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The measurement of elastic stresses and energy in cubic single-crystal films by x-ray diffraction

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Anisotropic elasticity calculations have been made for use in conjunction with strain measurements by x-ray diffraction for sputtered single-crystal films. Only the cubic case has been treated. Data from InSb films with (100) and (111) orientations on similarly oriented GaAs substrates are given. It was found that nearly alike planar strains ϵ yield lower planar stresses σ_1' and σ_2' and stored energy density U for the (100) orientation. The (100) films exhibit a relatively large strain perpendicular to the film ϵ_3.

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I. INTRODUCTION

In a previous paper by Vook and Witt,[1] anisotropic elasticity calculations were carried out to determine the strains normal to the free surface within evaporated polycrystalline films. These results demonstrated that the ratio of normal strain ϵ_3 to the strain within the plane of the film ϵ depends upon the orientation (hkl). It was assumed that: (1) the film is firmly attached to the substrate, (2) the thermal expansion of the film and substrate are isotropic in the plane of the substrate, (3) the stress on the film in a direction normal to the plane of the film is zero, and (4) the shear strain in the plane of the films is zero. With these assumptions, useful relations were obtained for the (100), (111), (311), (420), and (422) planes of cubic crystals. Additional transformations were calculated by Rao[2] for (310) and (321) planes. These were used to determine normal strains in sputtered BCC films.

This paper deals with the x-ray measurement of the planar and normal strain within anisotropic cubic single-crystal films. Special attention is given to sputtered films deposited onto a dissimilar single-crystal substrate. Anisotropic elasticity theory is used to calculate the planar stresses, their maximum and minimum directions, and stored elastic energies for any film orientation. The final equations are given in simplified forms in terms of the elastic constant C_{ij} and the film orientation.

Sputtered films may contain additional stresses due to special defects introduced during the deposition of atoms having higher energies than those that are available during evaporation. Therefore, in addition to the assumptions made by Vook and Witt, one must also assume that: (5) the defects introduced by sputtering develop an additional isotropic strain in the plane of the film ϵ_{in}. This assumption is analogous with assumption (2) dealing with the strain contribution from differential thermal expansions or contractions ϵ_{th}. In sputtered films, inert gas atoms can cause a change in the interplanar spacing of the atomic planes within a crystal which remains when the film is removed from the substrate. This material may be treated as a solid solution between the target material and atomic species from the sputtering gas.

The x-ray method and elastic calculations are applied to strain and stress determinations in a sputtered InSb film on a GaAs substrate.

II. THEORY

It is convenient to begin with the strain ellipsoid.[3] Each point on the ellipsoidal surface represents the component of normal strain, whose direction and magnitude are those of the radius vector to this point. The strain point corresponding to the angles χ (collateral angle) and ϕ (rotation about normal to the film) is given by

$$\epsilon_{\phi\chi} = \epsilon_1 \sin^2\chi \cos^2\phi + \epsilon_2 \sin^2\chi \sin^2\phi + \epsilon_3 \cos^2\chi. \quad (1)$$

Because of strain isotropy in the plane of the film (i.e., $\epsilon_1 = \epsilon_2 = \epsilon$), this simplifies to

$$\epsilon_\chi = (\epsilon - \epsilon_3)\sin^2\chi + \epsilon_3. \quad (2)$$

Equation (2) can be related to the various stresses σ_i by using the two sets of relations:
For the (001) orientation in the cubic system,

$$\sigma_1 = \sigma_2 = (C_{11} + C_{12})\epsilon + C_{12}\epsilon_3, \quad (3a)$$

$$\sigma_3 = 2C_{12}\epsilon + C_{11}\epsilon_3, \quad (3b)$$

or for all other (hkl) planes,

$$\sigma_1' = (C_{11}' + C_{12}')\epsilon + C_{13}'\epsilon_3, \quad (4a)$$

$$\sigma_2' = (C_{21}' + C_{22}')\epsilon + C_{23}'\epsilon_3, \quad (4b)$$

$$\sigma_3' = (C_{31}' + C_{32}')\epsilon + C_{33}'\epsilon_3. \quad (4c)$$

To obtain an explicit expression for the stress, one must transform the matrix of elastic constants into a new set of C_{ij}' constants. By substituting into Eqs. 4(a)–(c) and using the results of the transformations as given in the Appendix, one obtains

