MODELING OF X-RAY DIFFRACTION STRESS ANALYSIS IN POLYCRYSTALLINE INTERCONNECTS WITH SHARP FIBER TEXTURES

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ABSTRACT

The microstructural model of a polycrystalline aggregate and an associated finite element model have been developed to help interpret the x-ray diffraction experimental results of strain measurements in terms of relations between the measured strains and macroscopic stress states in polycrystalline aluminum and copper interconnects. The interconnects had a sharp [111] fiber textures or a combination of [111] and [100] fiber texture components. The sin²ψ vs. εᵧᵧ plots based on finite element simulations of thermal expansion mismatch stresses were constructed for both aluminum and copper interconnects. The effects of the single crystal anisotropy, grain orientation (texture), and associated plastic inhomogeneity on the strain distribution and shape of the sin²ψ versus εᵧᵧ plots were probed. The strain distributions in two distinct groups of grains having [111] and [100] orientations were used to discuss the problems associated with reconstructing the macroscopic stress state from x-ray diffraction measurements of strains.

BACKGROUND

The x-ray diffraction is the most commonly used technique for measuring stresses in thin metal lines, or interconnects on semiconductor devices. The strain (residual or applied) is measured as a change in the inter-atomic spacing in groups of grains favorably oriented for diffraction at several tilt angles measured from the surface normal, that is, the so-called sin²ψ technique. For an elastically isotropic, homogeneous material the macroscopic stress is then calculated using the tensor transformation and elasticity theory, e.g. [Noyan87]. For micron or sub-micron thick and wide, strongly textured (therefore elastically anisotropic and only periodically homogeneous) polycrystalline interconnect lines the diffracting grain population is small and the boundary conditions for the elastic fields are different from those for a blanket thin film. A fundamental issue, addressed in this project, is whether the macrostress can be recalculated unambiguously from local strains measured by x-ray diffraction in these interconnects. The local strains originate from the elastic anisotropy (grain-to-grain interactions) and nonhomogeneous plastic deformation (orientation dependent yield function).

The microstructure of the metallic interconnect is simulated as a Laguerre tessellation (Fig.1) which has been proven to be a topologically correct representation of a single-phase alloy [Xue97a]. The model interconnect, shown schematically in Figure 2, is composed of 20 grains representing a near-bamboo structure, typical for conventional
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(not damascene) deposition processes. Each grain is divided into a large number of finite elements. Totally, 40,000 3-D elements are used, with the elastic and plastic properties consistent with its crystallographic orientation. The distribution of the thermal expansion mismatch strains and stresses in such a polycrystalline aggregate is studied for aluminum and copper interconnects deposited on an [100]-orientated silicon single crystal. The most common [111] fiber texture [Hurd98, Tracy94] with a random in-plane rotation is considered for aluminum interconnects. A more complex case is studied for Cu interconnects which contain different volumetric fractions of [111] and [200] fiber textures as well as a random texture component [Harper97, Tracy93].

The residual strains are calculated at a specific ($\phi$, $\psi$) direction defined in Figure 3 in order to simulate the x-ray diffraction experiments. The $\sin^2\psi$ versus strain ($\varepsilon_{\psi}$) plots are constructed for both aluminum and copper interconnects. The effects of the single crystal anisotropy, grain orientation (crystallographic texture), and associated plastic inhomogeneity on the strain distribution and shape of $\sin^2\psi$ vs. $\varepsilon_{\psi}$ plots are discussed. The numerical simulations of x-ray diffraction experiments are used to interpret the experimental results in terms of relations between the measured strains and macroscopic stress states in interconnects.

Figure 1. Aluminum thin film bounded on silicon substrate is idealized as a Laguerre tessellation. An interconnect is a portion of the tessellation as shown in the center of the film.
Figure 2. A schematic of a metal interconnect. In state-of-the-art IC's, the grains, denoted as g₁ to g₅ in this figure, have the so-called columnar structure. The top and underneath dielectric materials are multiple layers.

Figure 3. Three coordinate systems used. Pᵢ, specimen coordinate system; Lᵢ, laboratory coordinate system; Xᵢ, crystal coordinate system.

