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Thermoelastic stresses in a cylinder or disk with cubic anisotropy[1]

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Abstract

The thermoelastic stresses in a crystal in the shape of a circular cylinder or disk are considered. The crystal is a cubically-orthotropic linear elastic solid, with three independent elastic properties. The cubic anisotropy renders the problem asymmetric, despite the axisymmetry of the geometry and thermal loading. This problem is motivated by a thermoelastic model used for certain crystal growth processes. Two simplifying assumptions are made here: (a) the problem is two-dimensional with plane strain or plain stress conditions, and (b) the elastic properties do not depend on the temperature. A new Fourier-type perturbation method is devised and an analytic asymptotic solution of a closed form is obtained, based on the weak cubic anisotropy of the crystal as a perturbation parameter. A general solution technique is described which yields the asymptotic solution up to a desired order. Numerical results are presented for typical parameter values. © 1999 Elsevier Science Ltd. All rights reserved.

1. Introduction

Single crystals of various materials are required for some high-performance electronic and opto-electronic devices. Crystal applications include semiconductors, laser modulators, electromechanical transducers and solar panels. Techniques for bulk crystal growth with good quality control have improved dramatically in the last 40 years (Hurle, 1993), but full understanding of the processes involved is still lacking.

One of the most popular bulk crystal growth techniques, with wide applications to semiconductors, is the Czochralski method (CZ), or its variant, Liquid Encapsulated Czochralski (LEC) (Hurle and Cockayne, 1994). This method is based on pulling the crystal from the melt. A rod holding an oriented seed is lowered to the surface of the melt contained in a crucible, and, after a

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[1] This paper is dedicated to Professor Avinoam Libai on the occasion of his 69th birthday.

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solid crystal with the desired diameter initiated, the rod is slowly pulled upwards. The crucible is externally heated in a controlled manner, to maintain the lower surface of the crystal near the melting temperature. Large-diameter cylindrical silicon (Si) crystals can be grown in this manner at a rate of a few centimetres per hour. III–V compound crystals, such as Gallium Arsenide (GaAs) and Indium Phosphide (InP), are more difficult to grow than Si, in terms of yield and quality control (Iseler, 1984).

During the bulk growth process, the main load that acts on the solid crystal is the thermal load due to the non-uniform temperature distribution that exists in the CZ growth chamber and, as a consequence, in the crystal itself. Si, GaAs and InP are all anisotropic crystals with *cubic symmetry*. The thermal load gives rise to a stress field, which in turn induces a field of dislocations in the crystal that has a very important effect on its quality. Therefore, it is important to estimate the thermal stress distribution in the crystal.

There have been various attempts to mathematically model the stress problem in cylindrical crystals. Some of the models are based on linear thermoelasticity (Jordan et al., 1981, 1984), and others on thermo-viscoplasticity (Lambropoulos et al., 1983; Volkl and Muller, 1989). Typically the CZ process is extremely slow compared to the solid-mechanics time scale, and so the elastic or viscoplastic problem may be regarded as quasi-static, and no inertia effects have to be considered. Full CZ models should be three-dimensional and anisotropic, although it is common to consider two-dimensional (axisymmetric) and isotropic models for simplicity (Iwaki and Kobayashi, 1981, 1986). The problem is inherently three-dimensional even when the geometry and temperature distribution are axisymmetric, due to the cubic orthotropy of the crystal. However, the deviation from two-dimensional isotropic conditions is typically not very large, and thus the simplified models may sometimes be useful in providing crude solutions. Lambropoulos (1987) investigated the regimes of validity of the isotropic assumption. The anisotropic problem has been attacked using numerical methods, such as finite element analysis (Dupret and van den Bogaert, 1994; Tsai, 1991).

In this paper, we consider the thermoelastic stresses in a cylindrical crystal. The crystal is a cubically-orthotropic linear elastic solid, with *three* independent elastic properties. Thus, the geometry of the problem is cylindrical whereas the material properties are Cartesian. We devise a new Fourier-type regular perturbation method, and obtain an asymptotic solution, based on the weak cubic anisotropy of the crystal. That is, we use the deviation of the elastic moduli tensor from that of an isotropic material as a perturbation parameter, and expand the solution in a perturbation series in powers of that parameter. This results in a *closed-form analytical solution* to the problem. We derive the first-order solution in detail, and we also show how to obtain a high-order solution for any desired order. The measure of anisotropy of the crystal material determines the required number of terms in the perturbation series. Also, the higher the order of the asymptotic solution is, the larger is the number of cylindrical harmonics that can be captured in it.

In developing the solution, we make two main simplifying assumptions:

(a) the problem is two-dimensional with plane strain or plane stress conditions, namely variation in the axial direction is neglected, and
(b) the elastic properties do not depend on the temperature, and thus the crystal is homogeneous.

Assumption (a) is the more limiting one. It is physically justified only *if the axial temperature* *gradient is much smaller than the radial gradient*, or if the crystal under consideration is a *thin disk*. In the former case, the axial gradients may be neglected compared to the in-plane gradients, which justifies a plane strain assumption for each plane. Thus, the three-dimensional problem can be replaced by a sequence of independent two-dimensional problems, each of which is associated with a certain cross section of the cylinder. Although the case of small axial gradients is not very common (since it means a slow crystal growth rate), it does exist and is of interest in practice since a small gradient in the growth direction in a CZ process ensures a high quality crystal (Borolev et al., 1995). The case of a disk is relevant if the crystal is grown as a thin film on a circular wafer (Hurle, 1994). In this case the plane stress assumption is justified.

The advantage of the present approach is fourfold. First, to the best of our knowledge this is the *first closed-form analytical solution* available which takes into account the *anisotropy* of the crystal. Also, the present approach of using a measure of the anisotropy as a perturbation parameter is unique. Analytic solution for the solid crystal problem do exist, even in three dimensions (e.g., Iwaki and Kobayashi, 1981, 1986), but only under the assumption of isotropy. The availability of an analytical solution that does not depend on the performance of a specific numerical code is certainly important. Second, such an analytic solution can be very useful in serving as a simple *benchmark* in testing and evaluating the performance of numerical codes. Third, the solution presented here is useful in *solving certain practical problems* in solid crystals, in the limited cases mentioned in the previous paragraph. Finally, the approach adopted here may serve as the *first step in developing a three-dimensional solution procedure* which is appropriate for more general problems. Such a procedure is currently under investigation.

Following is the outline of the paper. In Section 2, we state the thermoelastic problem under investigation. In Section 3, we present the asymptotic solution to this problem. We employ the well-known zero-order isotropic solution (Landau and Lifshitz, 1986) to deduce the first- and higher-order analytic approximations to the exact solution. The solution is presented simultaneously for the plane strain and the plain stress cases. In Section 4, some specific solutions are worked out for typical parameters. We conclude the paper with some remarks in Section 5.