$$\sigma_1' = [C_{11} + (A+1)C_{12} + C_{an}(A-1)\Omega_1]\epsilon, \quad (4d)$$

$$\sigma_2' = [C_{11} + (A+1)C_{12} + C_{an}(A-1)\Omega_2]\epsilon, \quad (4e)$$

where

$$C_{an} = C_{44} - \frac{1}{2}(C_{11} - C_{12}), \quad (4f)$$

$$A=\frac{\epsilon_3}{\epsilon}=\frac{-2C_{12}+C_{an}\Omega_{hkl}}{C_{11}+C_{an}\Omega_{hkl}}, \tag{4g}$$

$$\Omega_{hkl}=4(\alpha_3^2\beta_3^2+\alpha_3^2\gamma_3^2+\beta_3^2\gamma_3^2), \tag{4h}$$

$$\Omega_1=4(\alpha_1\beta_1\alpha_3\beta_3+\alpha_1\gamma_1\alpha_3\gamma_3+\beta_1\gamma_1\beta_3\gamma_3), \tag{4i}$$

$$\Omega_2=4(\alpha_2\beta_2\alpha_3\beta_3+\alpha_2\gamma_2\alpha_3\gamma_3+\beta_2\gamma_2\beta_3\gamma_3). \tag{4j}$$

Equation (4g) was obtained by setting Eq. (4c) equal to zero and solving for A. Combining Eqs. (2), (4d), and (4c) gives

$$\epsilon_\chi=f_1'\sigma_1^{s\prime}\sin^2\chi-f_1''\sigma_1^{e\prime}, \tag{5a}$$

$$\epsilon_\chi=f_2'\sigma_2^{s\prime}\sin^2\chi-f_2''\sigma_2^{e\prime}, \tag{5b}$$

with

$$f_1'=\frac{1-A}{[C_{11}+(A+1)C_{12}+C_{an}(A-1)\Omega_1]}, \tag{6a}$$

$$f_1''=\frac{-A}{[C_{11}+(A+1)C_{12}+C_{an}(A-1)\Omega_1]}, \tag{6b}$$

$$f_2'=\frac{1-A}{[C_{11}+(A+1)C_{12}+C_{an}(A-1)\Omega_2]}, \tag{6c}$$

$$f_2''=\frac{-A}{[C_{11}+(A+1)C_{12}+C_{an}(A-1)\Omega_2]}. \tag{6d}$$

If the data are free of errors, the value of the stress obtained from the slope of Eqs. 5(a) and (b) is equal to the corresponding extrapolated stress

$$\sigma_1^{s\prime}=\sigma_1^{e\prime}=\sigma_1',$$

$$\sigma_2^{s\prime}=\sigma_2^{e\prime}=\sigma_2'.$$

In case of an isotropic film, Eqs. 5(a) and (b) simplify to

$$\epsilon_\chi=\frac{1+\nu}{E}\sigma^s\sin^2\chi-\frac{2\nu}{E}\sigma^e, \tag{5c}$$

where σ^s and σ^e are the isotropic plane stresses obtained from the slope and by extrapolation. This requires that $f'_{\rm iso}=(1+\nu)/E$ and $f''_{\rm iso}=2\nu/E$, which is obtained with $C_{an}=0$ giving

$$f_1'=f_2'=f'_{\rm iso}=\frac{1-A_{\rm iso}}{C_{11}+(A_{\rm iso}+1)C_{12}}=\frac{C_{11}+2C_{12}}{C_{11}(C_{11}+C_{12})-2C_{12}^2}, \tag{7a}$$

and

$$f_1''=f_2''=f''_{\rm iso}=\frac{-A_{\rm iso}}{C_{11}+(A_{\rm iso}+1)C_{12}}=\frac{2C_{12}}{C_{11}(C_{11}+C_{12})-2C_{12}^2}. \tag{7b}$$

Lamés constants (λ,μ) are introduced to provide connecting relationships between the elastic moduli (C_{11}, C_{12}), Young's modulus (E) and Poisson's ratio (ν), i.e.,

$$\lambda=\frac{\nu E}{(1+\nu)(1-2\nu)}=C_{11},$$

and

$$\mu=\frac{E}{2(1+\nu)}=\frac{1}{2}(C_{11}-C_{12}).$$

Solving for C_{12} and substituting into Eqs. 7(a) and (b), provides the isotropic limit as previously given by Eq. (5c).