METHOD

The residual stresses due to thermal expansion coefficient mismatch are calculated when the system temperature changes from deposition or annealing temperature (which may be as high as 400°C) to 25°C. By weighting the element stresses with its volume, that is

\[ \sigma_{y}^{w} = \frac{v}{\bar{v}} \sigma_{y} \]  \hspace{1cm} (1)

where \( v \) is the volume of an element, and \( \bar{v} = \sum_{m} v/m \) is the mean volume of elements in the interconnect composed of \( m \) elements, we calculate macrostress tensor in the form:
\[ \bar{\sigma}_v = \frac{1}{m} \sum_m \sigma_i^w \]  

(2)

This tensor is used as a reference in assessing different methods of stress calculations.

The simulated x-ray diffraction data are generated from the FEM-computed residual microstresses at 25°C as follows. Denoting the direction specified by angles \( \psi \) and \( \phi \) as direction \((\psi, \phi)\) (see Figure 3), and the microstrain in an FEM element as \( \varepsilon = [\varepsilon_{11} \, \varepsilon_{22} \, \varepsilon_{12} \, \varepsilon_{13} \, \varepsilon_{23}] \), the volume-weighted microstresses of the element \( \varepsilon_{33}^{Lw} \) are calculated with Equation 3 by replacing \( \sigma_i^w \) with volume-weighted microstresses \( \sigma^w_{ij} \).

\[ \varepsilon_{33}^{Lw} = \varepsilon_{11} \cos^2 \phi \sin^2 \psi + \varepsilon_{12} \sin 2\phi \sin^2 \psi + \varepsilon_{22} \sin 2\phi \sin^2 \psi + \varepsilon_{33} \cos^2 \psi + \varepsilon_{13} \cos \phi \sin 2\psi + \varepsilon_{23} \sin \phi \sin 2\psi \]  

(3)

where:

\( \varepsilon_{ij} = S^{w}_{ij} \sigma_{ij} \)

For different crystallographic orientations, each grain has a different compliance coefficient matrix:

\[ S_{ijkl}^{w} = a_{im} a_{jn} a_{kp} a_{lq} S_{mpq} \]

where \( a_{ij} \) are the direction cosines between sample coordinate system \( P_i \) and the [100] crystal axes of the grain, or the \( X_i \) coordinate system. Given an orientation matrix of the grain, nine direction cosines are known, whereby, the value of \( S_{ijkl}^{w} \) can be computed. The Al and Cu single crystal compliance coefficient matrix \( S \) is given by

\[
S = \begin{bmatrix}
S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\
S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\
S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & S_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & S_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & S_{44}
\end{bmatrix}
\]

The elastic compliance's of Al and Cu single crystal (in units of \( 1/P\alpha \), [Tanaka97a, Noyan87]) are

\[\text{Al} : \begin{align*}
S_{11} &= 1.59 \times 10^{-11} \\
S_{12} &= -5.78 \times 10^{-12} \\
S_{44} &= 3.54 \times 10^{-11}
\end{align*} \]

\[\text{Cu} : \begin{align*}
S_{11} &= 1.50 \times 10^{-11} \\
S_{12} &= -6.30 \times 10^{-12} \\
S_{44} &= 1.33 \times 10^{-11}
\end{align*} \]

The volume-weighted macrostrain in direction \((\psi, \phi)\) is consequently calculated as:

\[ \bar{\varepsilon}_{33}^{Lw} = \frac{1}{m} \sum_m \varepsilon_{33}^{Lw} \]  

(4)

RESULTS AND DISCUSSION

The finite element model was used to simulate the x-ray diffraction measurements of residual stresses in textured polycrystals. The most common technique for measuring residual strains is based on Equation 3, e.g., [Noyan 87]. It uses the \( \sin^2 \psi \) versus strain \( \varepsilon_{33} \) plots determined experimentally at different \( \psi \) angles (at least three \( \psi \) orientations are...
needed for determination of a full strain tensor, e.g., $\psi=0, 45^\circ$, and $90^\circ$). The $\sin^2 \psi$ versus $\epsilon_{\phi\psi}$ plots were constructed for the following cases.

1. **Strong [111] fiber texture.** In this case we studied the effects of crystallographic texture and single crystal anisotropy on the shape of the $\sin^2 \psi$ plots. The elastic anisotropy of the shear moduli of the face centered cubic (fcc) crystals is conveniently described by the Zener parameter:

$$A = 2c_{44}/(c_{11} - c_{12})$$

where $c_{ij}$ are the stiffness constants. The parameter $A$ is 1 for isotropic crystals and it’s excursion from unity represents the degree of elastic anisotropy. For aluminum $A=1.23$; copper is highly anisotropic with $A=3.21$. The examples of simulation results for unpassivated aluminum (cooled from 400°C) and copper (cooled from 500°C) interconnects are shown in Figures 4 and 5. In both cases the grains had the $\langle 111 \rangle$ directions spread in the range of 20 degrees from the interconnect plane.