2. Mathematical preliminaries. Problem formulation

We consider a long elastic cylinder under plane strain conditions. The cross section of the cylinder is a circle of radius R centred at the origin of the XY-plane. For any system of orthogonal coordinates (η_1, η_2) the equilibrium equations in the elastic stresses σ_{ij}, $i, j = 1, 2$ takes the form (Landau and Lifshitz, 1986)

$$\boldsymbol{div}\,\sigma(\eta_1,\eta_2)+\boldsymbol{F}(\eta_1,\eta_2) = 0; \quad \sigma = \{\sigma_{ij}\}; \quad \sigma_{12} = \sigma_{21} \tag{2.1}$$

The detailed expressions for the divergence of a symmetrical tensor involve the metric of the coordinate system (Landau and Lifshitz, 1975).

In the above $\boldsymbol{F} = (f_1, f_2)$ designates the mass forces of various physical nature. Particularly, for a non-uniformly heated solid, $\boldsymbol{F}$ is proportional to the temperature gradient:

$$\boldsymbol{F} = A\,\boldsymbol{grad}\,T(\eta_1,\eta_2) \tag{2.2}$$

From here on Cartesian (x, y) and polar coordinates (r, θ) will be used in parallel. In both systems the elastic response of an *isotropic* material is described by the following constitutive relation

$$\begin{pmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{12}\end{pmatrix} = \gamma\begin{pmatrix}C_{11} & C_{12} & 0\\ C_{12} & C_{11} & 0\\ 0 & 0 & C_{44}\end{pmatrix}\begin{pmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{12}\end{pmatrix} \tag{2.3}$$

$$C_{11} = \chi_1; \quad C_{12} = \chi_1 + 2\chi_2; \quad C_{44} = C_{11} - C_{12} = -2\chi_2$$

$$\gamma = \frac{E}{2(1+v)(1-2v)}; \quad \chi_1 = 2(1-v); \quad \chi_2 = -(1-2v) \tag{2.4}$$

that involves only two material constants—the Young modulus E and the Poisson ratio v.

In the relation (2.3) the strain tensor $\varepsilon = \{\varepsilon_{ij}\}$ represents the covariant gradient of the displacement vector $\boldsymbol{u} = (u_1, u_2)$

$$\varepsilon = \tfrac{1}{2}(\text{grad}\,\boldsymbol{u} + \text{grad}^T\,\boldsymbol{u}) \tag{2.5}$$

Using (2.3)–(2.5), the eqn (2.1) may be expressed equivalently in terms of $\boldsymbol{u}(\eta_1, \eta_2)$

$$\chi_1\,\boldsymbol{grad}\,\text{div}\,\boldsymbol{u} + \chi_2\,\boldsymbol{rot}\,\boldsymbol{rot}\,\boldsymbol{u} = -\gamma^{-1}\boldsymbol{F} \tag{2.6}$$

eqn (2.6) holds in a thin disk (plane stress conditions) too, provided that the coefficients involved are obtained from (2.4) by the formal transformation (Landau and Lifshitz, 1975)

$$E \to \frac{E(1+2v)}{(1+v)^2}; \quad v \to \frac{v}{1+v}$$

so that

$$\gamma = \frac{E}{2(1-v)};' \quad \chi_1 = \frac{2}{1+v}; \quad \chi_2 = -\frac{1-v}{1+v}$$

This resemblance enables us to perform further analysis in a uniform manner for both plane strain and plane stress cases.

The components of the strain——displacement differential relation (2.5) are dependent on the coordinate system. For instance we have in the polar system (Landau and Lifshitz, 1986)

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r}; \quad \varepsilon_{\theta\theta} = \frac{1}{r}\frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r}; \quad 2\varepsilon_{r\theta} = \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r} + \frac{1}{r}\frac{\partial u_r}{\partial \theta} \tag{2.7}$$

When passing to the Cartesian system the strains (2.7) are transformed by (Landau and Lifshitz, 1986)

$$\begin{aligned}\varepsilon_{rr} + \varepsilon_{\theta\theta} &= \varepsilon_{xx} + \varepsilon_{yy}\\ \varepsilon_{\theta\theta} - \varepsilon_{rr} + 2i\varepsilon_{r\theta} &= \exp\{2i\theta\}(\varepsilon_{yy} - \varepsilon_{xx} + 2i\varepsilon_{xy})\end{aligned} \tag{2.8}$$

A *square symmetric orthotropic* crystal aligned with the (x, y) coordinate axes corresponds to the Cartesian form (2.3) of constitutive relation in which the entry C_{44} is not necessarily equal to $C_{11} - C_{12}$ but may take an admissible value. The energetically reasonable bounds on C_{44} are discussed by Ting (1996). The constant

$$\mu_* = \gamma C_{44}/2$$

is termed the second shear modulus of an orthotropic crystal in distinction to the shear modulus

$$\mu = \gamma(C_{11}-C_{12})/2$$

The moduli E and v related to C_{11}, C_{12} by (2.4) will be also in use. The dimensionless factor

$$\omega = 2(\mu_*-\mu)/\gamma = C_{44}-C_{11}+C_{12} \tag{2.9}$$

is conveniently introduced (Landau and Lifshitz, 1986) to measure the anisotropy of a square symmetric medium. Typically, ω lies in the range of 0.44–0.66 (Lambropoulos, 1987). From (2.4) it follows that ω vanishes for an isotropic material.

Combining now relations (2.1), (2.3), (2.5) and (2.9) in the ($\eta_1 = x, \eta_2 = y$) coordinates (when $\varepsilon_{11} = \varepsilon_{xx}$, $\varepsilon_{22} = \varepsilon_{yy}$, $\varepsilon_{12} = \varepsilon_{xy}$ and $f_1 = f_x$, $f_2 = f_y$) we arrive at the following Cartesian form of equilibrium equations

$$\chi_1 \operatorname{grad}_x \operatorname{div} \boldsymbol{u}+\chi_2 \operatorname{rot}_x \operatorname{rot}\boldsymbol{u} +\omega\frac{\partial\varepsilon_{xy}}{\partial y} = -\gamma^{-1}f_x; \quad \boldsymbol{u} = (u_x, u_y)$$

$$\chi_1 \operatorname{grad}_y \operatorname{div} \boldsymbol{u}+\chi_2 \operatorname{rot}_y \operatorname{rot}\boldsymbol{u} +\omega\frac{\partial\varepsilon_{xy}}{\partial x} = -\gamma^{-1}f_y; \quad 2\varepsilon_{xy} = \frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x} \tag{2.10}$$

in which the isotropic and anisotropic terms are separated explicitly. Note that if $\omega = 0$, eqn (2.10) reduce to the isotropic eqn (2.6).