Equations 5(a) and (b) are based upon Eq. (2), and since $(\epsilon-\epsilon_3)$ as well as ϵ_3 are obtainable from direct measurements of ϵ_χ vs $\sin^2\chi$, the following relations are used to determine the stresses

$$f_1'\sigma_1^{s\prime}=f_2'\sigma_2^{s\prime}=\epsilon-\epsilon_3, \tag{8a}$$

$$f_1''\sigma_1^{e\prime}=f_2''\sigma_2^{e\prime}=\epsilon_3. \tag{8b}$$

One may also obtain the average plane stresses $<\sigma^s>$ and $<\sigma^e>$ from

$$<\sigma^s>=\frac{1}{2}\left[\frac{1}{f_1'}+\frac{1}{f_2'}\right](\epsilon-\epsilon_3), \tag{9a}$$

and

$$<\sigma^e>=\frac{1}{2}\left[\frac{1}{f_1''}+\frac{1}{f_2''}\right]\epsilon_3, \tag{9b}$$

with

$$\frac{1}{f_1'}+\frac{1}{f_2'}=\frac{2[C_{11}+(A+1)C_{12}]}{1-A}+C_{an}\Omega_{hkl}, \tag{10a}$$

$$\frac{1}{f_1''}+\frac{1}{f_2''}=\frac{-2[C_{11}+(A+1)C_{12}]}{A}+\frac{C_{an}(A-1)}{A}\Omega_{hkl}. \tag{10b}$$

Although it would appear that Eqs. 9(a) and (b) are redundant, two separate determinations of the average plane stress provides a crosscheck on the assumptions made in arriving at Eq. (2).

For biaxial strain, ϵ_3 is of opposite sign to ϵ due to either a Poisson expansion or contraction along the 3 direction. The sign reversal requires that ϵ_χ cross the $\sin^2\chi$ axis. And, this must occur at

$$\sin^2\chi_0=1/(1-\epsilon/\epsilon_3) \tag{11a}$$

or in terms of the elastic constants:
for (100) type planes

$$\sin^2\chi_0=2C_{12}/(C_{11}+2C_{12}), \tag{11b}$$

and for all others,

$$\sin^2\chi_0=(2C_{12}+C_{an}\Omega_{hkl})/(C_{11}+2C_{12}). \tag{11c}$$

For isotropic films the corresponding value is

$$\sin^2\chi_0=2\nu/(1+\nu). \tag{11d}$$

The crossover point $\sin^2\chi_0$ is required to correct the x-ray diffraction data for solid solution effects in films which are not usually present in a bulk standard.

The strain energy per unit volume is readily calculated for the anisotropic case using

$$U=\frac{1}{2}\epsilon_i'\epsilon_j'C_{ij}',$$

where a summation over i and j is implied. For the general case, this reduces to

$$U_{hkl}=\frac{1}{2}[C_{11}(2+A^2)+2C_{12}(1+2A)+C_{an}(1-A)^2\Omega_{hkl}]\epsilon^2 \tag{12a}$$

and for the (100) orientation, is given by

$$U_{100} = \left[C_{11} + C_{12} + 2A_{100}C_{12} + \frac{1}{2}A_{100}^{2}C_{11}\right]\epsilon^2. \qquad (12b)$$

The energy per unit volume for an isotropic film is

$$U_{iso} = \frac{E}{(1+\nu)(1-2\nu)}\,[1 + 2\nu A_{iso} + (1-\nu)A_{iso}{}^2]\epsilon^2. \qquad (12c)$$

