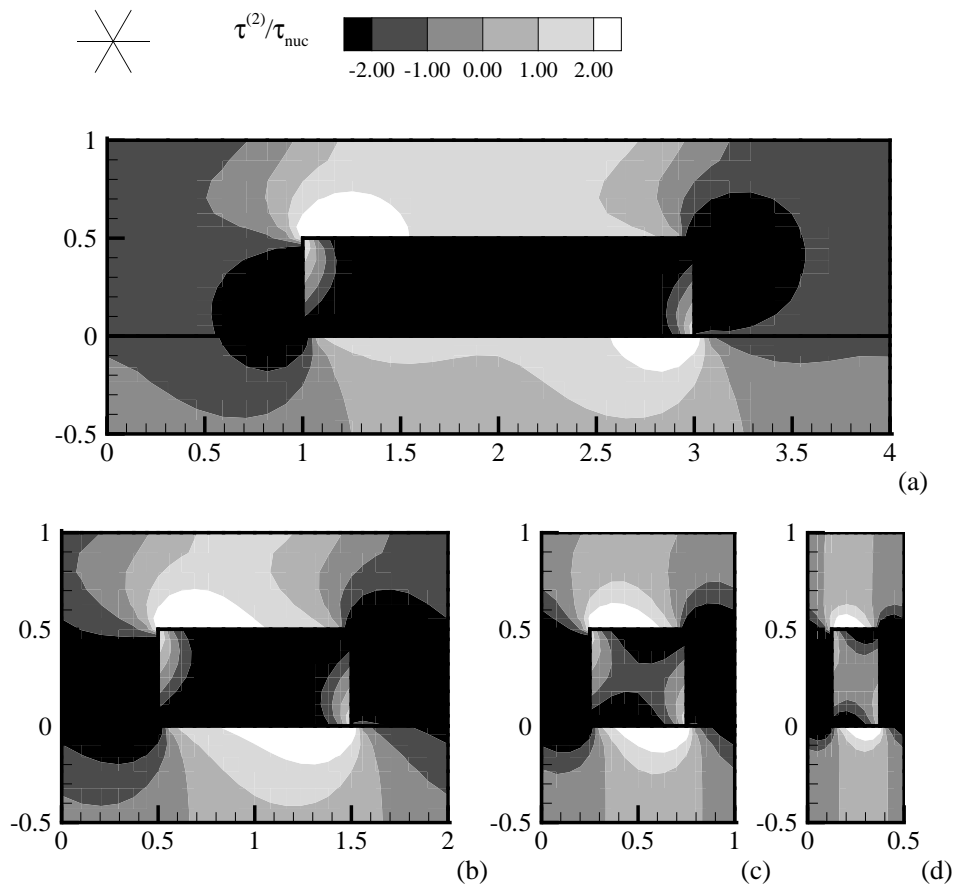
interfaces becomes significant, the nucleation rate decreases and the material response becomes harder. This is similar to the findings in [15] for thin films, but even more pronounced due to the four-sided constraints on dislocation motion (note that the formation of long pile-ups is a consequence of the interfaces of the line with the passivation layer and with the substrate being modeled as impenetrable). In lines with  $h/w \geq 1$  the yield strength is relatively high (in comparison with the nucleation strength  $\tau_{\text{nuc}} = 25\text{MPa}$ ); for  $h/w < 1$ :  $\sigma_{11}^y \simeq 100\text{MPa}$  with  $h/w = 1$  and  $\sigma_{11}^y \simeq 150\text{MPa}$  with  $h/w = 2$ . The trend in these calculations is that stress relaxation by dislocation motion is more effective for smaller aspect ratio lines. Results presented in the following subsection show that this does not hold in general.



**Figure 4.5** Average  $\sigma_{11}$  in the line versus imposed temperature for the four lines with aspect ratios shown in Fig. 4.4.

In order to understand why stress relaxation by dislocation motion is more effective for lines with  $h/w < 1$ , Fig. 4.6 shows the resolved shear stress at  $60^\circ$  in the four elastic lines normalized by the nucleation strength  $\tau_{\text{nuc}}$ . In the line with  $h/w = 2$  (Fig. 4.6d) there are only two very small regions near the line corners where the resolved shear stress  $\tau^{(2)}$  on the slip planes at  $\phi^{(2)} = 60^\circ$  exceeds the

nucleation strength. Only sources in these regions can nucleate dislocations. In flat lines,  $h/w < 1$ , the resolved shear stress magnitude is greater and distributed more homogeneously in the line, so that almost all sources available can be activated. It is also important to note that the small aspect ratio lines,  $h/w < 1$ , have more dislocation sources than the lines with  $h/w \geq 1$ ; since  $h$  is fixed, lines with  $h/w < 1$  have a larger cross-sectional area but the same source density as lines with  $h/w > 1$ .



