

Diffusion-induced stresses in a long bar under an electric field

Chi-Chuan Hwang[†], Ke-Ming Chen and Jin-Yuan Hsieh

Department of Mechanical Engineering, Chung Yuan University, Chung-Li, Taiwan 32023, Republic of China

Received 17 May 1994, in final form 12 July 1994

Abstract. Diffusion-induced stresses in a long bar with a square cross section under an electric field are calculated. We obtain in advance analytical solutions of the concentration, then with these results, the diffusion-induced stresses are also calculated analytically by introducing the displacement potential and Airy stress function. The results show that the electric field can depress the stresses and deviate the positions of local maximum stresses, and these effects are more apparent at short times than at long times.

1. Introduction

Diffusion-induced stresses in semiconductor materials during diffusion processes have been studied extensively over recent decades, because they can cause dislocation generation which affects solute distribution and subsequent electronic properties [1]. The diffusion-induced stresses are built up by composition inhomogeneity during mass transfer, i.e. they are caused by concentration gradients, similar to those caused by temperature gradients in an otherwise unstressed body. Prussin [2] was the first to analyse the transverse stresses developed in a thin plate during the diffusion process. The diffusion-induced stresses related to the dislocation density were studied in detail by Tuck [3]. Li [4] solved the diffusion-induced stresses in a single-phase elastic medium of various geometries and corrected an error made by Prussin [2]. Further, Lee and Li [5] proposed that the most rapid diffusion processes occur without generation of dislocation. Chu and Lee [6] investigated diffusion-induced stresses in two-phase elastic media. However, the above calculations of diffusion-induced stresses only treated one-dimensional systems because of geometric symmetry. Chu and Lee [7] further carried out a study of diffusion-induced stresses in a long bar of square cross section. In their work, the concentration distribution was obtained in an analytic form, while the displacement and the stress fields were obtained numerically using a Jacobi iterative method.

Besides natural diffusion, the forced diffusion of charged impurities can also occur if an electric field is applied during the diffusion process. In this work we take such a problem into consideration. A long bar of square cross section is considered. We use a two-step diffusion process as follows. In the short first

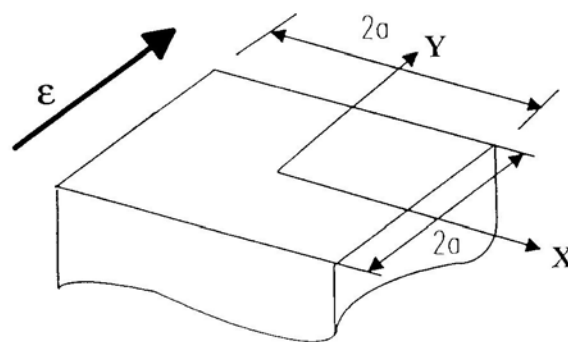


Figure 1. Physical configuration of a long bar under an electric field.

step (the prediffusion) the desired amount of solute is absorbed at the surface. Under proper conditions we can maintain a constant solute concentration at the surface. In the second step (the redistribution) the solute near the surface diffuses into the long bar.

We will obtain the analytic solution of concentration in advance. Then, by introducing a displacement potential and an Airy stress function, we can derive the analytic forms of the diffusion-induced stresses. This kind of method has been successfully implemented in solving the thermal stresses during Czochralski growth process [8,9]. The results are compared with those obtained by Chu and Lee [7], and effects of the applied electric field are discussed.