For $\omega < 1$ this enables us to approximate the solution of (2.10) analytically by expressing the vector $\boldsymbol{u}$ as a perturbation series in ω (Holmes, 1995)

$$\boldsymbol{u} = \sum_{j=0}^{\infty} \omega^j \boldsymbol{u}^{(j)} \tag{2.11}$$

In view of (2.2), substituting (2.11) into (2.10) gives the isotropic problem (2.6) of the zeroth-order

$$\chi_1 \boldsymbol{grad}\operatorname{div} \boldsymbol{u}^{(0)}+\chi_2 \boldsymbol{rot\,rot}\,\boldsymbol{u}^{(0)} = -\gamma^{-1}A\,\boldsymbol{grad}\,T \tag{2.12}$$

and the successive higher-orders

$$\chi_1 \boldsymbol{grad}\operatorname{div} \boldsymbol{u}^{(j)}+\chi_2 \boldsymbol{rot\,rot}\,\boldsymbol{u}^{(j)} = -\boldsymbol{F}^{(j-1)} \quad j = 1, 2, \ldots \tag{2.13}$$

Here we incorporate the mass pseudo forces $\boldsymbol{F}^{(j)}(x, y) = (\partial\varepsilon_{xy}^{(j)}/\partial y; \partial\varepsilon_{xy}^{(j)}/\partial x); j \geqslant 0$ which result from the preceding equation. Although the original anisotropic equation simplifies to (2.10) only in the Cartesian coordinates, the isotropic approximating problems (2.12), (2.13) of any order are handled with equal ease in any orthogonal system (η_1, η_2). For this purpose it remains to express the functions $\boldsymbol{F}^{(j)}(\eta_1, \eta_2)$ using the well-known formulae of vector analysis. Particularly, by (2.7), (2.8) we have for $\boldsymbol{F}^{(j)}(r, \theta) = (f_r^{(j)}, f_\theta^{(j)})$ after some algebra

$$f_r^j = \frac{\partial \varepsilon_{xy}^{(j)}}{\partial x}\sin\theta + \frac{\partial \varepsilon_{xy}^{(j)}}{\partial y}\cos\theta = \frac{\partial E_r^{(j)}}{\partial r}\sin^2 2\theta + \frac{1}{2r}\frac{\partial E_r^{(j)}}{\partial \theta}\sin 4\theta + \frac{2}{r}E_r^{(j)}\cos^2 2\theta$$
$$+\frac{1}{2}\frac{\partial \varepsilon_{r\theta}^{(j)}}{\partial r}\sin 4\theta + \frac{1}{r}\frac{\partial \varepsilon_{r\theta}^{(j)}}{\partial \theta}\cos^2 2\theta - \frac{1}{r}\varepsilon_{r\theta}^{(j)}\sin 4\theta \quad (2.14)$$

and similarly

$$f_\theta^{(j)} = \frac{\partial \varepsilon_{xy}^{(j)}}{\partial x}\cos\theta - \frac{\partial \varepsilon_{xy}^{(j)}}{\partial y}\sin\theta = \frac{1}{2}\frac{\partial E_r^{(j)}}{\partial r}\sin 4\theta + \frac{1}{r}\frac{\partial E_r^{(j)}}{\partial \theta}\sin^2 2\theta - \frac{1}{r}E_r^{(j)}\sin 4\theta$$
$$+\frac{1}{2}\frac{\partial \varepsilon_{r\theta}^{(j)}}{\partial r}\cos^2 2\theta - \frac{1}{2r}\frac{\partial \varepsilon_{r\theta}^{(j)}}{\partial \theta}\sin 4\theta + \frac{1}{r}\varepsilon_{r\theta}^{(j)}\sin^2 2\theta \quad (2.15)$$

where

$$2E_r^{(j)} = \varepsilon_{rr}^{(j)} - \varepsilon_{\theta\theta}^{(j)} \quad (2.16)$$

We complete the problem formulation by expanding the prescribed boundary conditions in powers of ω, and appending them to (2.12) and (2.13).

3. Solution technique

To be more specific, let the boundary $r = R$ be free of applied traction

$$\sigma_{rr}(R,\theta) = \sum_{j=0}^{\infty} \omega^j \sigma_{rr}^{(j)}(R,\theta) = 0; \quad \sigma_{r\theta}(R,\theta) = \sum_{j=0}^{\infty} \omega^j \sigma_{r\theta}^{(j)}(R,\theta) = 0$$

Thus the elastic stresses are caused solely by the temperature gradient. Assume further that the temperature distribution is axially symmetric, so that $T = T(r)$. When solving the successive problems (2.12), (2.13) the above boundary conditions should likewise be met separately for each approximation step:

$$\sigma_{rr}^{(j)}(R,\theta) = 0; \quad \sigma_{r\theta}^{(j)}(R,\theta) = 0; \quad j = 0, 1, 2, \ldots \quad (3.1)$$

By virtue of (2.3), (2.7) they are expressed in terms of the displacements and their first derivatives.

We also impose the natural requirement for the strains to be finite at the point $r = 0$. In view of (2.7) this means that

$$u^{(j)}(0,\theta) = 0; \quad j = 0, 1, 2, \ldots \quad (3.2)$$

3.1. The zeroth-order approximation

For the square symmetry, the multiplier A in (2.2) processes the form (Landau and Lifshitz, 1986)

$$A = -\tfrac{2}{3}\alpha\gamma(1+\nu) \quad (3.3)$$

where α is the scalar coefficient of thermal expansion.

Due to the axial symmetry the second left-hand term in eqn (2.12) vanishes thus resulting (Landau and Lifshitz, 1986) in the following second-order equation in $\boldsymbol{u}^{(0)}(r) = (u_r^{(0)}(r), 0)$

$$\frac{3(1-\nu)}{(1+\nu)}\frac{\mathrm{d}}{\mathrm{d}r}\left[\frac{1}{r}\frac{\mathrm{d}(ru_r^{(0)}(r))}{\mathrm{d}r}\right] = \alpha T'(r)$$

This equation is easy to integrate, and yields the solution

$$u_r^{(0)} = \frac{\alpha(1+\nu)}{3(1-\nu)}\left\{\frac{1}{r}\int_0^r T_0(\rho)\rho\,\mathrm{d}\rho + (1-2\nu)\frac{r}{R^2}\int_0^R T_0(\rho)\rho\,\mathrm{d}\rho\right\} \tag{3.4}$$

where

$$T_0(r) = T(r) - T(R)$$

The integration constants in (3.4) have been chosen as to satisfy the zeroth-order boundary conditions (3.1), (3.2): $\sigma_{rr}^{(0)}(R,\theta) = 0$; $u_r^{(0)}(0) = 0$.