**Figure 4.6** Distribution of the shear stress resolved on the slip planes at  $60^\circ$ , normalized by the nucleation strength  $\tau_{\text{nuc}}$  for four lines of height  $h = 0.5 \mu\text{m}$  with various aspect ratios: (a)  $h/w = 0.25$ , (b)  $h/w = 0.5$ , (c)  $h/w = 1$  and (d)  $h/w = 2$ .

### 4.2.2 Size effects

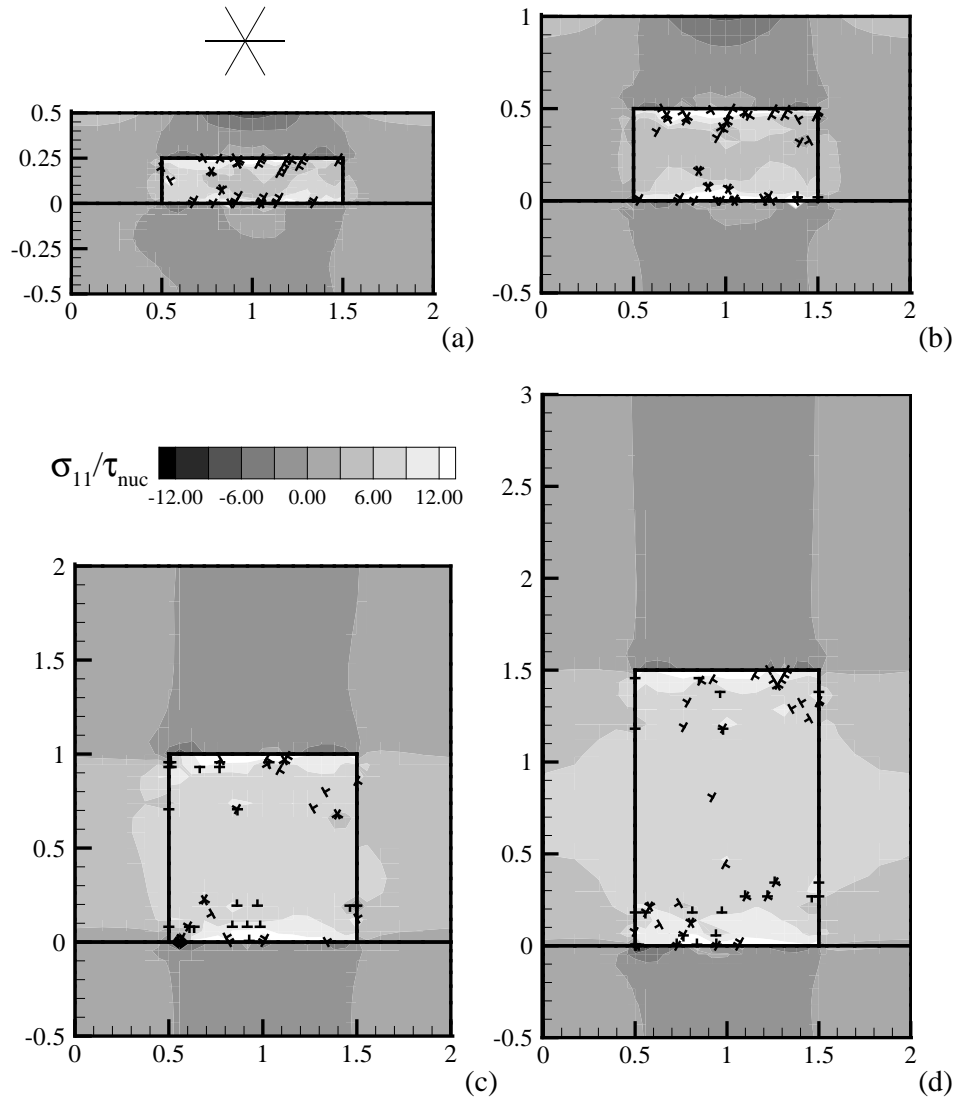
To investigate the role of source availability on stress relaxation in the lines, we analyze a set of lines with varying aspect ratio but with the width fixed. The line width is now fixed at  $w = 1\mu\text{m}$  while the line height  $h$  ranges between  $0.25\mu\text{m}$  and  $1.5\mu\text{m}$ , so that the aspect ratio range remains between  $h/w = 0.25$  and  $1.5$  for comparison with the previous results. The line area fraction is the same as in Fig. 4.3 and the elastic response of the lines is size independent. The use of a fixed width ensures that the ratio between the passivation layer thickness and the line height remains  $h_p/h = 2$  and the ratio between pitch and line width is still  $2p/w = 1$ . The  $\sigma_{11}$  stress and dislocation distributions at 400K are shown in Fig. 4.7. The line shown in Fig. 4.7a has the same aspect ratio ( $h/w = 0.25$ ) as the line in Fig. 4.4a, but the cross-sectional area ( $0.25\mu\text{m}^2$ ) and the number of Frank-Read sources is the same as for the line in Fig. 4.4c. Despite the reduced number of sources (15 for the line in Fig. 4.7a versus 60 for the line in Fig. 4.4a), there is considerable dislocation activity and the stress in the line core has relaxed significantly. The availability of sources is greater in the present lines with  $h/w \geq 1$ , Figs. 4.7c and d, and the number of dislocations nucleated during the simulation is larger by a factor between 2 and 10 than for the lines in Figs. 4.4c, d. This is mainly due to the higher probability of a source being located in the zones with a high resolved shear stress. Nevertheless, despite the higher nucleation activity, stress relaxation in the lines has not been effective. This is seen in Fig. 4.8, where the average stress in the line,  $\langle\sigma_{11}\rangle$ , is plotted as a function of temperature. The response of lines with  $h/w \geq 1$  is still almost elastic as in Fig. 4.5.