2. Concentration distribution

Consider a long bar with square cross section in the region $-a \leq X, Y \leq a$, as shown in figure 1. Initially there is no charged impurity inside the bar, and as the process begins, the concentration at the outer surface is maintained constant at C_0 during diffusion. An electric

[†] To whom all correspondence should be addressed.

field causing charged impurity drift in the Y direction is applied simultaneously. Hence the concentration $C(X, Y, t)$ must obey the modified Fick's law [3]:

$$\left[D \left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} \right) - v \frac{\partial}{\partial Y} \right] C = \frac{\partial}{\partial t} C \quad (1)$$

where D is a constant representing the isotropic diffusivity and v is the mean drift velocity of the particles. Under the influence of the field, $v = B\varepsilon$, where B is the mobility and ε the applied field. The mobility B is related to a diffusion coefficient by Einstein's relation [3]:

$$\frac{D}{B} = \frac{kT}{qz} \quad (2)$$

where k is Boltzmann's constant, q the electronic charge, qz the ionic charge, and T the absolute temperature. The corresponding initial and boundary conditions just mentioned are

$$\begin{aligned} C(X, Y, t) &= 0 \\ C(\pm a, Y, t) &= C_0 \\ C(X, \pm a, t) &= C_0. \end{aligned} \quad (3)$$

Equations (1) and (3) can be transformed into dimensionless forms by using the following scalings:

$$\begin{aligned} x &= \frac{X}{a} & y &= \frac{Y}{a} & \tau &= \frac{Dt}{a^2} \\ p &= \frac{va}{D} & c &= \frac{C}{C_0} \end{aligned} \quad (4)$$

then one has

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - p \frac{\partial}{\partial y} \right) c = \frac{\partial}{\partial \tau} c \quad (5)$$

and

$$\begin{aligned} c(x, y, \tau) &= 0 \\ c(\pm 1, y, \tau) &= 1 \\ c(x, \pm 1, \tau) &= 1. \end{aligned} \quad (6)$$

Solving the above equations and omitting the details of calculation, one finds

$$c(x, y, \tau) = 1 + \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A_{mn} e^{py/2} e^{-\lambda_{mn}\tau} \cos \alpha_n x \cos \omega_m y \quad (7)$$

where

$$\begin{aligned} A_{mn} &= -\frac{8(-1)^{m+n} e^{p^2/4} \omega_m (1 + e^{-p})}{\alpha_n (p^2 + 4\omega_m^2)} \\ \lambda_{mn} &= \alpha_n^2 + \omega_m^2 + \frac{p^2}{4} \\ \alpha_n &= \frac{2n+1}{2} \pi \\ \omega_m &= \frac{2m+1}{2} \pi. \end{aligned} \quad (8)$$

3. The diffusion-induced stresses

As the concentration distribution is obtained one can proceed to find the diffusion-induced stress distributions. A plane strain problem is considered. We first introduce the dimensionless displacement potential ϕ_0 and the Airy stress function ϕ_A which respectively have to satisfy

$$\Delta \phi_0 = c(x, y, \tau) \quad (9)$$

$$\Delta \Delta \phi_A = 0 \quad (10)$$

where $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ and $c(x, y, \tau)$ is shown by equation (7). Then the diffusion-induced stresses are given by

$$\sigma_{ij} = \sigma_{0ij} + \sigma_{Aij} \quad (11)$$

where

$$\begin{aligned} \sigma_{0xx} &= -2\mu \frac{\partial^2 \phi_0}{\partial y^2} \\ \sigma_{0yy} &= -2\mu \frac{\partial^2 \phi_0}{\partial x^2} \\ \sigma_{0zz} &= -2\mu \Delta \phi_0 \\ \sigma_{0xy} &= 2\mu \frac{\partial^2 \phi_0}{\partial x \partial y} \end{aligned} \quad (12)$$

and

$$\begin{aligned} \sigma_{Axx} &= \frac{\partial^2 \phi_A}{\partial y^2} \\ \sigma_{Ayy} &= \frac{\partial^2 \phi_A}{\partial x^2} \\ \sigma_{Azz} &= \nu \Delta \phi_A \\ \sigma_{Axy} &= -\frac{\partial^2 \phi_A}{\partial x \partial y}. \end{aligned} \quad (13)$$