In the case of aluminum (low elastic anisotropy) the $\sin^2 \psi$ versus $\epsilon_{\phi\psi}$ plot is linear despite the strong [111] texture. Such linear plots have been observed experimentally using x-ray diffraction, e.g. [Tanaka97b]. In contrast the blanket films usually display some deviation from linearity [Tanaka97a]. The fact that the $\sin^2 \psi$ versus $\epsilon_{\phi\psi}$ plots are linear is of practical importance. In materials with sharp texture the x-ray diffraction experimental data can be limited to two or maximum three points corresponding to the intensity poles of reflection, which enforces the assumption of linearity.

In the case of copper (high elastic anisotropy) the $\sin^2 \psi$ versus $\epsilon_{\phi\psi}$ plots show some curvature as well as some deviation in strain caused by the elastic grain-to-grain interactions (different grain orientation sets). If the grain population is not kept constant during the x-ray diffraction measurements, the experimental $\sin^2 \psi$ versus $\epsilon_{\phi\psi}$ plots may show oscillations. The range of oscillations could be determined from the upper and lower limits on the simulated curves.

![Figure 4. Residual strains in the direction parallel to the aluminum interconnect lines as a function of $\sin^2 \psi$. The standard deviation of $\epsilon_{\phi\psi}$ is too small to be represented in the graph. Aluminum line was modeled as elastic-linear strain hardening-perfectly plastic [Xue97].](image_url)
2. [111] and [100] fiber texture components with orientation independent yield criterion.

In this case we studied the distribution of strains between two distinct groups of grains. In a passivated copper interconnect section with 20 grains, 17 grains had a [111] crystallographic orientation (81% volume) and the remaining 3 grains had a [100] crystallographic orientation (19% volume). The thermal stresses were calculated when the system temperature changed from 100°C to 25°C. All grains were modeled as elastic-perfectly plastic with the yield strength σ_y = 470 MPa at room temperature and von Mises yield criterion. Therefore, the strain inhomogeneity was caused mostly by the elastic anisotropy. The stress tensors were calculated for each grain population and for the entire interconnect, respectively. The results are presented in Table 1. The simulated sin²ψ versus εψ plots are shown in Figures 6-8. During cooling from 100°C to 25°C the deformation is predominantly elastic since the average von Mises stresses for [111] and [100] grains are approximately 170 MPa and 90 MPa, respectively. The sin²ψ versus εψ plots show that the strains in the [100] population are higher than those in the [111] population due to the higher in-plane stiffness of the [111] oriented grains (the ratio of Young’s moduli in the ⟨111⟩ and ⟨100⟩ directions for copper single crystal is 3.2). For the same reason the residual stresses are higher in the [111] population when the proper, orientation dependent elastic moduli are used. The use of the “bulk” elastic moduli would have led to the erroneous results. The issues related to reconstructing the macrostresses from strains measured in specific grain populations are discussed in the next section.
3. [111] and [100] fiber texture components with orientation dependent yield criteria. The model described in the previous section was used. However, recognizing that each grain deforms like a single crystal, i.e. by slip on (111)<110> slip systems, the orientation dependent yield criteria were applied to the [100] oriented grains. The yield stress of a particular grain with the <hkl> orientation is determined as follows [e.g., Jawarani95]:

$$\sigma_y = \frac{\tau_c}{\cos \theta \cos \lambda \sin \alpha}$$

where: $\tau_c$ is the critical resolved shear stress, $\theta$ is the angle between the projection of the <111> direction of the grain on the wafer plane and the longitudinal direction of the interconnect, $\lambda$ is the angle which the Burger vector makes with the wafer plane, and $\alpha$ is the angle between (hkl) direction and <111> direction. It was assumed that all grains with the <111> orientation had the same yield stress $\sigma_y = 470$ MPa at room temperature, and the yield stress of the [100]-oriented grains was a function of their in-plane orientation (i.e., a function of angle $\theta$). The orientation dependent yield criterion allowed us to study the residual stresses due to inhomogeneous deformation. Generally speaking the [100] oriented grains deformed plastically at lower stress levels than the [111] grains, which is in agreement with the experimental observations, e.g. [Schwarzer93]. The results of simulations are summarized in Table 2 and Figures 9-11.