The inefficiency of relaxation for  $h/w \geq 1$  is because the stress state in these lines is very close to being hydrostatic, as is shown in Fig. 4.9a, plotting  $\langle\sigma_{11}\rangle$ ,  $\langle\sigma_{22}\rangle$  and the average hydrostatic stress,

$$\langle\sigma_h\rangle = \frac{1}{3}[\langle\sigma_{11}\rangle + \langle\sigma_{22}\rangle + \langle\sigma_{33}\rangle], \quad (4.9)$$

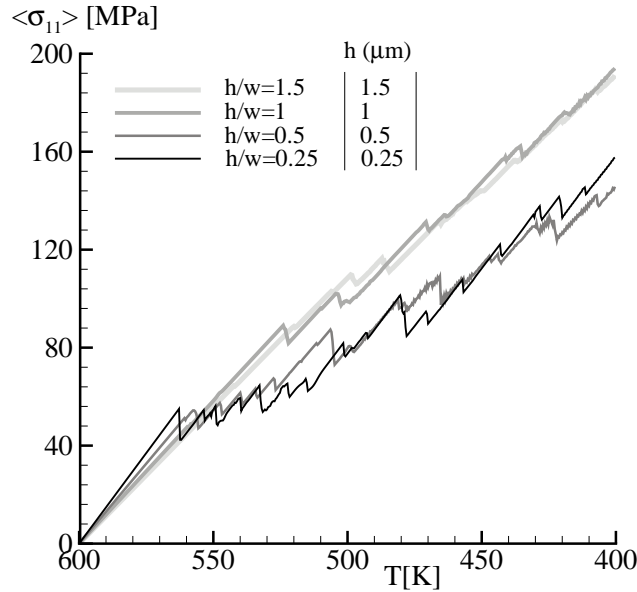
in a line with  $w = h = 1\mu\text{m}$ . Figure 4.9b shows similar plots for a line with  $h/w = 0.25$ ,  $w = 2\mu\text{m}$  and  $h = 0.5\mu\text{m}$ . The elastic stress in this flatter line is less hydrostatic, and  $\langle\sigma_{11}\rangle$  is reduced, even though  $\langle\sigma_{22}\rangle$  is not affected by dislocation glide. From Fig. 4.9a it seems that when dislocations nucleate,  $\langle\sigma_{11}\rangle$  reduces but the transverse stress  $\langle\sigma_{22}\rangle$  increases somewhat, thus maintaining the same hydrostatic stress state.

Taking a closer look at the dislocations in Figs. 4.4 and 4.7 one can see that lines with  $h/w < 1$  are characterized by many dislocation pile-ups at the top and



**Figure 4.7** Contours of  $\sigma_{11}$ , normalized by the nucleation strength  $\tau_{\text{nuc}}$  and dislocation distribution at final temperature for four lines of width  $w = 1\mu\text{m}$  with various aspect ratios: (a)  $h/w = 0.25$ , (b)  $h/w = 0.5$ , (c)  $h/w = 1$  and (d)  $h/w = 1.5$ .

at the bottom of the lines. The magnitude of the net Burgers vector at the top of the line corresponds approximately to a super-dislocation with Burgers vector in the  $-x_1$  direction. The dislocations at the bottom are equivalent to a super-