Here μ is the Lamé constant and ν is Poisson's ratio. It should be noted that the dimensionless forms of ϕ_0 , ϕ_A and σ_{ij} are given by

$$\phi_0 = \frac{\Phi_0}{\Lambda} \quad \phi_A = \frac{\Phi_A}{\Lambda} \quad \sigma_{ij} = \frac{\Sigma_{ij}}{\Lambda} \quad (14)$$

where Φ_0 , Φ_A , Σ_{ij} are the dimensional displacement potential, the Airy stress function and stresses respectively, and $\Lambda = 0.01(1+\nu)\bar{V}C_0/(1-\nu)$. Here $\bar{V}$ is the lattice contraction coefficient. The traction-free boundary conditions are adopted, i.e.

$$\begin{aligned} \sigma_{xx}(x, \pm 1, \tau) &= \sigma_{yy}(x, \pm 1, \tau) = 0 \\ \sigma_{xy}(\pm 1, y, \tau) &= \sigma_{xy}(\pm 1, y, \tau) = 0. \end{aligned} \quad (15)$$

Since the dimensionless concentration c has been found in the preceding section, we have a particular solution of equation (9):

$$\phi_0 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} B_{mn}(y) e^{-\lambda_{mn}\tau} \cos \alpha_n x + \frac{1}{4}(x^2 + y^2) \quad (16)$$

where

$$\begin{aligned} B_{mn}(y) &= e^{py/2} (M_{mn} \cos \omega_m y + N_{mn} \sin \omega_m y) \\ M_{mn} &= \frac{A_{mn}(p^2/4 - \omega_m^2 + \alpha_n^2)}{p^2 \omega_m^2 + (p^2/4 - \omega_m^2 + \alpha_n^2)} \\ N_{mn} &= \frac{A_{mn} p \omega_m}{p^2 \omega_m^2 + (p^2/4 - \omega_m^2 + \alpha_n^2)}. \end{aligned} \quad (17)$$

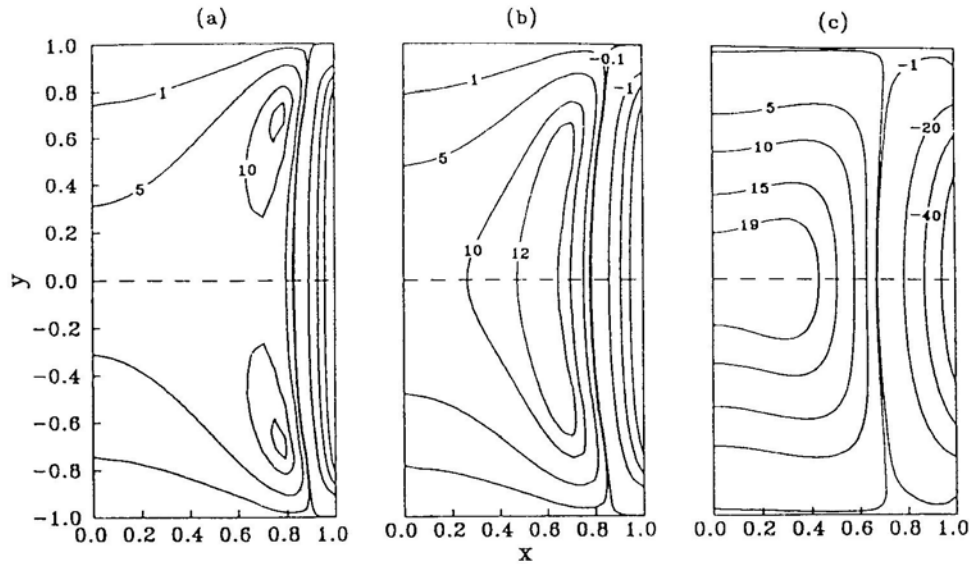


Figure 2. σ_{yy} contours for $p = 0$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

