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EFFECTS OF TRANSVERSE TEMPERATURE FIELD NONUNIFORMITY ON STRESS IN SILICON SHEET GROWTH

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Stress and strain rate distributions are calculated using finite element analysis for steady-state growth of thin silicon sheet with temperature nonuniformities imposed in the transverse (sheet width) dimension. Significant reductions in residual stress are predicted to occur for the case where the sheet edge is cooled relative to its center provided plastic deformation with high creep rates is present.

1. Introduction

Growth speed limitations arise in attempts to produce thin silicon sheet because high interface region axial temperature gradients required to maintain growth stability lead to thermoelastic stresses that are sufficient to buckle the ribbon and make it unsuitable for fabrication into solar cells [1,2]. A number of observations have led to the conjecture that transverse temperature variations, i.e., those occurring across the sheet width, can lead to reduction of stress by compensating for the stress produced by axial temperature nonuniformities [3]. If transverse isotherm shapes can be found that can be experimentally imposed, and are consistent with the high axial interface temperature gradients necessary to maintain stable growth, then it may be possible to achieve greater growth speeds before buckling occurs. In principle, for stress-driven inelastic deformation (powerlaw creep, for example) it is possible to demonstrate via a static thermoelastic analysis that there exist two-dimensional temperature distributions with transverse isotherm variations which produce zero stress in the sheet [4]. However, the temperature distributions required do not appear to be practical for maintaining high speed sheet growth. For the temperature distributions considered earlier [1], which are compatible with maintaining the necessary high interface temperature gradients, stresses will inevitably appear, and the sensitivity of high temperature creep to stress levels will lead to optimal profiles which then are quite different.

We have previously shown that plastic deformation has a dominant influence on the stress distributions set up in a thin silicon sheet grown under steady-state conditions [1]. Stress and strain rate distributions were calculated for several axial temperature profiles used to achieve interface gradients sufficient to sustain growth speeds of 3 cm/min and above for thin $(200-300 \, \mu \text{m})$ silicon sheet. Only the effect of temperature nonuniformities in one dimension, the axial (growth) direction, was examined. Uncertainty in the form of the constitutive relationship for creep appropriate for describing stress relaxation during growth limited

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quantitative application of the results and only secondary creep was modeled. More recent experimental studies [5,6] indicate that creep rates are likely to be even higher than those assumed in these initial modeling attempts.

We extend our initial analysis here by considering the influence of temperature nonuniformities in two dimensions, along the growth direction and in the transverse or sheet width direction, on sheet stress distributions and on residual (room temperature) stress. Creep rates are increased by a factor of one hundred over those used earlier. The details for the temperature field and creep representation are discussed in section 2. Results and discussion of implications of stress on growth limits are presented in sections 3 and 4.

2. Temperature field and creep representations

Axial temperature profiles used in high speed sheet growth usually have interface temperature gradients in the solid of the order of 500–1000°C/cm. They may either monotonically decrease to room temperature thereafter or include a reheat region to maintain temperatures above 1100°C, where there is sufficient creep, for a longer time to anneal out residual stress that is large enough to fracture or buckle the sheet. For

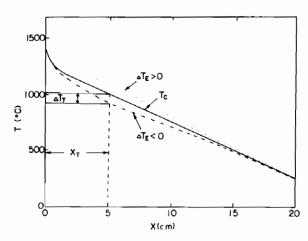


Fig. 1. Details of temperature profile nonuniformities imposed on sheet with cooler (dashed line) or hotter (dotted line) edges in relation to the centerline (solid line).

simplicity, we consider here axial temperature profiles of the shape shown in fig. 1 for the sheet centerline and edge. At the sheet centerline we use a profile T_c consisting of a high temperature exponential portion and a linear region:

$$T_{\rm c}(x) = T_0 \exp\left[-(G_{\rm I} - G_{\rm R})x/T_0\right] + G_{\rm R}(L - x) + T_{\rm R},$$
 (1)

with

$$T_0 = T_{\rm M} - T_{\rm R} - G_{\rm R}L,$$

where $T_{\rm M}$ and $T_{\rm R}$ are the silicon melting point (1685 K) and room temperature (300 K), respectively, and the centerline temperature falls to $T_{\rm R}$ at a growth distance x equal to L (taken to be 20 cm). The profile is parameterized by an interface (x=0) temperature gradient $G_{\rm I}$ and a room (x=L) gradient $G_{\rm R}$.

The transverse isotherm variation is represented by a function $\Delta T_{\rm E}(x, y)$ such that the two-dimensional sheet temperature field is written:

$$T(x,y) = T_c(x) + \Delta T_E(x,y), \tag{2}$$

where $\Delta T_{\rm E}$ represents the deviation from $T_{\rm c}$ at each axial location x.