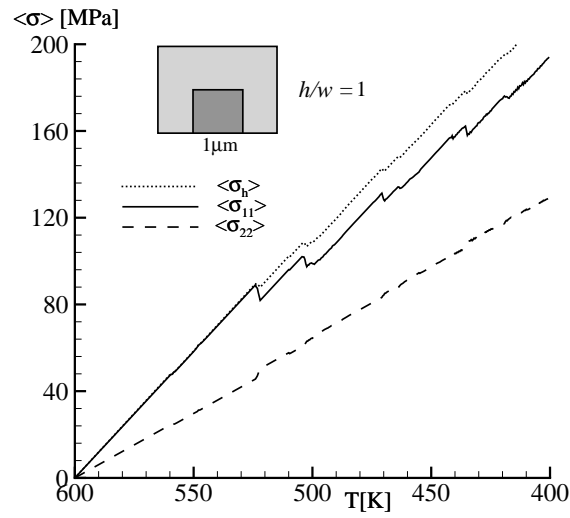


**Figure 4.8** Average  $\sigma_{11}$  in the line versus imposed temperature for the four lines with width  $w = 1\mu\text{m}$  and aspect ratios: (a)  $h/w = 0.25$ , (b)  $h/w = 0.5$ , (c)  $h/w = 1$  and (d)  $h/w = 1.5$  of Fig. 4.7.

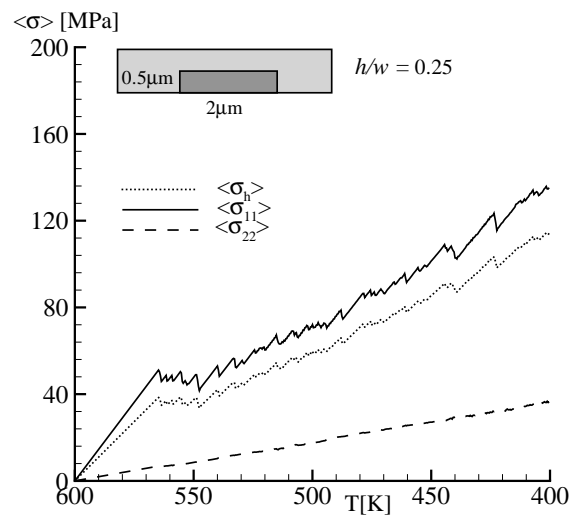
dislocation with the opposite-signed Burgers vector. This dislocation structure is efficient in the relaxation of  $\langle \sigma_{11} \rangle$ , since it corresponds to the idealized picture of misfit dislocations at the top and at the bottom of the line. According to the same idealized picture, relaxation of  $\langle \sigma_{22} \rangle$  would require misfit dislocations at the line edges with their Burgers vector pointing in the  $x_2$  direction on the left-hand edge and in the  $-x_2$  direction on the other side. However, during the simulations, opposite net Burgers vectors develop on these sides. This observation emphasizes that a high dislocation density is not always effective in relaxing the stresses; what matters is the plastic straining, which depends on the distance that dislocations travel on the slip planes, and on the slip plane orientation. Dislocations on slip planes parallel to the line-substrate interface are not effective in relaxing  $\langle \sigma_{11} \rangle$ .

Comparison of Fig. 4.8 with Fig. 4.5 shows that the lines with  $h/w = 0.25$  but of different size exhibit different hardening behaviors; the stress increase in the small line in Fig. 4.7a, after 560K, is higher than in the two times larger one in Fig. 4.4a. In fact, the  $h/w = 0.25$  line in Fig. 4.8 hardens at least as fast the one with  $h/w = 0.5$ . One possible explanation is that the pile-ups which form in the line with





(a)



(b)

**Figure 4.9** Average stress versus imposed temperature in lines with the same line area but with different aspect ratios: (a)  $h/w = 1$ ; (b)  $h/w = 0.25$ .

$h = 0.25\mu\text{m}$  are on average closer to the dislocation sources, so that their back stress inhibits nucleation. The back stress works against the formation and glide of new dislocations, which would make the pile-ups longer, and therefore hinders stress relaxation. This is similar to the size-dependent hardening mechanism seen in thin single-crystal films in [15]. Effective relaxation of  $\langle\sigma_{11}\rangle$  for smaller aspect ratio lines, i.e. lines with  $h/w < 1$ , only occurs if the height of the line is large compared to the length of dislocation pile-ups. The width is not a limitation, because stress relaxation by glide is an effective mechanism only when  $w > h$ . In all the simulations with  $w > h$  the average distance of dislocation sources from the top and the bottom of the lines is smaller than from the sides. Moreover, dislocation pile-ups rarely form at the lateral edges of the line.