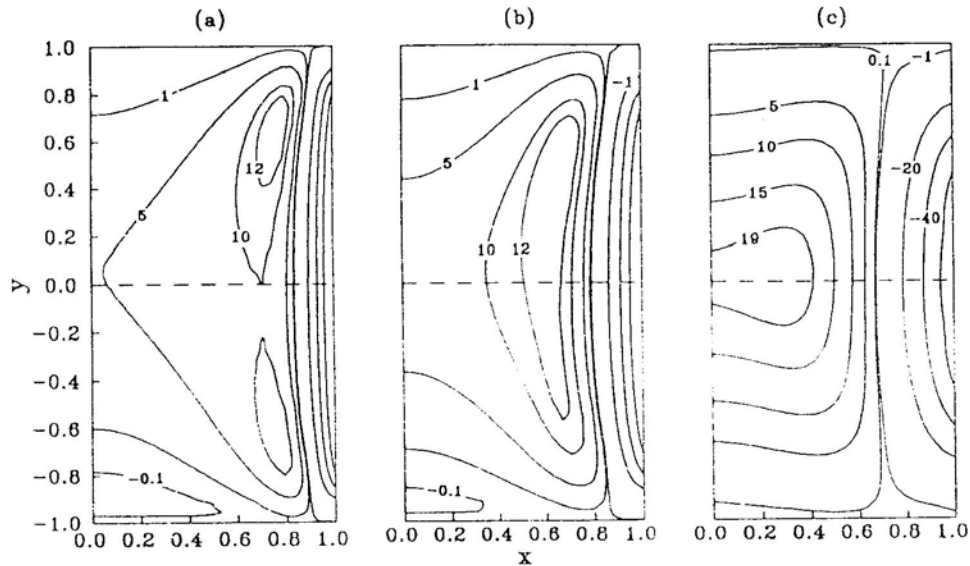


Figure 3. σ_{yy} contours for $p = 0.05$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

The Airy stress function is constructed in the form

$$\phi_A = \phi_1 + \phi_2 \quad (18)$$

thus

$$\sigma_{Aij} = \sigma_{1ij} + \sigma_{2ij} \quad (19)$$

where the stresses σ_{1ij} and σ_{2ij} are derived from ϕ_1 and ϕ_2 respectively. The function ϕ_1 has the form

$$\phi_1 = \sum_{n=0}^{\infty} (E_n \cosh \alpha_n y + F_n \sinh \alpha_n y G_n y \cosh \alpha_n y + H_n y \sinh \alpha_n y) \cos \alpha_n x + \frac{\mu}{2} (x^2 + y^2) \quad (20)$$

where the unknowns E_n , F_n , G_n and H_n are determined by the boundary conditions

$$\begin{aligned} \sigma_{0yy}(x, \pm 1, \tau) + \sigma_{1yy}(x, \pm 1, \tau) &= 0 \\ \sigma_{0xy}(x, \pm 1, \tau) + \sigma_{1xy}(x, \pm 1, \tau) &= 0. \end{aligned} \quad (21)$$

Consequently, one has

$$\begin{aligned} E_n &= \mu (e^{p/2} - e^{-p/2}) (\sinh \alpha_n + \alpha_n \cosh \alpha_n) \\ &\times \sum_{m=0}^{\infty} N_{mn} (-1)^m e^{-\lambda_{mn} \tau} - \mu (e^{p/2} + e^{-p/2}) \sinh \alpha_n \\ &\times \sum_{m=0}^{\infty} \left(\frac{p}{2} N_{mn} - \omega_m M_{mn} \right) (-1)^m e^{-\lambda_{mn} \tau} / \Delta_{1n} \\ F_n &= \mu (e^{p/2} + e^{-p/2}) (\cosh \alpha_n + \alpha_n \sinh \alpha_n) \\ &\times \sum_{m=0}^{\infty} N_{mn} (-1)^m e^{-\lambda_{mn} \tau} - \mu (e^{p/2} - e^{-p/2}) \cosh \alpha_n \\ &\times \sum_{m=0}^{\infty} \left(\frac{p}{2} N_{mn} - \omega_m M_{mn} \right) (-1)^m e^{-\lambda_{mn} \tau} / \Delta_{2n} \\ G_n &= \mu (e^{p/2} - e^{-p/2}) \sinh \alpha_n \end{aligned}$$