Two different transverse isotherm functional dependences have been investigated. In the one case a parabolic change in temperature between the center and edge was modeled; the other case studied was a sinusoidal variation. These introduce extremes in transverse isotherm shape that give a profile which has either a maximum or a zero gradient at the sheet edge, respectively. Qualitatively, the results are similar, but the latter represents more closely the experimental situation encountered in a thin sheet. Transverse temperature gradients that can be supported in practice are a function of the thickness for a given sheet ambient temperature field, because conduction tends to smooth out radiation field variations. The case of a finite width ribbon in an enclosure with varying parabolic transverse wall temperature has been studied in detail [7]. For a ribbon thickness of 300 µm and an imposed 100°C temperature difference between the enclosure wall centerline and edge, the ribbon can support a temperature

difference of only 55°C, with maximum transverse gradients of the order of 30-40°C/cm. These values increase as sheet thickness decreases, so that temperature differences of the order of 100°C can be supported between the sheet center and edge in practice.

The following discussion, therefore, will concern results obtained with $\Delta T_{\rm E}$ given by

$$\Delta T_{\rm E}(x,y) = \Delta T(x) \sin^2(\pi y/2W), \tag{3}$$

where 2W is the sheet width (taken to be 5 cm). $\Delta T(x)$ represents the temperature difference between center and edge,

$$\Delta T(x) = \Delta T_{\rm T} (x/x_{\rm T})^2 \exp[2(1-x/x_{\rm T})],$$
 (4)

and is parameterized by a maximum amplitude, $\Delta T_{\rm T}$, and the distance from the interface at which that maximum is imposed, $x_{\rm T}$. $\Delta T(x)$ is zero and has zero gradient at the interface and for large x (see fig. 1). Both the cases of the sheet cooled ($\Delta T_{\rm T} < 0$) and heated ($\Delta T_{\rm T} > 0$) with respect to the centerline are considered.

Recent experimental work [5] on steady-state creep determinations suggests that secondary creep in silicon above 1000°C is more intense than even the "high creep" representation used in ref. [1], with a factor of 40 increase not untypical. In addition, primary creep intensities for very short times (up to 10 s) are comparably large [6]. A

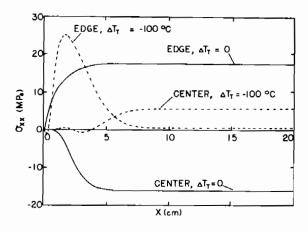


Fig. 2. Comparison of σ_{xx} variations along the sheet centerline and edge for cases of flat transverse isotherms ($\Delta T_{\rm T} = 0$) and cooler edges ($\Delta T_{\rm T} = -100\,^{\circ}$ C), with V = 1 cm/min and $x_{\rm T} = 1$ cm.

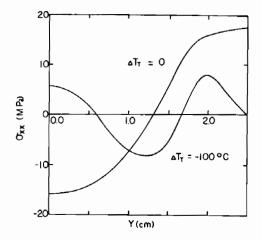


Fig. 3. Comparison of σ_{xx} variations across the sheet width at room temperature (x = 20 cm) for conditions as in fig. 2.

means to incorporate primary creep into the present formalism does not appear to be warranted because it would simply lead to replacement of one set of constants in the constitutive relation by another, for example, involving unknown dislocation nucleation and multiplication rates. This does not appear to allow new physics to be introduced at this time because of a scarcity of relevant data. Thus, we choose to retain the creep representation used in ref. [1] to study the effects of transverse isotherm nonuniformity in the present work.

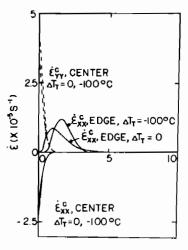


Fig. 4. Comparison of creep strain rates along sheet centerline and edge for conditions as in fig. 2.

3. Results

Stress and strain rate distributions and residual stress reductions predicted to occur with transverse isotherm nonuniformities are presented in figs. 2-5. The case of $G_1 = 500\,^{\circ}\text{C/cm}$ and $G_R = 60\,^{\circ}\text{C/cm}$, with the creep intensity increased by a factor of 100 over the "high creep" case of ref. [1], is illustrated in detail in figs. 2-4. Graphs of the principal stress component σ_{xx} along the sheet centerline and at its edge with no transverse isotherm curvature are compared to the case of $\Delta T_T = -100\,^{\circ}\text{C/cm}$ and $x_T = 1\,\text{cm}$ at $V = 1\,\text{cm/min}$

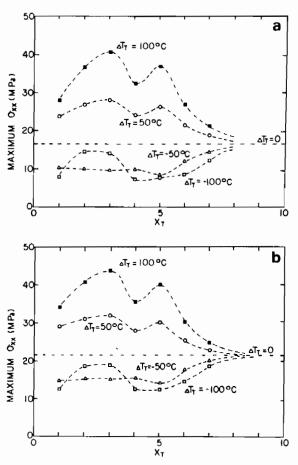


Fig. 5. Maximum residual stress reductions as a function of the degree of heating and cooling of the sheet edge (ΔT_T) and of the distance from the interface where the maximum isotherm distortion occurs (x_T) at growth speeds of (a) 1 cm/min and of (b) 3 cm/min.

in fig. 2. Residual stress (σ_{xx}) distributions across the sheet width are compared in fig. 3. The creep strain rate components (ϵ_{ij}^c) along the sheet centerline and edge are illustrated in fig. 4. Fig. 5 shows the dependence of the maximum residual stress on $\Delta T_{\rm T}$ and $x_{\rm T}$ for this same profile at V=1 and 3 cm/min for cases of cooling and heating of the sheet edge relative to the centerline.