3.2. *The first-order approximation*

In view of the symmetry of the zeroth-order solution (3.4) we have

$$\frac{\partial \varepsilon_{rr}^{(0)}}{\partial \theta} = \frac{\partial \varepsilon_{\theta\theta}^{(0)}}{\partial \theta} = \varepsilon_{r\theta}^{(0)} = \sigma_{r\theta}^{(0)} \equiv 0$$

everywhere in the circle. With this result the zeroth-order mass force $\boldsymbol{F}^{(0)}(r,\theta) = (f_1, f_2)$ becomes [see (2.14), (2.15)]

$$f_r^{(0)}(r,\theta) = \frac{\mathrm{d}E_r^{(0)}(r)}{\mathrm{d}r}\sin^2 2\theta + \frac{2}{r}E_r^{(0)}(r)\cos^2 2\theta = E_1(r) - E_2(r)\cos 4\theta$$

$$f_\theta^{(0)}(r,\theta) = E_2(r)\sin 4\theta \tag{3.5}$$

In the above

$$E_1(r) = \frac{\mathrm{d}E_r^{(0)}(r)}{\mathrm{d}r} + 2r^{-1}E_r^{(0)}(r); \quad E_2(r) = \frac{\mathrm{d}E_r^{(0)}(r)}{\mathrm{d}r} - 2r^{-1}E_r^{(0)}(r) \tag{3.6}$$

Now, it is convenient to express the temperature $T_0(r)$ as a power series in r (although other forms of $T_0(r)$ can also be considered). Such a series can be obtained by using a Taylor expansion about $r = 0$. Also, if discrete T_0 values are given via numerical or experimental data, $T_0(r)$ can be defined by polynomial interpolation (see Section 4):

$$T_0(r) = \sum_{k=0}^{\infty} \tilde{T}_k r^k$$

In this case, $u_r^{(0)}$ in (3.4) can also be expressed as a power series not involving, by (3.2), (3.4), a constant term:

$$u_r^{(0)}(r) = \sum_{k=1}^{\infty} \beta_k r^k$$

$$\beta_1 = \frac{\alpha(1+\nu)}{3(1-\nu)}\left\{\frac{\tilde{T}_0}{2} + (1-2\nu)\sum_{m=0}^{\infty}\frac{R^m}{m+2}\tilde{T}_m\right\}; \quad \beta_k = \frac{\alpha(1+\nu)}{3(k+1)(1-\nu)}\tilde{T}_{k-1}; \quad k > 1 \tag{3.7}$$

Due to (2.7), (2.16) and (3.7) the quantities (3.6) take the form:

$$2E_1(r) = \frac{\mathrm{d}^2 u_r^{(0)}(r)}{\mathrm{d}r^2} + \frac{\mathrm{d}u_r^{(0)}(r)}{r\,\mathrm{d}r} - \frac{u_r^{(0)}(r)}{r^2} = 2\sum_{k=0}^{\infty} c_{k+2} r^k; \quad 2c_k = (k^2+4k-3)\beta_k$$

$$2E_2(r) = \frac{\mathrm{d}^2 u_r^{(0)}(r)}{\mathrm{d}r^2} - 3\frac{\mathrm{d}u_r^{(0)}(r)}{r\,\mathrm{d}r} + 3\frac{u_r^{(0)}(r)}{r^2} = 2\sum_{k=2}^{\infty} d_{k+2} r^k; \quad 2d_k = (k^2-1)\beta_k \tag{3.8}$$

We note in passing that the linear term $\beta_1 r$ in (3.7) makes no contribution to (3.8) and hence to the high-order solutions. In keeping with (2.3), (2.4), (2.7) this function corresponds only to the zeroth-order homogeneous stress field $\sigma_{rr} = \sigma_{\theta\theta} = \gamma\beta_1$; $\sigma_{r\theta} = 0$.

Equation (2.13) and the specific dependence of the mass force $\boldsymbol{F}^{(0)}(r,\theta)$ in (3.4) on θ, permits us to write the sought-for first-order solution $\boldsymbol{u}^{(1)} = (u_r^{(1)}(r,\theta), u_\theta^{(1)}(r,\theta))$ as linear combinations of the same trigonometric functions:

$$u_r^{(1)}(r,\theta) = w_0(r) + w_1(r)\cos 4\theta$$
$$u_\theta^{(1)}(r,\theta) = w_2(r)\sin 4\theta \tag{3.9}$$

These relations provide the required reflection symmetry with respect to the x, y-axes:

$$u_r^{(1)}(r,\theta) = u_r^{(1)}(r,-\theta); \quad u_\theta^{(1)}(r,\theta) = -u_\theta^{(1)}(r,-\theta)$$

In view of (2.3), (2.7) and (2.8) substituting (3.9) into the homogeneous boundary conditions (3.1) leads to the boundary expressions:

$$\nu w_0'(R) + (1-\nu)\frac{w_0(R)}{R} + \left[\nu w_1'(R) + \frac{1-\nu}{R}(w_1(R) + 4w_2(R))\right]\cos 4\theta = 0$$

$$\left(w_2'(R) - \frac{w_2(R)}{R} - \frac{4w_1(R)}{R}\right)\sin 4\theta = 0 \tag{3.10}$$

Because the differential operators in eqn (2.13) leave the structure of (3.9) unchanged, the functions $w_0(r)$ and $(w_1(r); w_2(r))$ may be found separately by equating the same trigonometric terms in both sides of (2.13). In doing so we first arrive at the boundary sub-problem of finding the axially symmetric function $w_0(r)$:

$$\chi_1 \frac{d}{dr}\left[\frac{1}{r}\frac{d(rw_0(r))}{dr}\right] = -E_1(r)$$

$$w_0(0) = 0; \quad vw_0'(R) + (1-v)\frac{w_0(R)}{R} = 0 \tag{3.11}$$

where the two-point boundary conditions are obtained from (3.2) and (3.10), respectively.

Similarly to (3.4), straightforward integration of this equation yields, on account of (3.7), (3.8)

$$w_0(r) = C_0 r - \frac{1}{\chi_1 r}\int_0^r \rho \, d\rho \int_0^\rho E_1(\rho_0)\, d\rho_0 = C_0 r - \frac{1}{\chi_1}\sum_{k=0}^{\infty} \frac{\alpha(1+v)(k^2+4k-3)}{6(1-v)(k+1)^2(k+3)}\tilde{T}_{k-1} \tag{3.12}$$

The constant C_0 is employed to satisfy the boundary condition (3.11) at the point $r = R$ while the condition (3.2) $w_0(0) = 0$ is met by (3.12) automatically.

The second sub-problem involves a system of two differential equations in $w_1(r)$, $w_2(r)$. We write these equations in a general form which is valid for the case where the angular argument in (3.9) is taken to be $l\theta$, $l = 1, 2, \ldots$ (rather than the fixed argument 4θ).

$$-\frac{\chi_1}{r^2}\left[\frac{d}{dr}(rw_1(r)) + lw_2(r)\right] + \frac{\chi_1}{r}\left[\frac{d^2}{dr^2}(rw_1(r)) + l\frac{d}{dr}w_2(r)\right]$$
$$+\frac{\chi_2 l}{r^2}\left[lw_1(r) + \frac{d}{dr}(rw_2(r))\right] = E_2(r)$$

$$-\frac{\chi_1 l}{r^2}\left[\frac{d}{dr}(rw_1(r)) + lw_2(r)\right] - \chi_2\frac{d}{dr}\left\{\frac{1}{r}\left[+lw_1(r) + \frac{d}{dr}(rw_2(r))\right]\right\} = -E_2(r) \tag{3.13}$$

We note that the functions $E_1(r)$, $E_2(r)$ are separated in the right-hand sides of the sub-problems (3.11), (3.13).