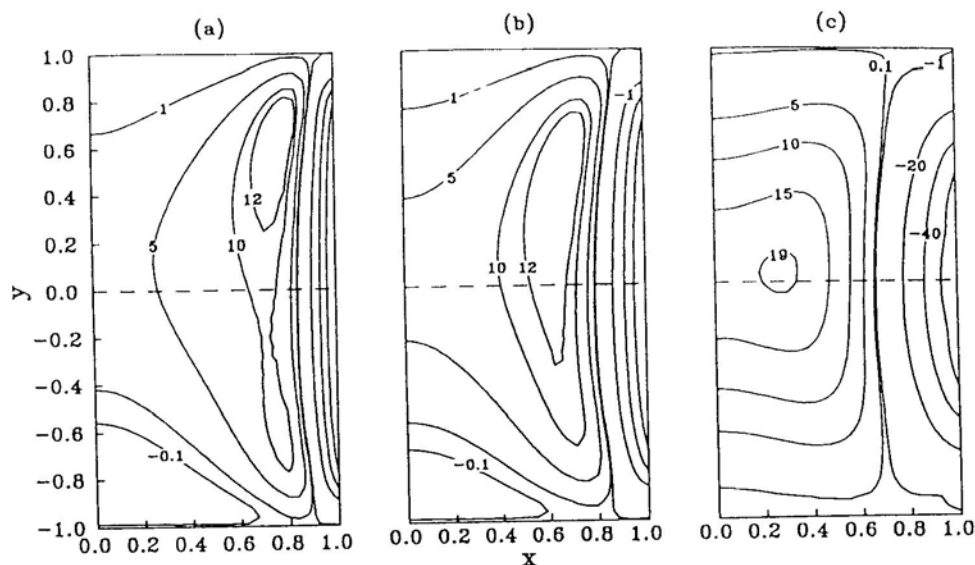


Figure 4. σ_{yy} contours for $p = 0.1$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

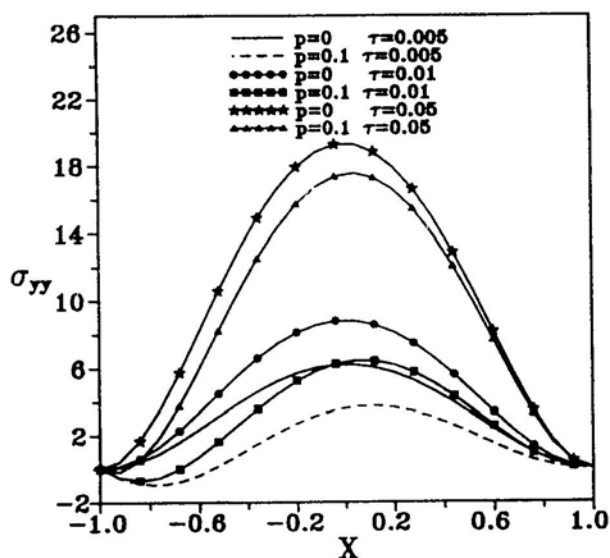


Figure 5. σ_{yy} distribution along the y axis.

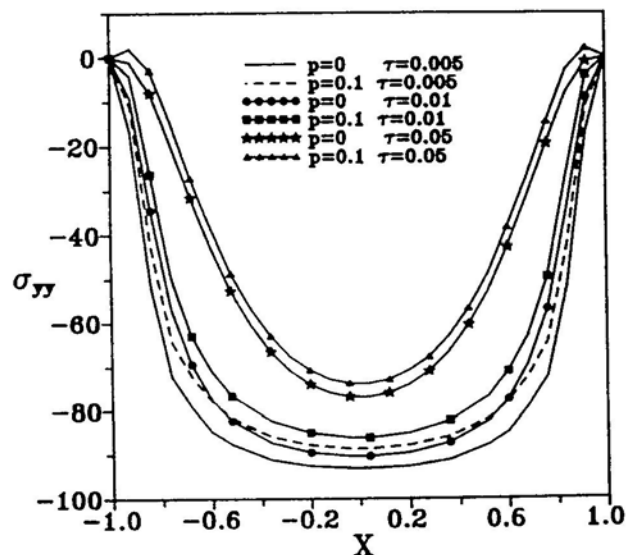


Figure 6. σ_{yy} distribution along $x = 1$.