A. Maximum and minimum stress directions in the plane of the film

Even though the plane strain is isotropic, it need not follow that the plane stress must be isotropic when $C_{an} \neq 0$. On the other hand, it is possible to select certain planes in the cubic system when $C_{an} \neq 0$ such that $\sigma_1' = \sigma_2'$. This is true for the (001) and (111) orientations. For other planes, $\sigma_1' \neq \sigma_2'$ and a complete description of the planar stresses requires a knowledge of the maximum (minimum) stress direction in the plane of the film. Details of this calculation are given in the Appendix. The maximum (minimum) stress direction is obtained by maximizing (minimizing) the stress σ_1' subject to the condition that the direction cosines of the unit vector 1′ along the 1′-2′-3′ directions be orthogonal to the normal of the planes (hkl). The normal and orthogonal conditions are achieved by introducing two Lagrange multipliers. A solution to the following equations provides the direction cosines α_1, β_1, and γ_1 which define the maximum and minimum stress direction 1′ and 2′ in terms of the edge directions of the cubic unit cell for the plane (hkl)

$$\left.\begin{aligned} &l(k^2-h^2)\alpha_1\beta_1 + k(h^2-l^2)\alpha_1\gamma_1 + h(l^2-k^2)\beta_1\gamma_1 = 0\\ &\alpha_1 h + \beta_1 k + \gamma_1 l = 0\\ &\alpha_1^2 + \beta_1^2 + \gamma_1^2 - 1 = 0. \end{aligned}\right\} \qquad (13a)$$

With each pair of solutions, a set of direction cosines is constructed with respect to the edges of the unit cell (Table I). Substituting these values into Eqs. 4(d) and (e) allows the maximum (minimum) plane stresses to be determined.

B. Stresses and strains in (100) and (111) oriented single-crystal InSb films on GaAs substrates.

The strain difference $\epsilon - \epsilon_3$, as well as ϵ_3 can be obtained entirely by x-ray diffraction. These are obtained most accurately from a set of hkl reflections selected at high 2θ angles over a range of χ values. The interplanar χ angles are measured between the plane of the film and those (hkl) planes selected for the strain analysis. These highly localized reflections are found by systematically varying ϕ, χ, and 2θ for maximum intensity. When an intensity maximum is found in 2θ, χ, and ϕ, a 2θ scan is made for a final determination of the maximum. Subsequently, the shift $\Delta\, 2\theta = 2\theta - 2\theta_0$ is determined relative to the target material $(2\theta_0)$ as a standard substance, and the strain is obtained from

$$\epsilon_\chi = -\frac{1}{2}\,[\cot\theta(hkl)]\Delta\, 2\theta. \qquad (13b)$$

Two orientations of InSb single-crystal films are used to illustrate the procedure and results: one has a (100) orientation while the second a (111). Both are deposited onto corresponding orientations of GaAs substrates.

An examination of the elastic constants for InSb films indicates that this material is anisotropic, as is demonstrated by

$$C_{an} = 1.50,$$

with $C_{11} = 6.72$, $C_{12} = 3.67$, and $C_{44} = 3.02$ all expressed in 10^{11} dyn/cm^2.[4]

Single-crystal (100) and (111) oriented films are especially simple to treat because the plane stress is isotropic when the plane strain is isotropic. The elastic anisotropy produces large differences in the elastic parameters used to calculate the stress from strain for the (100) and (111) orientations. These parameters are listed in Table II along with χ_0 values which are required to correct the strain data. The elastic parameters vary by a factor of 2 to 3, whereas χ_0 is much less sensitive to crystal orientation.

X-ray strain data are given in Figs. 1 and 2 along with the reflection plane from which each point was obtained. A least-squares fit to the (100) data gives

$$\epsilon - \epsilon_3 = -4.23\times 10^{-3},$$
$$\epsilon_{xr} + \epsilon_3 = 2.70\times 10^{-3},$$

and a mean-square error of $\pm 0.22\times 10^{-3}$ in the linear fit. The corresponding data for (111) planes gives

$$\epsilon - \epsilon_3 = -3.08\times 10^{-3},$$
$$\epsilon_{xr} + \epsilon_3 = 1.37\times 10^{-3},$$

with a mean-square error of $\pm 0.13\times 10^{-3}$. The accuracy of these residual stress measurements is comparable to the ac-

TABLE I. Direction cosine matrix (a) illustrating general notation.