### 4.2.3 Optimization

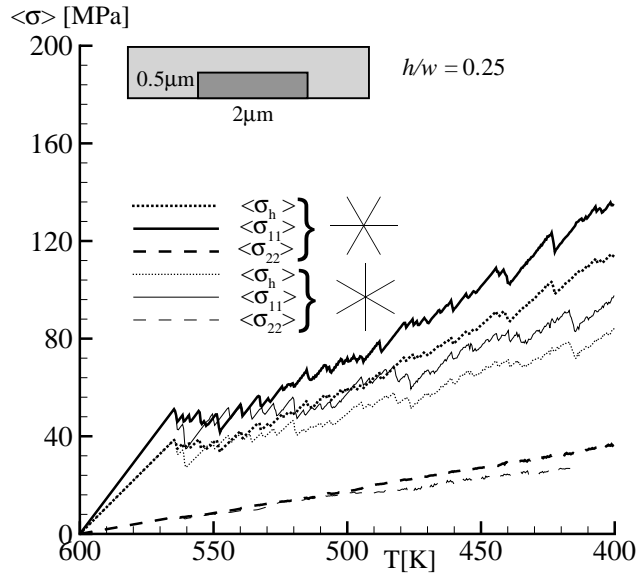
Since the hydrostatic stress plays a key role in void formation, it is of interest to reduce it as much as possible. We now consider only lines with  $h/w < 1$ , because relaxation of the  $\langle\sigma_{11}\rangle$  stress is effective and because  $\langle\sigma_{22}\rangle$  in these lines is smaller than  $\langle\sigma_{11}\rangle$  (Fig. 4.9). The average hydrostatic stress in such lines at 400K is significantly lower than in lines with  $h/w > 1$  but still around 120MPa.

### Effect of slip plane orientation

More effective relaxation of  $\langle\sigma_{11}\rangle$  is achieved by changing the slip plane orientation. In this Section, lines with slip planes oriented at  $\phi^{(\alpha)} = (30^\circ, 90^\circ, 150^\circ)$  are considered which corresponds to a  $30^\circ$  rotation of the FCC-like orientation in the previous calculations. This can also be considered as corresponding to a BCC-type orientation [12].

The calculation for the line with  $h = 0.5\mu\text{m}$  and  $w = 2\mu\text{m}$  is repeated in the rotated orientation. A comparison is given in Fig. 4.10 of the evolution of the average normal stresses  $\langle\sigma_{11}\rangle$ ,  $\langle\sigma_{22}\rangle$  and the hydrostatic stress  $\langle\sigma_h\rangle$  for the two orientations. The line with the rotated orientation more effectively relaxes  $\langle\sigma_{11}\rangle$ : at 400K  $\langle\sigma_{11}\rangle \simeq 90\text{MPa}$  for the BCC-type orientation while  $\langle\sigma_{11}\rangle \simeq 140\text{MPa}$  for the FCC-type orientation. The number of dislocations piled-up at the top and at the bottom of the line in the BCC-type orientation is approximately the same as in the line with the FCC-type orientation, but, due to the orientation of their Burgers vector they are equivalent to  $\sqrt{3}$  times more misfit dislocations than in the FCC-type crystal. The dislocation structure in the BCC-type crystal is more effective

in relieving the  $\langle \sigma_{11} \rangle$  stress. The BCC-type orientation is also slightly favorable for decreasing  $\langle \sigma_{22} \rangle$  and the hydrostatic stress.

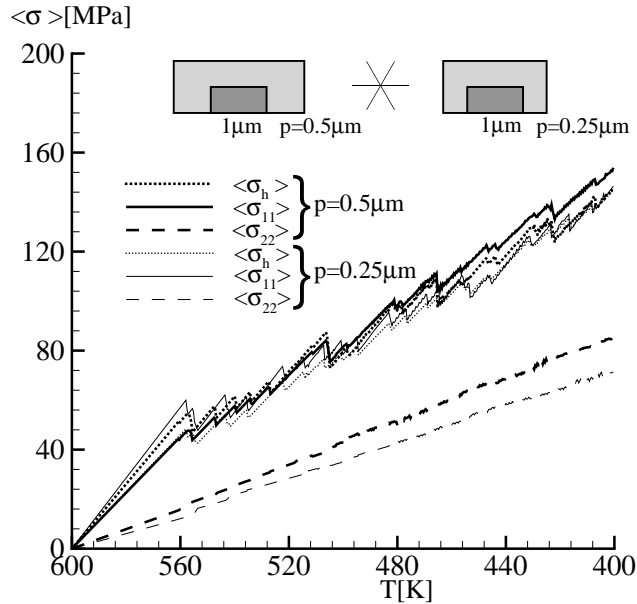


**Figure 4.10** Average stresses versus imposed temperature in a line with aspect ratio  $h/w = 0.25$  for FCC-type,  $\phi^{(\alpha)} = (0^\circ, 60^\circ, 120^\circ)$ , and BCC-type,  $\phi^{(\alpha)} = (30^\circ, 90^\circ, 150^\circ)$ , orientations.