Table 1. Macrostresses in passivated, plastically homogeneous copper interconnects with two texture components. The volume-weighted stresses in entire interconnects and in these two textures are computed separately.

<table>
<thead>
<tr>
<th>Stress component</th>
<th>Macrostress (MPa)</th>
<th>Stress in [111] population (MPa)</th>
<th>Stress in [100] population (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{11}$</td>
<td>215</td>
<td>247</td>
<td>188</td>
</tr>
<tr>
<td>$\sigma_{22}$</td>
<td>128</td>
<td>131</td>
<td>125</td>
</tr>
<tr>
<td>$\sigma_{33}$</td>
<td>73</td>
<td>53</td>
<td>90</td>
</tr>
<tr>
<td>$\sigma_{12}$</td>
<td>-2</td>
<td>-2</td>
<td>-2</td>
</tr>
<tr>
<td>$\sigma_{13}$</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$\sigma_{23}$</td>
<td>0</td>
<td>-1</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2. Macrostresses in passivated, plastically inhomogeneous copper interconnects with two texture components. The volume-weighted stresses in entire interconnects and in these two textures are computed separately.

<table>
<thead>
<tr>
<th>Stress component</th>
<th>Macrostress (MPa)</th>
<th>Stress in [111] population (MPa)</th>
<th>Stress in [100] population (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{11}$</td>
<td>644</td>
<td>241</td>
<td>986</td>
</tr>
<tr>
<td>$\sigma_{22}$</td>
<td>402</td>
<td>130</td>
<td>632</td>
</tr>
<tr>
<td>$\sigma_{33}$</td>
<td>197</td>
<td>53</td>
<td>318</td>
</tr>
<tr>
<td>$\sigma_{12}$</td>
<td>-6</td>
<td>-2</td>
<td>-9</td>
</tr>
<tr>
<td>$\sigma_{13}$</td>
<td>-24</td>
<td>5</td>
<td>-45</td>
</tr>
<tr>
<td>$\sigma_{23}$</td>
<td>-50</td>
<td>-1</td>
<td>-91</td>
</tr>
</tbody>
</table>
Figure 6. Mean strains in $(\phi, \psi)$-direction when $\phi=0$ in the interconnect where all grains have the same yield strength. Legend: $\bullet$ stands for the mean strain in the entire interconnect, $\triangle$ stands for the mean strain in [111] texture, $\blacksquare$ stands for the mean strain in [100] texture. The strain curve starts at $\psi=0$ and terminates at $\psi=\pi/2$ or $-\pi/2$.

Figure 7. Mean strains in $(\phi, \psi)$-direction when $\phi=45^\circ$ in the interconnect where all grains have the same yield strength. Legend: $\bullet$ stands for the mean strain in the entire interconnect, $\triangle$ stands for the mean strain in [111] texture, $\blacksquare$ stands for the mean strain in [100] texture. The strain curve starts at $\psi=0$ and terminates at $\psi=\pi/2$ or $-\pi/2$.

Large residual strains developed in the [100]-oriented grain population. High hydrostatic stresses are present as well as relatively high shear stresses which cause so called “$\psi$-splitting”. The stresses in the [111] population have not changed as compared with the case studied in Section 2.
Figure 8. Mean strains in (φ, ψ)-direction when φ=90° in the interconnect where all grains have the same yield strength. Legend: ● stands for the mean strain in the entire interconnect, ▲ stands for the mean strain in [111] texture, ■ stands for the mean strain in [100] texture. The strain curve starts at ψ=0 and terminates at ψ=π/2 or -π/2.

Figure 9. Mean strains in (φ, ψ)-direction when φ=0 in the interconnect where each individual grain in [100] texture has its specific yield strength σ_y depending its in-plane rotation. Legend: ● stands for the mean strain in entire interconnect, ▲ stands for the mean strain in [111] texture, ■ stands for the mean strain in [100] texture. The strain curve starts at ψ=0 and terminates at ψ=π/2 or -π/2.

The x-ray diffraction analysis would need to account for the triaxial stress state and the presence of the shear stresses. The two available solutions are the Dölle-Hauk method [Dölle77] and the generalized least-squares method [Winholtz88]. They can be used to determine the residual strain tensor. The stress analysis is complicated by several issues discussed below.
Figure 10. Mean strains in (ψ, ψ)-direction when ϕ=45 in the interconnect where each individual grains in [100] texture has its specific yield strength σ, depending its in-plane rotation. Legend: ◇ stands for the mean strain in entire interconnect, ▲ stands for the mean strain in [111] texture. ■ stands for the mean strain in [100] texture. The strain curve starts at ψ=0 and terminates at ψ=π/2 or ~π/2.