4. Discussion

Some insight into the physical mechanisms operative in producing changes in sheet stress distributions as a result of transverse isotherm nonuniformity is gained by inspection of figs. 2-4. The variation of $\sigma_{\nu\nu}$ along the sheet is not significantly affected by the cooling of the sheet edge. The important change occurs in the σ_{xx} distribution. The sheet centerline stress is completely inverted from compressive to tensile along most of the length of the sheet, while the residual edge stress is significantly reduced from the flat isotherm value (fig. 2). However, the maximum σ_{xx} stress acting on the sheet is increased and has a peak at about 2 cm from the interface. The residual stress distribution across the sheet width increases in complexity. Fig. 3 shows that a region of compressive stress develops midway between the sheet centerline and edge as a consequence. Strain rate distributions are shown in fig. 4 for this case. The centerline $\dot{\epsilon}_{xx}^{c}$ and $\dot{\epsilon}_{yy}^{c}$ distributions are very little changed, with the major difference produced by the transverse isotherm nonuniformity being the shift of the edge $\dot{\epsilon}_{xx}^c$ distribution maximum to lower temperatures. These small changes are responsible for large proportional changes in residual stress.

Modeling of the sheet with edges heated relative to the center shows that only edge cooling produces lower sheet residual stress (fig. 5). The extent of the stress change is shown to be a complicated function of $\Delta T_{\rm T}$ and $x_{\rm T}$. A growth speed increase from 1.0 to 3.0 cm/min leads to higher residual stresses in all cases.

It should be noted that additional increases of edge cooling do not necessarily produce further decreases in residual stress. The changes are not simply related to $\Delta T_{\rm T}$ or $x_{\rm T}$ at any creep intensity, and will depend upon more detailed aspects of the temperature profile and of the creep representation. This analysis demonstrates the sensitivity of the residual stress distribution in silicon sheet to parameters such as the creep rate, $\Delta T_{\rm T}$, $x_{\rm T}$ and V. It is not intended to attach quantitative significance to the model results at this time because of the major uncertainty still surrounding the form of the creep law that is appropriate for representing stress relaxation in sheet growth. However, the results point to several fundamental effects that should not be invalidated at a qualitative level by this uncertainty:

- (1) Transverse isotherm nonuniformity can lead to higher maximum stresses in the sheet, and hence will increase the tendency for buckling to occur (see fig. 2). This will allow the sheet growth limits to be increased at low interface gradients (~500°C/cm) only while operation is well below the buckling threshold. We also find that the extent to which moderate transverse isotherm nonuniformities reduce the residual stress is inadequate to produce any significant compensation for axial temperature nonuniformities as the interface gradients are raised above 1000°C/cm in order to increase the growth speed capability. Thus, vertical sheet growth speed limits set by creep ultimately are not raised significantly through transverse isotherm variations within the present representation for the effects of creep.
- (2) Evidence that the residual stress distribution can be fundamentally altered (see fig. 3) and residual stress reduced by edge cooling is an encouraging sign that practical temperature distributions may be found for which residual stresses are essentially zero, although this will necessarily be accompanied by higher dislocation densities. Considerably more detailed information is required on the creep response in the critical region between 1000 and 1200°C, where the transverse isotherm

effects on edge strain rates are predicted to be largest in this model (fig. 4), in order to allow more quantitative significance to be attached to optimization studies that could predict these growth conditions. The detailed nature of the creep will affect the shape of the curves for $\Delta T_{\rm T} = -50\,^{\circ}{\rm C}$ and $-100\,^{\circ}{\rm C}$ shown in figs. 5a and 5b also. The minima in the region of $x_{\rm T} = 4.5$ cm appear to be a consequence of complicated interrelationships between higher temperature thermoelastic stresses and creep, in particular. Stress increases, such as in σ_{xx} in fig. 2, must be kept below levels producing buckling in order to achieve a viable solution for low residual stress growth configurations, however.

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References

- J.C. Lambropoulos, J.W. Hutchinson, R.O. Bell, B. Chalmers and J.P. Kalejs, J. Crystal Growth 65 (1983) 324.
- [2] R.G. Seidensticker and R.H. Hopkins, J. Crystal Growth 50 (1980) 221.
- [3] A.D. Morrison et al., Annual Progress Report DOE/JPL 954355/76-3 (October 29, 1975 to September 30, 1976), September 15, 1976.
- [4] S. Utku, S.K. Ray and B.K. Wada, Computers and Structures, in press.
- [5] H. Siethoff and W. Schroter, Scripta Met. 17 (1983) 393.
- [6] J.P. Kalejs et al., Quarterly Progress Report DOE/JPL 956312/84-09 (July 1, 1984 to September 30, 1984), December 15, 1984.
- [7] J.P. Kalejs et al., Quarterly Progress Report DOE/JPL 956312/83-04 (April 1, 1983 to June 30, 1983), August 15, 1983.

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