### Effect of a shorter pitch

In the calculation for the line with  $h/w = 0.5$  ( $h = 0.5\mu\text{m}$  and  $w = 1\mu\text{m}$ ), the pitch was  $2p = 1\mu\text{m}$ . We repeat this simulation keeping all the parameters fixed but changing the pitch to  $2p = 0.5\mu\text{m}$ . Neither the geometry of the line nor the number and position of sources are changed. Figure 4.11 shows a comparison of the average in-plane stress evolution in the two lines. When the lines are more closely spaced ( $p = 0.25\mu\text{m}$ ) the hydrostatic stress is reduced in the elastic range. At the end of the simulation, at 400K, the average hydrostatic stress in the line with  $p = 0.25\mu\text{m}$  is a little lower than in the line with  $p = 0.5\mu\text{m}$ . This is due to a reduced overall elastic stiffness against  $\langle \sigma_{22} \rangle$  for the passivation layer which is a consequence of the change in geometry; as  $p$  decreases, the passivation layer between lines is narrower and this reduces the overall stiffness even though the

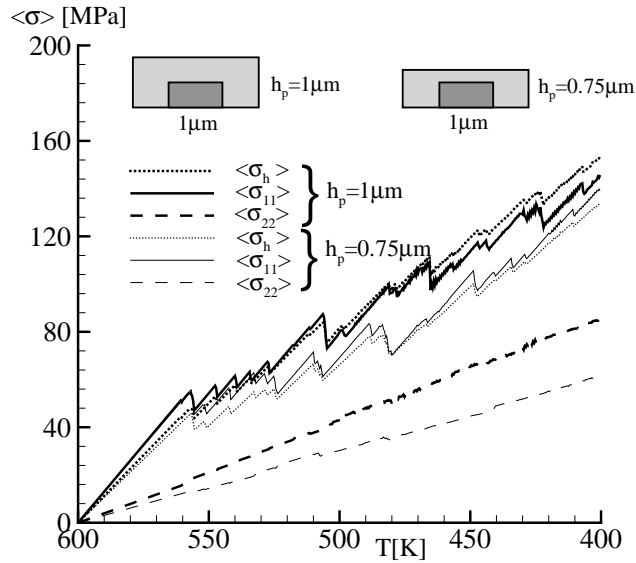
elastic properties remain the same.



**Figure 4.11** Average stresses versus imposed temperature in two lines with  $w = 1\mu\text{m}$  and  $h = 0.5\mu\text{m}$  which differ in the half-pitch:  $p = 0.25\mu\text{m}$  or  $p = 0.5\mu\text{m}$ .

### Effect of a thinner passivation layer

The simulation for the line with aspect ratio  $h/w = 0.5$  ( $h = 0.5\mu\text{m}$  and  $w = 1\mu\text{m}$ ) is repeated with all parameters unchanged except for the height of the passivation layer, which is now  $h_p = 0.75\mu\text{m}$  as compared with the previous value of  $h_p = 1\mu\text{m}$ . Figure 4.12 shows that the stress state that develops in the line with the thinner passivation layer is slightly less hydrostatic than in the line with the thicker layer. The value of  $\langle \sigma_{11} \rangle$  in the elastic range is the same in the two simulations, but because the hydrostatic component of the stress is reduced in the line with  $h_p = 0.75\mu\text{m}$ , the resolved shear stress on the slip planes is increased and stress relaxation is slightly more efficient. In the elastic regime, the value of  $\langle \sigma_{22} \rangle$  develops more slowly in the line with the thinner passivation layer. Thus, the average hydrostatic stress in the line is smaller if a thinner passivation layer is used.



**Figure 4.12** Average stresses versus imposed temperature in two lines with  $w = 1\mu\text{m}$  and  $h = 0.5\mu\text{m}$  for various heights of the passivation layer:  $h_p = 1\mu\text{m}$  and  $h_p = 0.75\mu\text{m}$ .