	1	2	3
(a) General notation			
1′	α_1	β_1	γ_1
2′	α_2	β_2	γ_2
3′	α_3	β_3	γ_3
(b) Values for (111) transformation.			
1′	$1/\sqrt{6}$	$1/\sqrt{6}$	$-2/\sqrt{6}$
2′	$1/\sqrt{2}$	$-1/\sqrt{2}$	0
3′	$1/\sqrt{3}$	$1/\sqrt{3}$	$1/\sqrt{3}$

TABLE II. Anisotropic elastic parameters required in Eqs. (6a) and (6b) for InSb.

hkl	χ_0(degrees)	$f_1' = f_2'$(cm^2/dyn)	$f_1'' = f_2''$(cm^2/dyn)
100	46.3	32.750	−17.100
111	38.1	16.540	−6.294

Calculated from:
$C_{11}' = C_{22}' = 0.0822$
$C_{31}' = C_{32}' = C_{23}' = C_{13}' = 0.0268$
$C_{12}' = C_{21}' = 0.0318$
$C_{33}' = 0.0872$
All expressed in dyn/cm^2.

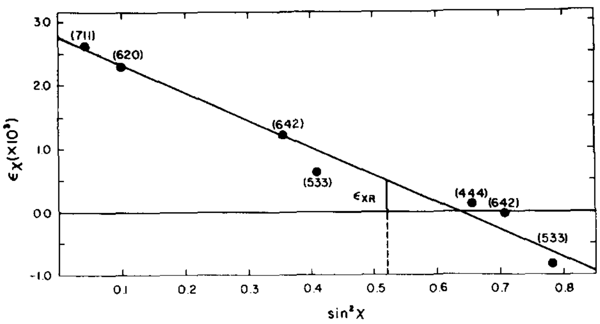

FIG. 1. Apparent strain, ϵ_χ vs $\sin^2\chi$ for (100) oriented InSb film on (100) GaAs.

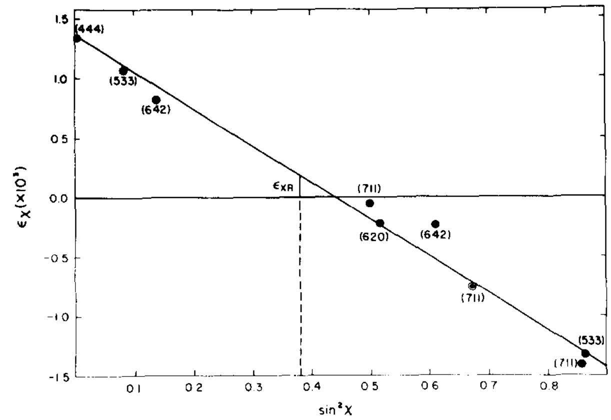

FIG. 2. Apparent strain, ϵ_χ vs $\sin^2\chi$ for (111) oriented InSb film on (111) GaAs.

curacy usually obtained using standard x-ray diffraction techniques.[5] Values of ϵ_{xr} were determined at the $\sin^2\chi_0$ crossover points as illustrated in Figs. 1 and 2 and are given in Table III.

The strain contribution, perpendicular to the plane of the film, is obtained from the differential thermal contractions of film and substrate material, i.e.,

$$\epsilon_{3th} = (\alpha_s - \alpha_f) A_{hkl} (T_D - T_R), \qquad (14)$$

where

$$A_{(100)} = -2C_{12}/C_{11}$$

and

$$A_{(111)} = -(2C_{12} + 4C_{an}/3)(C_{11} + 4C_{an}/3),$$

and $\alpha_s (= 6.13\times10^{-6})$ and $\alpha_f (= 5.7\times10^{-6})$ are the thermal expansion coefficients[6] for substrate and film, and T_D and T_R are the deposition and room temperatures. The planar intrinsic strain ϵ_{in} is obtained by subtracting ϵ_{th}, the thermal strain in the plane of the film, from the total strain ϵ. The thermal and intrinsic parts of the planar strain are related to their components perpendicular to the plane of the film ϵ_{3th} and ϵ_{3in}, respectively, through Eq. 4(g). These results as well as the related stresses may be found in Table III. It can be seen that the dominant stresses and strains are intrinsic. The apparent x-ray strains may extend over the ranges