The system (3.13) is linear. Hence its partial solution $\phi_i(r)$, $i = 1, 2$ should be combined with a general solution $\varphi_i(r)$ of the corresponding homogeneous system:

$$w_i(r) = \varphi_i(r) + \phi_i(r); \quad i = 1, 2 \tag{3.14}$$

The differential operators (3.13) are of the Euler type. Thus (Rice and Strange, 1989) both functions ($\varphi_i(r)$ possess the form of the same power in r

$$\varphi_i(r) = H_\lambda^{(i)} r^\lambda; \quad i = 1, 2 \tag{3.15}$$

Substituting (3.15) into the homogeneous counterpart of (3.13) gives the algebraic system to define the constants $H_\lambda^{(1)}$, $H_\lambda^{(2)}$:

$$\alpha_{11}(\lambda)H_\lambda^{(1)} + \alpha_{12}(\lambda)H_\lambda^{(2)} = 0$$
$$\alpha_{21}(\lambda)H_\lambda^{(1)} + \alpha_{22}(\lambda)H_\lambda^{(2)} = 0 \tag{3.16}$$

Here

$$\alpha_{11}(\lambda) = \chi_1(\lambda^2-1)+\chi_2 l^2; \quad \alpha_{12}(\lambda) = l[\chi_1(\lambda-1)+\chi_2(\lambda+1)]$$
$$\alpha_{21}(\lambda) = -l[\chi_1(\lambda+1)+\chi_2(\lambda-1)]; \quad \alpha_{22}(\lambda) = -\chi_1 l^2-\chi_2(\lambda^2-1) \tag{3.17}$$

In order to find non-trivial solutions of (3.16) we set up the polynomial equation in λ

$$(\lambda^2-1)^2-2l^2(\lambda^2-1)+4l^2+l^4 = 0 \tag{3.18}$$

that results from setting the determinant $\Delta(\lambda) = \alpha_{11}\alpha_{22}-\alpha_{12}\alpha_{21}$ of (3.16) equal to zero. Equation (3.18) has four integer roots:

$$\lambda_1 = l-1; \quad \lambda_2 = l+1; \quad \lambda_3 = -l-1; \quad \lambda_4 = -l-1$$

As would be expected, these roots are independent of the elastic constant χ_1, χ_2. They may be also identified in a somewhat different manner. Indeed, the displacement $(r^{\lambda}\cos l\theta, r^{\lambda}\sin l\theta)$ are generated by the Airy's biharmonic function $\Psi(r,\theta) = r^{\lambda+1}\cos l\theta$. By applying the biharmonic operator ∇^4 to $\Psi(r,\theta)$ in the polar coordinates

$$\nabla^4 r^{\lambda+1}\cos l\theta = [l^2-(\lambda+1)^2]\nabla^2 r^{\lambda-1}\cos l\theta = [l^2-(\lambda+1)^2][l^2-(\lambda-1)^2]\nabla^2 r^{\lambda-3}\cos l\theta = 0$$

we arrive at the same four roots.

We avoid singularities at $r = 0$ by discarding the negative roots $\lambda_{3,4}$. As a result the general solution $\varphi_i(r)$ takes the form containing only two arbitrary constants $H^{(1)}_{l\pm 1}$

$$\varphi_1(r) = H^{(1)}_{l-1}r^{l-1}+H^{(1)}_{l+1}r^{l+1}; \quad \varphi_2(r) = \xi_{l-1}H^{(1)}_{l-1}r^{l-1}+\xi_{l+1}H^{(1)}_{l+1}r^{l+1}$$
$$\xi_{l-1} = -\alpha_{12}(l-1)/\alpha_{11}(l-1) = -1; \quad \xi_{l+1} = -\alpha_{12}(l+1)/\alpha_{11}(l+1) \tag{3.19}$$

We next find the partial solution $\phi_i(r)$. By substituting the power expansion (3.8) for $E_2(r)$ the right-hand side of the system (3.13) takes the form

$$\sum_{k=0}^{\infty} d_{k+2}(r^k;-r^k) \tag{3.20}$$

From the preceding results it follows that except for the powers $k = l\pm 1$ any other individual term of (3.20) gives the following addition to the partial solution of (3.13)

$$(D^{(1)}_{k+2}r^k, D^{(2)}_{k+2}r^k); \quad k \neq l-1, \quad k \neq l+1$$
$$D^{(1)}_{k+2} = \Delta^{-1}(k)d_{k+2}(\alpha_{22}(k)-\alpha_{12}(k)); \quad D^{(2)}_{k+2} = -\Delta^{-1}(k)d_{k+2}(\alpha_{21}(k)+\alpha_{11}(k)) \tag{3.21}$$

The constants $D^{(1,2)}_{k+2}$ are obtained by solving the corresponding 2×2 non-degenerated algebraic system with the matrix (3.17) and the right-hand side $(d_{k+2}, -d_{k+2})$. This system is arrived at by substituting the term $(D^{(1)}_{k+2}r^k, D^{(2)}_{k+2}r^k)$ into (3.13), with the coefficients of r^k equated in the both sides. Summing the items (3.21) over k we obtain

$$\sum_{\substack{k=0 \\ k\neq l\pm 1}}^{\infty} (D^{(1)}_{k+2}r^k, D^{(2)}_{k+2}r^k) \tag{3.22}$$

The solutions $(\tau^{(1)}_{l-1}(r), \tau^{(2)}_{l-1}(r))$ and $(\tau^{(1)}_{l+1}(r), \tau^{(2)}_{l+1}(r))$ for the two remaining terms of (3.20)

$$(d_{k+2}r^k, -d_{k+2}r^k); \quad k = l\pm 1$$

should be derived in another way since the matrix (3.17) degenerates for these values of k. To this end we use the method of undefined coefficients (Rice and Strange, 1989) thus arriving at the following sought-for expressions which involves a logarithmic multiplier $\ln r$ and the parameters $\xi_{l\pm 1}$ in (3.19)

$$\tau_{l-1}^{(1)}(r) = Q_{l-1}^{(1)} r^{l-1} \ln r + Q_{l-1}^{(2)} r^{l-1}; \quad \tau_{l-1}^{(2)}(r) = \xi_{l-1} Q_{l-1}^{(1)} r^{l-1} \ln r + \xi_{l+1} Q_{l-1}^{(2)} r^{l-1}$$
$$\tau_{l+1}^{(1)}(r) = Q_{l+1}^{(1)} r^{l+1} + Q_{l+1}^{(2)} r^{l+1} \ln r; \quad \tau_{l+1}^{(2)}(r) = \xi_{l-1} Q_{l+1}^{(1)} r^{l+1} + \xi_{l+1} Q_{l+1}^{(2)} r^{l+1} \ln r \tag{3.23}$$