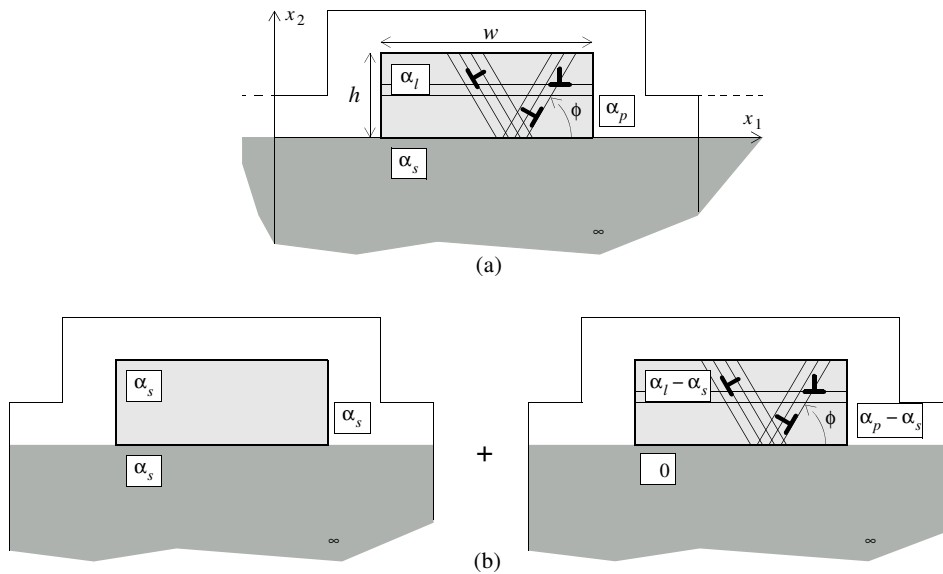
### 4.3 Lines with non-planar passivation

The planar passivation layer is mainly used in Cu lines obtained by Demascene process. The traditional deposition process for Al-Cu lines involves the use of a non planar capping layer.

In this section stress relaxation in lines with non-planar passivation layer is analyzed. The model is still based on an infinitely long array of single-crystalline lines, each having thickness  $h$  and width  $w$ , perfectly bonded to an infinitely large substrate and now capped by a non-planar passivation layer (Fig. 4.13).

Results are here presented of three simulations for lines with aspect ratios of  $w/h = 1.25, 2.5, 5$ . The height of the line is fixed at  $h = 0.4\mu\text{m}$ , while the width ranges from  $0.5$  to  $2\mu\text{m}$ . The thickness of the passivation layer is the same in all simulations.

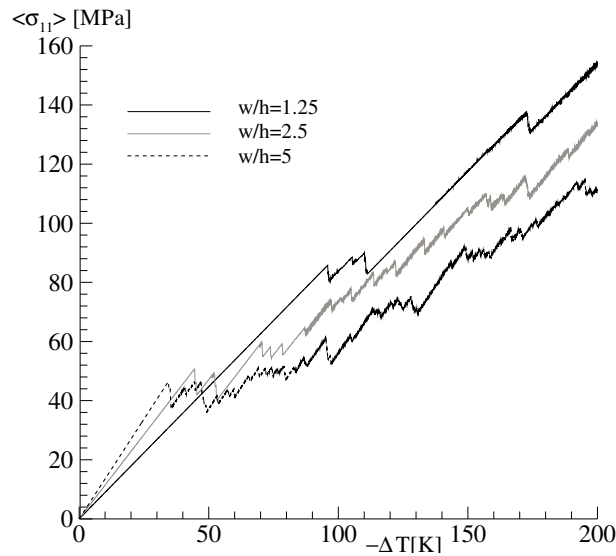
The evolution of the average value of  $\sigma_{11}$  in the line,  $\langle \sigma_{11} \rangle$ , is plotted as a function of the temperature reduction in Fig 4.14. The curves show that the elastic response depends on the line aspect ratio. With  $w/h = 5$ , the average stress in the



**Figure 4.13** Decomposition used to solve the fields in a dislocated line on a substrate with non planar passivation layer.

elastic regime builds up faster than in the lines with smaller aspect ratios. As a consequence, plastic deformation starts earlier and is more effective for larger width-to-height ratios.

Figure 4.15 shows the distribution of the dislocations and the transverse stress  $\sigma_{11}$  in the cell at the end of the cooling process. The stress is normalized by the nucleation strength. The compressive stress in the substrate (only its upper part is seen in the figure) is very low on average, because of the large thickness of the substrate. Only near the interface with the line do the stresses in the substrate reach high values, caused by the fields of the dislocations piled up there. The pile-ups formed at the top and bottom of the line lead to the development of two highly stressed boundary layers. The hard boundary layers are more distinct in the line with the largest aspect ratio  $w/h = 5$  (Fig. 2c), where plastic relaxation has been more effective. Stresses in the core of the line are very low in this case in comparison with the line with aspect ratio  $w/h = 1.25$  (Fig 4.15). With  $w/h = 1.25$ , there has been very little dislocation activity so that the final stress distribution is very similar to the elastic solution.