$$0.27\times10^{-3} < \epsilon_{xr}(100) < 0.71\times10^{-3}$$

and

$$0.07\times10^{-3} < \epsilon_{xr}(111) < 0.33\times10^{-3}$$

with central values of 0.49×10^{-3} and 0.20×10^{-3}. In view of the smallness of each of these strain terms and the possibility of overlap in values when the errors are considered, it would appear that an explanation of these differences may not be justified at this time.

The elastic energy density is readily calculated from Eqs. 12(a) and (b) giving $U = C(hkl)\epsilon^2$ with $C(100) = 0.0639$ and $C(111) = 0.0975$ in dyn/cm^2. These densities may be found in Table III. One finds the elastic energy density for the (111) oriented InSb film to be larger than for the (100) orientation. It is also evident from values of $C(hkl)$ that the (100) orientation allows much more strain to be developed for a given value of strain energy.

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APPENDIX

In general, the elastic constants required in Eqs. 4(a)–(c) depend upon the choice of the axes, i.e. 1′, 2′, and 3′. These can be calculated from the measured elastic constants C_{11}, C_{12}, and C_{44}. The latter are based upon the axes along edges of the cubic cell (1, 2, and 3), while the new axes are chosen such that 3′ is perpendicular to the film and 1′ and 2′ are mutually perpendicular in the plane of the film. For an isotropic film, the constants are independent of the choice of the orthogonal coordinate system.

The transformations required for general anisotropic materials are given in reference.[7] The transformed moduli may be obtained from the summation

$$C'_{ij} = \omega_i \omega_j \sum_{m=1}^{6} \sum_{n=1}^{6} \frac{C_{mn}}{\omega_m \omega_n} Q_{mi} Q_{ni}, \qquad (15)$$

with $\omega_k = 1$, for $k = 1, 2$, and 3 and $\omega_k = \frac{1}{2}$ for $k = 4, 5$, and

TABLE III. Listing of individual thermal, intrinsic, and ϵ_{xr} strains along with the corresponding stresses and energy densities. σ and U are in dyn/cm^2.

Specimen	ϵ_{3th}	ϵ_{3in}	ϵ_{th}	ϵ_{in}	ϵ_{xr}	σ_{th}	σ_{in}	$\sigma^{a)}$	U
	$X10^3$	$X10^3$	$X10^3$	$X10^3$	$X10^3$	$X10^{-8}$	$X10^{-8}$	$X10^{-8}$	$X10^{-6}$
(111)/400 °C	0.092	1.08	− 0.15	− 1.76	0.20	− 1.47	− 17.15	− 18.62	3.54
(100)/425 °C	0.175	2.04	− 0.16	− 1.86	0.49	− 1.02	− 11.90	− 12.91	2.60

a) $\sigma = \sigma_1 = \sigma_2$ for (100) and (111).

TABLE IV. General definition of Q_{ij} terms in terms of direction cosines of special axes 1′, 2′, and 3′.

$i \backslash j$	1	2	3	4	5	6
1	α_1^2	α_2^2	α_3^2	$2\alpha_2\alpha_3$	$2\alpha_3\alpha_1$	$2\alpha_1\alpha_2$
2	β_1^2	β_2^2	β_3^2	$2\beta_2\beta_3$	$2\beta_3\beta_1$	$2\beta_1\beta_2$
3	γ_1^2	γ_2^2	γ_3^2	$2\gamma_2\gamma_3$	$2\gamma_3\gamma_1$	$2\gamma_1\gamma_2$
4	$\beta_1\gamma_1$	$\beta_2\gamma_2$	$\beta_3\gamma_3$	$\beta_2\gamma_3+\beta_3\gamma_2$	$\beta_1\gamma_3+\beta_3\gamma_1$	$\beta_1\gamma_2+\beta_2\gamma_1$
5	$\gamma_1\alpha_1$	$\gamma_2\alpha_2$	$\gamma_3\alpha_3$	$\gamma_2\alpha_3+\gamma_3\alpha_2$	$\gamma_1\alpha_3+\gamma_3\alpha_1$	$\gamma_1\alpha_2+\gamma_2\alpha_1$
6	$\alpha_1\beta_1$	$\alpha_2\beta_2$	$\alpha_3\beta_3$	$\alpha_2\beta_3+\alpha_3\beta_2$	$\alpha_1\beta_3+\alpha_3\beta_1$	$\alpha_1\beta_2+\alpha_2\beta_1$