$$\begin{aligned}
 & \times \sum_{m=0}^{\infty} \left(\frac{p}{2} N_{mn} - \omega_m M_{mn} \right) (-1)^m e^{-\lambda_{mn} \tau} \\
 & - \mu (e^{p/2} + e^{-p/2}) \alpha_n \cosh \alpha_n \\
 & \times \sum_{m=0}^{\infty} N_{mn} (-1)^m e^{-\lambda_{mn} \tau} / \Delta_{2n} \\
 H_n &= \mu (e^{p/2} + e^{-p/2}) \cosh \alpha_n \\
 & \times \sum_{m=0}^{\infty} \left(\frac{p}{2} N_{mn} - \omega_m M_{mn} \right) (-1)^m e^{-\lambda_{mn} \tau} \\
 & - \mu (e^{p/2} - e^{-p/2}) \alpha_n \sinh \alpha_n \\
 & \times \sum_{m=0}^{\infty} N_{mn} (-1)^m e^{-\lambda_{mn} \tau} / \Delta_{1n}
 \end{aligned} \quad (22)$$

where

$$\begin{aligned}
 \Delta_{1n} &= \alpha_n + \frac{\sinh 2\alpha_n}{2} \\
 \Delta_{2n} &= -\alpha_n + \frac{\sinh 2\alpha_n}{2}.
 \end{aligned} \quad (23)$$

In determining ϕ_2 , the subsequent boundary conditions from the above calculation require

$$\sigma_{2xy}(x, \pm 1, \tau) = \sigma_{2yx}(x, \pm 1, \tau) = 0 \quad (24)$$

and

$$\begin{aligned}
 \sigma_{2xt}(\pm 1, y, \tau) &= -\sigma_{0xt}(\pm 1, y, \tau) - \sigma_{1xt}(\pm 1, y, \tau) \\
 \sigma_{2yt}(\pm 1, y, \tau) &= -\sigma_{0yt}(\pm 1, y, \tau) - \sigma_{1yt}(\pm 1, y, \tau).
 \end{aligned} \quad (25)$$

Assuming ϕ_2 is in the form

$$\phi_2 = \cos \gamma x (I \cosh \gamma y + J \gamma y \sinh \gamma y) \quad (26)$$

which automatically satisfies equation (10), then by condition (24), one finds that γ must be the root of the

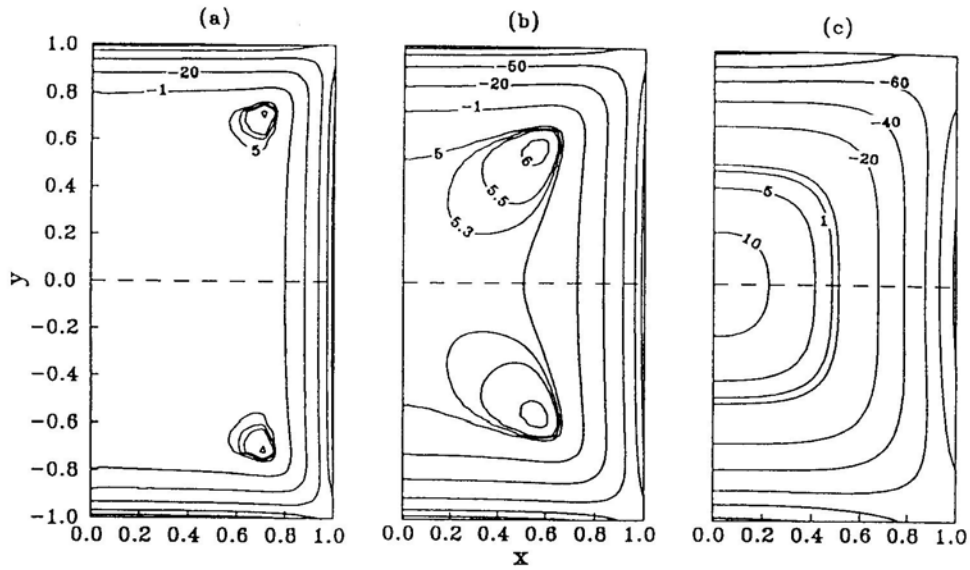


Figure 7. σ_{zz} contours for $p = 0$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