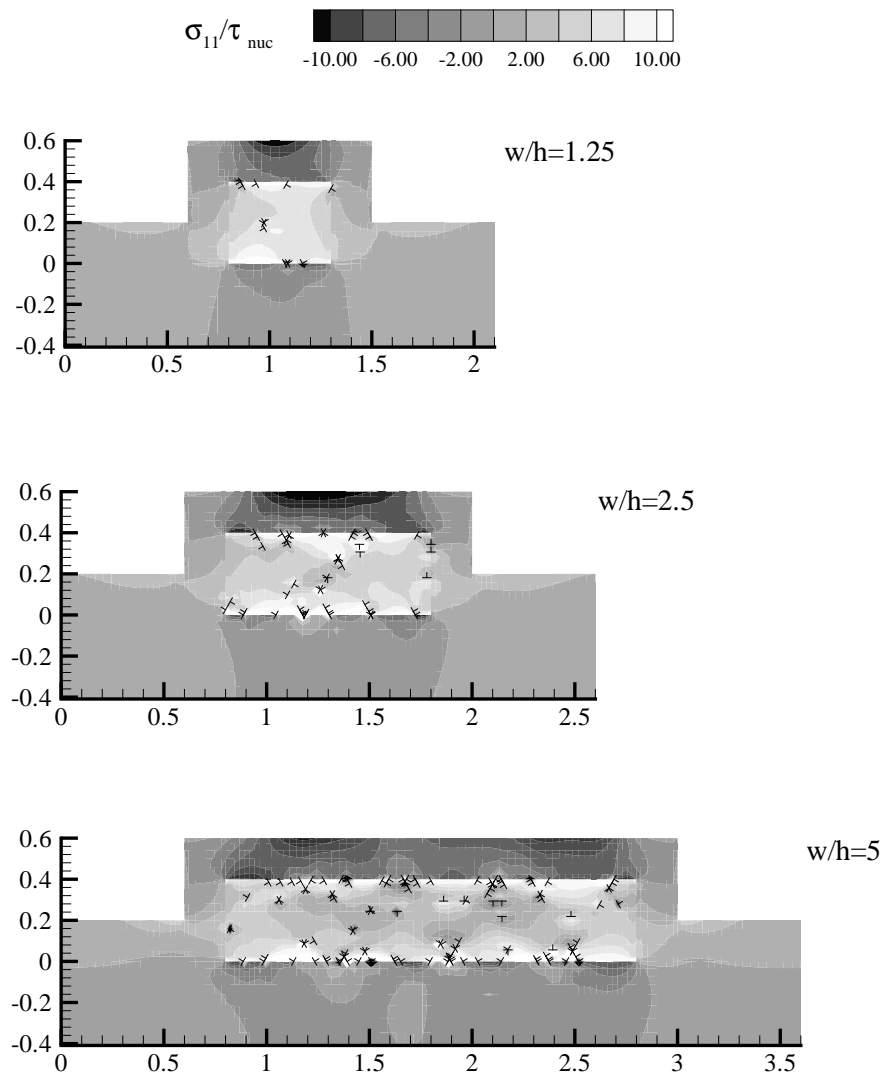


**Figure 4.14** Average in-plane stress as a function of  $\Delta T$  for lines with various aspect ratios.

#### 4.4 Conclusions

Discrete dislocation results have been presented on the evolution of thermal stresses in metal interconnects. A comparison of the mechanical response of lines characterized by the same cross-sectional area shows that:

- the stress that develops in lines with a height-to-width ratio near to or greater than one is nearly hydrostatic. As a consequence, plastic relaxation by dislocation motion is not effective in minimizing the internal stress in these lines;
- lines with a height-to-width ratio that is significantly less than one develop a stress state that has a large deviatoric part so that substantial relaxation by dislocation motion occurs. The dislocations form pile-ups at the substrate and passivation layer interfaces, which give rise to hard boundary layers;
- even if the height-to-width ratio is significantly less than one, plastic relaxation is inhibited if the height of the line is comparable to the dislocation nucleation length (the diameter of a stable loop nucleated from a Frank-Read source). In this case, the average distance of the sources to the line



**Figure 4.15** In-plane stress and dislocation distribution after cooling by 200K.

boundaries is small enough for the back stress associated with the boundary dislocation pile-ups to retard nucleation throughout the line;

- the effectiveness of plastic relaxation is orientation dependent. In the cal-



culations here, plastic relaxation is more effective for crystals with  $\phi^{(\alpha)} = (30^\circ, 90^\circ, 150^\circ)$  (BCC-type) than for crystals with  $\phi^{(\alpha)} = (0^\circ, 60^\circ, 120^\circ)$  (FCC-type);

- a shorter pitch tends to reduce the hydrostatic stress in the line, because of a reduction in the stress parallel to the line-substrate interface;
- the difference between the thermal expansion coefficients of the substrate and the passivation layer, as well as the elastic mismatch between the line, the passivation layer and the substrate have been neglected in the calculations here. Accounting for these differences will alter the hydrostatic part of the elastic stress state and thereby the subsequent stress relaxation.

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