6. The values of Q_{mi} are given in Tables IV and V. A sample calculation for C'_{11} is given below for a cubic material.

Summing Eq. (15) in m and n, and noting that for cubic crystals, $C_{11}=C_{22}=C_{33}$, $C_{12}=C_{21}=C_{23}=C_{32}=C_{13}=C_{31}$, $C_{44}=C_{55}=C_{66}$, and all other C_{ij}'s are equal to zero, one obtains

$$C'_{11}=C_{11}(Q_{11}^2+Q_{21}^2+Q_{31}^2)+2C_{12}(Q_{11}Q_{21}+Q_{11}Q_{31}+Q_{21}Q_{31})+4C_{44}(Q_{41}^2+Q_{51}^2+Q_{61}^2). \quad (16a)$$

Substituting the values of Q_{11}, Q_{21}, Q_{31}, Q_{41}, Q_{51}, and Q_{61} into Eq. 16(a) from Table IV gives

$$C'_{11}=C_{11}+4C_{an}(\alpha_1^2\beta_1^2+\gamma_1^2\alpha_1^2+\beta_1^2\gamma_1^2. \quad (17a)$$

Similarly, it can be shown that

$$C'_{12}=C_{12}+4C_{an}(\alpha_1\beta_1\alpha_2\beta_2+\alpha_1\gamma_1\alpha_2\gamma_2+\beta_1\gamma_1\beta_2\gamma_2), \quad (17b)$$

$$C'_{13}=C_{12}+C_{an}\Omega_1, \quad (17c)$$

$$C'_{22}=C_{11}+4C_{an}(\alpha_2^2\beta_2^2+\alpha_2^2\gamma_2^2+\beta_2^2\gamma_2^2), \quad (17d)$$

$$C'_{23}=C_{12}+C_{an}\Omega_2, \quad (17e)$$

$$C'_{33}=C_{11}+C_{an}\Omega_{hkl}, \quad (17f)$$

and

$$C'_{21}=C'_{12}, \quad (17g)$$

$$C'_{31}=C'_{13}, \quad (17h)$$

$$C'_{32}=C'_{23}. \quad (17i)$$

Specifically for a (111) oriented film, choosing the 1′, 2′, and 3′ directions as $(11\bar{2})$, $(1\bar{1}0)$, (111), respectively, and substituting these values into Eqs. 17(a)–(i), one gets

$$C'_{11}=0.5C_{11}+0.5C_{12}+C_{44}, \quad (18a)$$

$$C'_{12}=0.167C_{11}+0.833C_{12}-0.333C_{44}, \quad (18b)$$

TABLE V. Q_{ij} terms for (111) plane with 1′ selected along $[1\bar{1}2]$, 2′ and 3′ are along $[1\bar{1}0]$ and [111], respectively.

$i \backslash j$	1	2	3	4	5	6
1	1/6	1/2	1/3	$2/\sqrt{6}$	$2/\sqrt{18}$	$2/\sqrt{12}$
2	1/6	1/2	1/3	$-2/\sqrt{6}$	$2/\sqrt{18}$	$-2/\sqrt{12}$
3	4/6	0	1/3	0	$-4/\sqrt{18}$	0
4	−2/6	0	1/3	$-1/\sqrt{6}$	$-1/\sqrt{18}$	$2/\sqrt{12}$
5	−1/3	0	1/3	$1/\sqrt{6}$	$-1/\sqrt{18}$	$-2/\sqrt{12}$
6	1/6	−1/2	1/3	0	$2/\sqrt{18}$	0