The pairs of constants $Q_{l-1}^{(1)}$, $Q_{l-1}^{(2)}$ and $Q_{l+1}^{(1)}$, $Q_{l+1}^{(2)}$ in (3.23) are found by solving the algebraic systems

$$[\chi_1(l-2)-\chi_2 l]Q_{l-1}^{(1)} + l(1+\xi_{l+1})[\chi_1(l-2)+\chi_2 l]Q_{l-1}^{(2)} = d_{l-1}$$
$$[\chi_1 l-\chi_2(l-2)]Q_{l-1}^{(1)} + l(1+\xi_{l+1})[\chi_1 l+\chi_2(l-2)]Q_{l-1}^{(2)} = -d_{l-1} \tag{3.24}$$

and

$$2(\chi_1-\chi_2)lQ_{l+1}^{(1)} + [\chi_1(l\xi_{l+1}+2l+2)+\chi_2 l\xi_{l+1}]Q_{l+1}^{(2)} = d_{l+1}$$
$$2(\chi_1-\chi_2)lQ_{l+1}^{(1)} + [\chi_1 l+\chi_2(2l\xi_{l+1}+2\xi_{l+1}+l)]Q_{l+1}^{(2)} = -d_{l+1} \tag{3.25}$$

respectively. These systems are also derived by substituting (3.23) into (3.13), with the logarithmic terms cancelling each other in the resultant expressions. We then add (3.22) and (3.23) to obtain explicitly the partial solution $\phi_i(r)$

$$\phi_i(r) = \sum_{\substack{k=0 \\ k\neq l\pm 1}}^{\infty} D_{k+2}^{(i)} r^k + \tau_{l-1}^{(i)} + \tau_{l+1}^{(i)}; \quad i = 1,2 \tag{3.26}$$

We now summarize the first-order solution, and the steps needed to obtain it. In all the following calculations, we set $l = 4$, which is appropriate for the first-order solution.

The first step is preparatory. The relative temperature $T_0(r) = T(r) - T(R)$ is written as a power series in r, with coefficients $\tilde{T}_k$. Then, the coefficients β_k are calculated by using (3.7). When the β_k are known, the coefficients c_k and d_k are found from (3.8). Next, the quantities $\alpha_{ij}(k)$ are determined from (3.17) for integer values of k, as well as the determinant $\Delta(k) = \alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}$. We also calculate the ξ_3 and ξ_5 in (3.19), and the $D_{k+2}^{(i)}$ in (3.21) for $k \neq 3, 5$.

The second step is the determination of $w_0(r)$. This function is given by (3.12), where the constant C_0 is obtained from the second condition in (3.11).

The third step is the determination of $w_1(r)$ and $w_2(r)$. These functions are given by the decomposition (3.14). The functions $\varphi_i(r)$ are obtained from (3.19), and involve the constants $H_3^{(1)}$ and $H_5^{(1)}$ which will be determined later. To find the functions $\phi_i(r)$, we first calculate the quantities $Q_3^{(i)}$ and $Q_5^{(i)}$ by solving the two 2×2 systems of equations (3.24) and (3.25). Then we find $\tau_3^{(i)}$ and $\tau_5^{(i)}$ from (3.23). Then the $\phi_i(r)$ are given by (3.26).

Finally, the whole solution for the displacements is given by (3.9). By following all the steps above, the displacements are determined up to the unknown constants $H_3^{(1)}$ and $H_5^{(1)}$. To find these constants, the displacements are differentiated to obtain the strains and from them the stresses. Requiring the two stress boundary conditions (3.1) (with $j = 1$) to hold, yields $H_3^{(1)}$ and $H_5^{(1)}$. This completes the solution process.

3.3. Higher-order solutions

All the analytical tools now are at hand to construct further approximations in ascending order. An important point is that the trigonometric functions of the same argument appear in (3.9) only by pairs. For brevity, the vectors whose components are proportional to $\cos l\theta$ and $\sin l\theta$, respectively, will be referred to as l-type terms so that the first-order approximation (3.9) involves the zeroth-type term and the fourth-type term.

In preparation for each approximation step the following factors that result from the structure of the right side vector (2.14), (2.15) must be kept in mind:

- substituting an axially symmetric term of zeroth type invariantly gives a zeroth-type term and a fourth-type term which are handled exactly as was done above for the first-order approximation;
- any l-type term ($l = 4m, m = 1, 2\ldots$) gives in turn three terms of $4(m-1)$, $4m$, and $4(m+1)$ type which may be found following the same guidelines.

Whilst the proposed method leads to rather cumbersome expressions, it provides a good quantitative insight to the problem.

4. Numerical examples

To illustrate the solution obtained in the previous section, we now present some numerical results for typical data, taken from Jordan et al. (1984). We consider a LEC GaAs boule, with radius 2.5 cm and length of 5 cm, pulled at a rate of 0.0004 cm/s, with a temperature difference of 200 K between the melting temperature (1511 K) at the bottom and the ambient temperature. The temperature distribution is axisymmetric, and depends on the radial coordinate r as well as on the axial coordinate z. We concentrate on the cross section $z = 1.5$ cm, and neglect the axial temperature variation, to enable plane strain conditions in the thermoelastic problem. We characterize the radial variation using the following four data points:

r [cm]	0	1	2	2.5
T [K$^\circ$]	1411	1404	1395	1371

We interpolate these data points using the third-degree Lagrange polynomial which passes through them. This yields the radial temperature function $T(r)$ in the circular cross section $0 \leqslant r \leqslant 2.5$. The elastic displacement and stress fields generated by this temperature field depend linearly on the thermal expansion coefficient α [see (3.3) and (2.2)]. Henceforth we normalize all the results by α. The stresses obtained using our perturbation technique do not depend on the elastic properties C_{11}, C_{12} and C_{44} separately, since each problem in the perturbation sequence is isotropic-like. The stresses only depend on the anisotropy parameter $\omega = C_{44} - C_{11} + C_{12}$, which has been used as a perturbation parameter [see (2.11)]. They also depend on Poisson's ratio ν. We set $\nu = 0.3$ and $\omega = 0.5$, which are typical, and obtain the asymptotic solution up to first order.