Figure 11. Mean strains in (ψ, ψ)-direction when ϕ=90 in the interconnect where each individual grains in [100] texture has its specific yield strength σ, depending its in-plane rotation. Legend: ◇ stands for the mean strain in entire interconnect, ▲ stands for the mean strain in [111] texture. ■ stands for the mean strain in [100] texture. The strain curve starts at ψ=0 and terminates at ψ=π/2 or ~π/2. The oscillatory curve represents a hypothetical data obtained from two different grain orientations.

In strongly textured materials such as interconnects the x-ray diffraction measurements of residual strains/stresses are based on limited data. In general, only the diffraction peaks at the intensity poles are detectable. For example, while using CuKα radiation and (331) reflection on copper interconnect the following tilt angles ψ are used:

- for the [111]-oriented grains ψ=22° 0’, 48°32’, 82°23’,
- for the [100] oriented grains ψ=46°30’, 76°44’.
From Figures 9–11 it is obvious that:
- Measuring strains in one population only would lead to significant errors in residual stress determination. Due to orientation dependent yield stresses (plastic inhomogeneity) the strains in each population are significantly different.
- Due to \( \psi \)-splitting the measurements need to be done at positive and negative \( \psi \)-tilts.
- Combining data from \( \psi \)-tilts corresponding to intensity pole from different grain populations would result in oscillatory curves and incorrect stress values. Such a hypothetical curve is shown in Figure 11. It was derived by connecting the data points corresponding to intensity poles for [100] and [111] populations.
- Strains need to be measured in both populations.
- Macroscopic residual stress may be determined unambiguously through modeling of grain interactions.
- While calculating stresses from measured strains the proper elastic constants have to be used. The methodology for converting strains to stresses in strongly textured polycrystals has been developed and is presented elsewhere in these proceedings.

**SUMMARY**

The microstructural model of a polycrystalline aggregate and an associated finite element model have been developed to help interpret the x-ray diffraction experimental results of strain measurements in terms of relations between the measured strains and macroscopic stress states in polycrystalline aluminum and copper interconnects. The modeled interconnects had a sharp [111] fiber texture or a combination of [111] and [100] fiber texture components. The \( \sin^2 \psi \) versus \( \varepsilon_{\psi\psi} \) plots based on finite element simulations of thermal expansion mismatch stresses were constructed for both aluminum and copper interconnects. The effects of the single crystal anisotropy, grain orientation (texture), and associated plastic inhomogeneity on the strain distribution and shape of the \( \sin^2 \psi \) vs. \( \varepsilon_{\psi\psi} \) plots were probed. The strain distributions in two distinct groups of grains having [111] and [100] orientations were used to discuss the problems associated with reconstructing the macroscopic stress state from x-ray diffraction measurements of strains.

For aluminum interconnects with predominantly one texture component, i.e. [111] fiber, the \( \sin^2 \psi \) plots are linear. The fact that the \( \sin^2 \psi \) plots are linear is of practical importance since due to sharp texture the x-ray diffraction experimental data is usually limited to two or three points corresponding to the intensity poles of the reflection used for measurements. In the case of copper (high elastic anisotropy) the \( \sin^2 \psi \) plots show some curvature as well as some deviation in strain caused by the elastic grain-to-grain interactions. If the grain population is not kept constant during the x-ray diffraction measurements, the experimental \( \sin^2 \psi \) plots may show oscillations.

In the case of textures composed of two distinct orientations with comparable volume fractions the strains in each grain populations are significantly different due to elastic grain-to-grain interactions and inhomogeneous plastic deformation. The modeling allows one to design and interpret the x-ray diffraction experiments. In particular the following observations were derived:
- Measuring strains in one population only would lead to significant errors in residual stress determination.
- Due to \( \psi \)-splitting the measurements need to be done at positive and negative \( \psi \)-tilts.
-Combining data from $\psi$-tilts corresponding to intensity pole from different grain populations would result in oscillatory curves and incorrect stress values.
-Macroscopic residual stress may be determined unambiguously through modeling of grain interactions.
-To calculate stresses from measured strains the proper elastic constants have to be used. The methodology for converting strains to stresses in strongly textured polycrystals has been developed and is presented elsewhere in these proceedings.

REFERENCES