TABLE VI. $\Omega_{hkl}/4$, $\Omega_1/4$, maximum and minimum stress directions for various hkl planes.

hkl	$\Omega_{hkl}/4$	Directions Maximum & Minimum		$\Omega_1/4$ 1	2
100	0	Isotropic		0	0
110	0.25	$1\bar{1}0$,	001	−1/4	0
111	0.333	Isotropic		−1/6	−1/6
311	0.157	233,	011	−27/242	−1/22
331	0.27	$1\bar{1}0$,	$11\bar{6}$	−9/38	−27/722
420	0.16	$1\bar{2}0$,	$00\bar{1}$	−4/25	0
211	0.25	$\bar{1}11$,	$01\bar{1}$	−1/6	−1/12
310	0.09	$\bar{1}30$,	001	−9/100	0

$$C'_{13}=0.333C_{11}+0.667C_{12}-0.667C_{44}, \quad (18c)$$

$$C'_{33}=0.333C_{11}+0.667C_{12}-1.333C_{44}, \quad (18d)$$

and

$$C'_{22}=C'_{11}, \quad (18e)$$

$$C'_{21}=C'_{12}, \quad (18f)$$

$$C'_{31}=C'_{13}=C'_{23}=C'_{32}. \quad (18g)$$

From Eq. (4d),

$$\sigma'_1=[C_{11}+(A+1)C_{12}+C_{an}(A-1)\Omega_1]\epsilon.$$

To determine the maximum (minimum) stresses in the plane of the film, $\Omega_1=\alpha_1\beta_1hk+\alpha_1\gamma_1hl+\beta_1\gamma_1kl$ has to be maximized (minimized). This has been written in terms of h, k, and l using

$$\alpha_3=\frac{h}{(h^2+k^2+l^2)^{1/2}},$$

$$\beta_3=\frac{k}{(h^2+k^2+l^2)^{1/2}},$$

and

$$\gamma_3=\frac{l}{(h^2+k^2+l^2)^{1/2}}.$$

Since direction 1′ is perpendicular to direction 3′ and is a unit vector, the following conditions must also be imposed

$$\left.\begin{array}{l}\alpha_1h+\beta_1k+\gamma_1l=0\\ \alpha_1^2+\beta_1^2+\gamma_1^2=1\end{array}\right\}. \quad (19)$$

This problem can be solved using the method of Lagrange. A function F is formed as follows:

$$F=\alpha_1\beta_1hk+\alpha_1\gamma_1hl+\beta_1\gamma_1kl+\lambda_1(\alpha_1^2+\beta_1^2+\gamma_1^2-1)+\lambda_2(\alpha_1h+\beta_1k+\gamma_1l),$$

where λ_1 and λ_2 are constants. Setting

$$\partial F/\partial\alpha_1,\ \partial F/\partial\beta_1,\ \partial F/\partial\gamma_1,\ \partial F/\partial\lambda_1,$$

and

$$\partial F/\partial\lambda_2,$$

equal to zero, leads to the following five equations involving α_1, β_1, γ_1, λ_1, and λ_2:

$$\left.\begin{array}{l}(\gamma_1kl+\alpha_1hk)+2\lambda_1\beta_1+\lambda_2k=0,\\ (\beta_1kl+\alpha_1hl)+2\lambda_1\gamma_1+\lambda_2l=0,\\ (\gamma_1hl+\beta_1hk)+2\lambda_1\alpha_1+\lambda_2h=0,\\ \alpha_1h+\beta_1k+\gamma_1l=0,\\ \alpha_1{}^2+\beta_1{}^2+\gamma_1{}^2=1.\end{array}\right\} \quad (20)$$

Eliminating λ_1 and λ_2 from the first three equations and retaining the last two equations, one gets Eq. 13(a), which defines the maximum or minimum stress direction (α_1, β_1, γ_1). In the case of a (111) oriented film, the first equation in Eq. 13(a) drops out, and hence, all the directions in the plane of the film have the same stress. Sample calculations are given in Table VI.

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