In Fig. 1(a) and 1(b), the contour lines of the displacement components u_r and u_θ are shown, respectively. They are plotted on a quarter-disk domain, although due to the symmetry a one-eighth of a disk domain is sufficient. The contour patterns of u_r clearly deviate from the isotropic

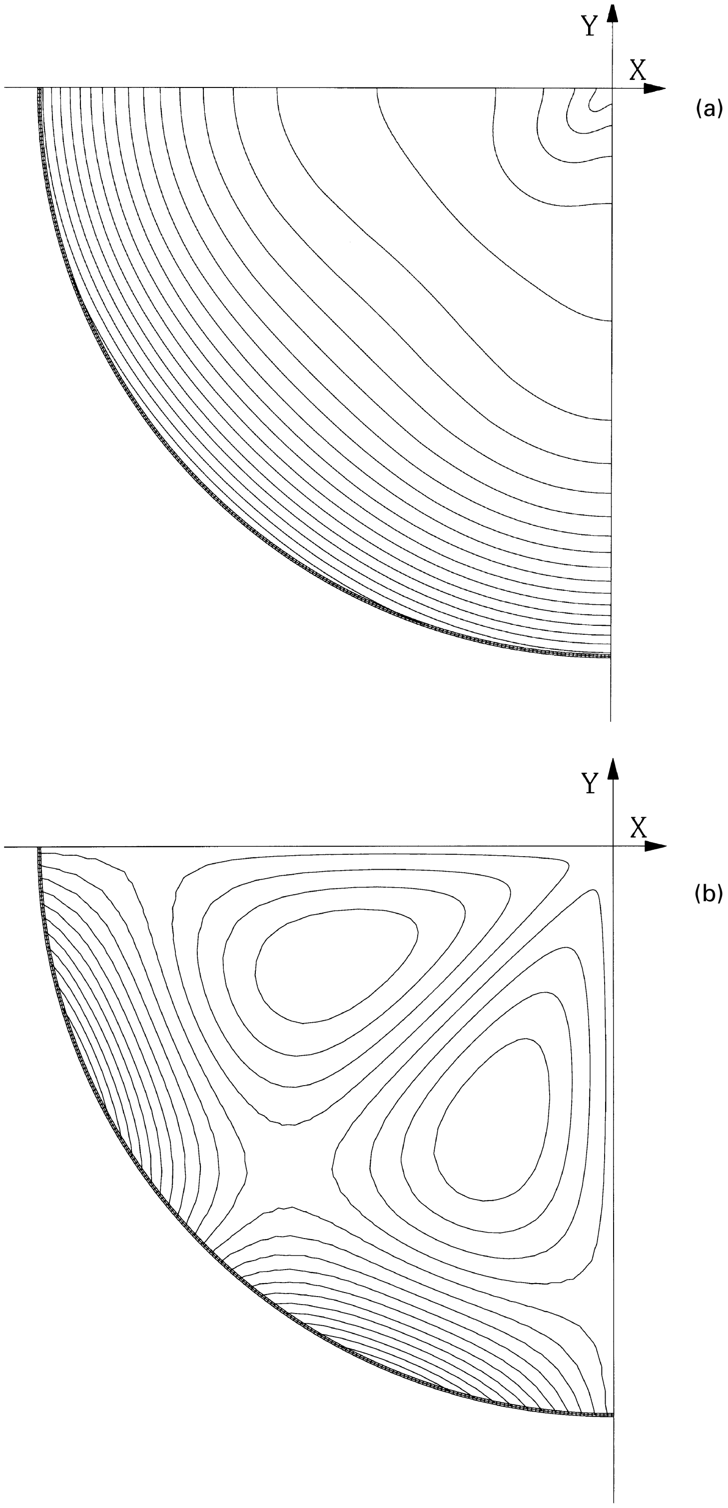

Fig. 1. Displacement contour lines of (a) u_r, (b) u_θ.

(axi-symmetric) pattern of concentric circles, which is obtained by the zero-order solution. The displacement u_θ is non-zero, as opposed to the isotropic case. The maximal value of u_r is 32.90, and it is attained on the boundary of the cylinder in a 45° direction relative to the crystal symmetry axes (x, y). The maximal value of u_θ is 1.343, also on the boundary, but in a 22.5° orientation. On the other hand, along the 45° direction, u_θ vanishes.

Figure 2(a)–(d) are contour plots of the stress components σ_{rr}, $\sigma_{\theta\theta}$, $\sigma_{r\theta}$, and the von Mises effective stress $\sigma_e = ((\sigma_{rr}+\sigma_{\theta\theta})^2+3\sigma_{r\theta}^2-3\sigma_{rr}\sigma_{\theta\theta})^{1/2}$, respectively. They are shown on a quarter-disk domain, although due to the symmetry a one-eight of a disk domain is sufficient. In comparison, the isotropic solution (which is also the zero-order solution in the perturbation expansion) consists of perfectly circular contour lines for σ_{rr}, $\sigma_{\theta\theta}$ and σ_e, while $\sigma_{r\theta}$ vanishes. Figure 2 shows that the hoop stress $\sigma_{\theta\theta}$ is almost axisymmetric, whereas the other stress components have more asymmetric features. The maximal stress values are as follows:

$\sigma_{rr} = 24.958$, attained at the point $r = 0$,
$\sigma_{\theta\theta}$ takes the same maximal value 24.958, attained at the same point $r = 0$,
$\sigma_{r\theta} = 10.399$, attained at the point $(r = 0.5R, \theta = 22.5°)$,
$\sigma_e = 28.161$, attained at the same point $(r = 0.5R, \theta = 22.5°)$

We have also obtained other results with different parameter values and temperature distributions. We remark that the results obtained for stresses and displacements have been found to be quite sensitive to the temperature distribution function $T(r)$, not just quantitatively, but qualitatively as well (i.e., in terms of the contour line patterns). This implies that a good knowledge on the temperature distribution in the boule prior to stress analysis is important.

5. Concluding remarks

In this paper, we have devised a Fourier-type perturbation method for the problem of finding the thermoelastic stresses in a circular cylinder or disk with a cubic anisotropy. The cubic anisotropy renders the problem asymmetric, despite the axisymmetry of the geometry and of the thermal loading. We have shown how to obtain a closed-form asymptotic solution, up to a desired order.

The problem has been motivated by a thermoelastic model used for certain crystal growth processes. Our model takes into account the weak anisotropy of the crystal, as opposed to some of the previous works which neglected it altogether. At the same time, however, we have made two simplifying assumptions: (a) the problem is two-dimensional with plane strain or plane stress conditions; and (b) the elastic properties do not depend on the temperature, and thus the crystal is homogeneous. These assumptions limit the applicability of the solution. However, the present approach is still advantageous in several respects: it is the first analytic solution available which takes the anisotropy of the crystal into account, it can serve as a benchmark to numerical schemes, it is a practical solution for crystal growth problems under certain conditions (see Introduction), and it serves as a basis for a more general solution procedure.

We currently investigate ways to obtain solutions that do not necessitate these assumptions. In particular, we consider the full three-dimensional problem, where the stresses vary in the axial direction z as well. Our approach is based on restating the problem as a perturbation problem in terms of the anisotropy parameter ω (as we have done in the present paper), and thus obtaining a

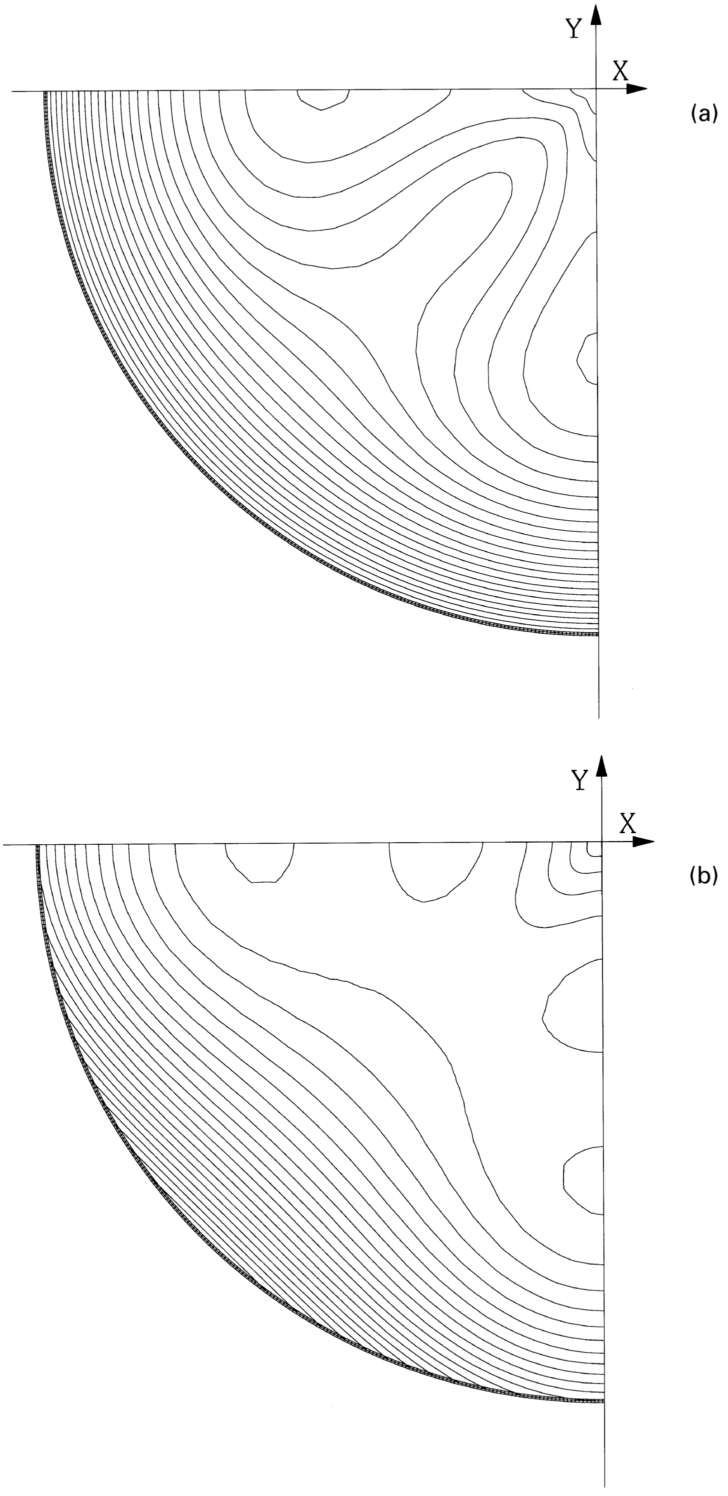

Fig. 2. Thermoelastic stress contours of (a) σ_{rr}, (b) $\sigma_{\theta\theta}$, (c) $\sigma_{r\theta}$, (d) the von Mises stresses.

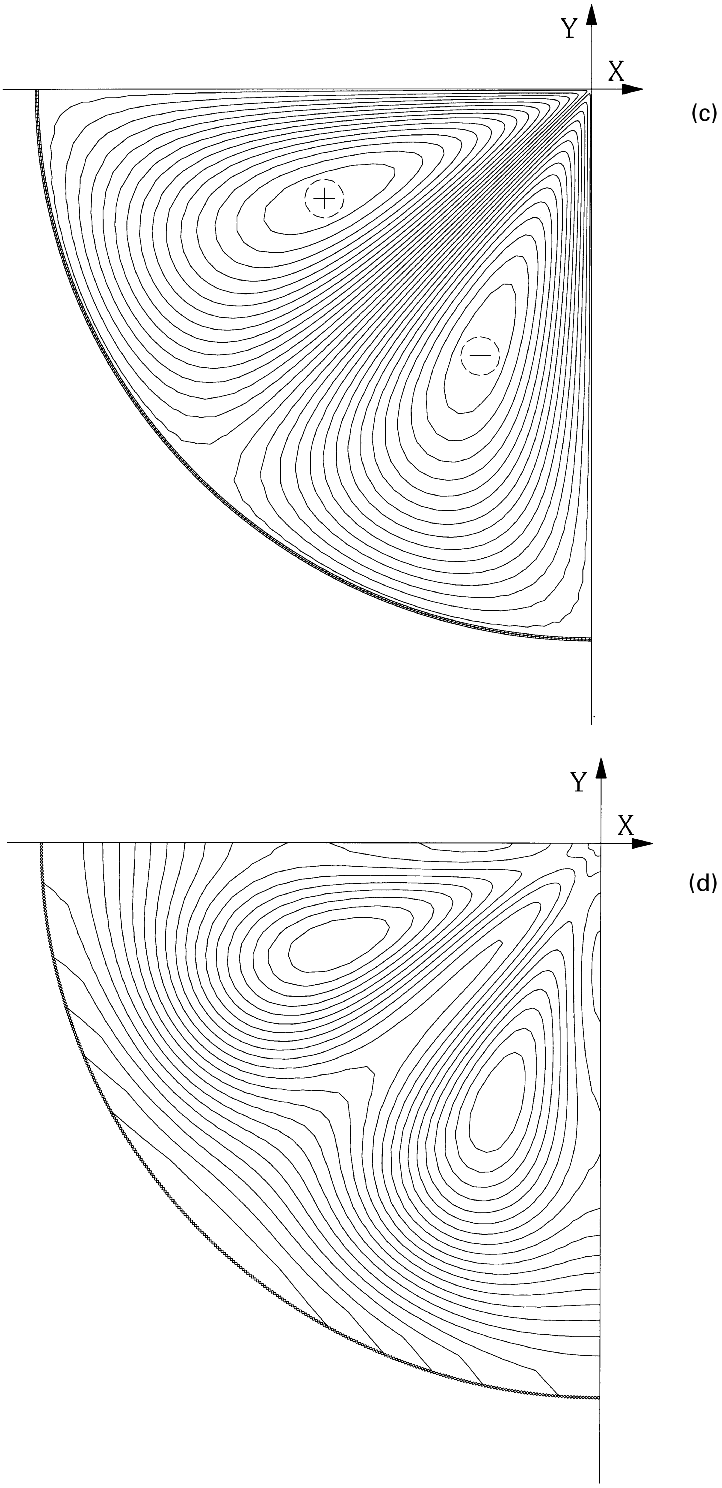

Fig. 2.—*Continued.*

sequence of isotropic-like two-dimensional elastic problems. Each of these problems is then solved, either analytically (in case this is possible), or numerically by the finite element method. In the latter case, this approach amounts to reducing the dimensionality of the numerical problem from three to two, with the obvious associated computational advantages.

Also under investigation are models for prediction dislocation densities, based on the asymptotic solutions mentioned above. This has a direct bearing on the analysis of the crystal growth process. We shall report on progress in these directions in a future publication.

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