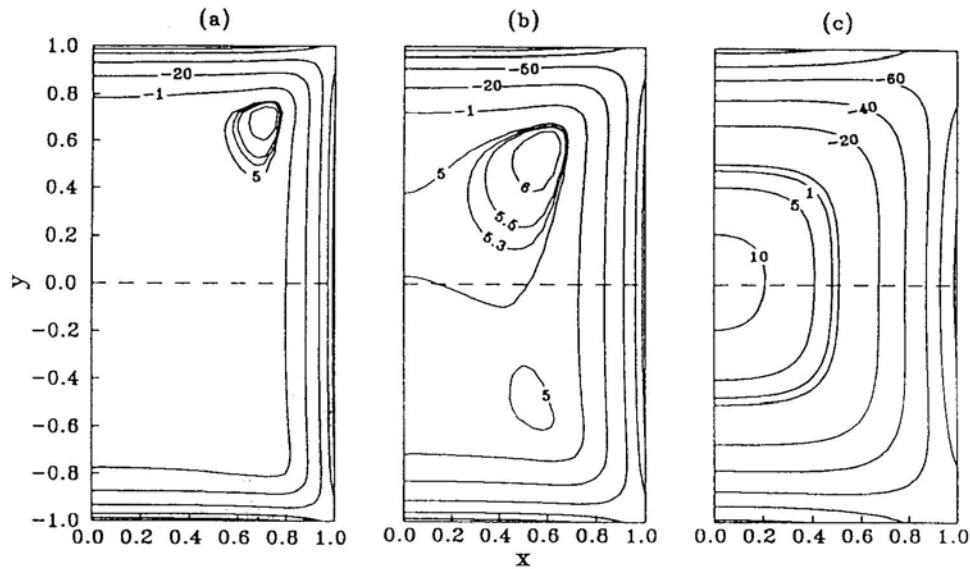


Figure 8. σ_{zz} contours for $p = 0.05$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

transcendental relation

$$\sinh 2\gamma + 2\gamma = 0 \quad (27)$$

with

$$I = -\frac{\gamma \sinh \gamma}{\cosh \gamma} J. \quad (28)$$

Equation (27) has infinitely many complex roots. Let γ_n be the n th root and thus ϕ_2 now can be expressed as the following series

$$\phi_2 = \sum_{n=0}^{\infty} K_n f_n(x, y) \quad (29)$$

where

$$f_n(x, y) = \cos \gamma_n x (-\sinh \gamma_n \cosh \gamma_n y + y \cosh \gamma_n \sinh \gamma_n y) \quad (30)$$

and values of K_n are unknown complex coefficients. The remaining work of solving ϕ_2 is to determine K_n values by using equation (25). By using equation (29) with (30), for the left-hand side of (25) and by using the known functions ϕ_0 and ϕ_1 for the right-hand side of (25), the exact solution is expected. However, due to the constraint of the form of power series, these coefficients can only be approximately determined by numerical methods. In this work they are determined by the method of least squares, so the boundary conditions of equation (25) may be satisfied at a number of midpoints ($y_m, m = 1, 2, \dots, M$) across the surfaces at $x = \pm 1$. Thus, we can establish the simultaneous equations

$$[\mathbf{S}]_{2M \times 2N} [\mathbf{U}]_{2N \times 1} = [\mathbf{V}]_{2M \times 1} \quad (31)$$

where the elements of each matrix in equation (31) are shown in the appendix. After ϕ_0, ϕ_1 and ϕ_2 have been

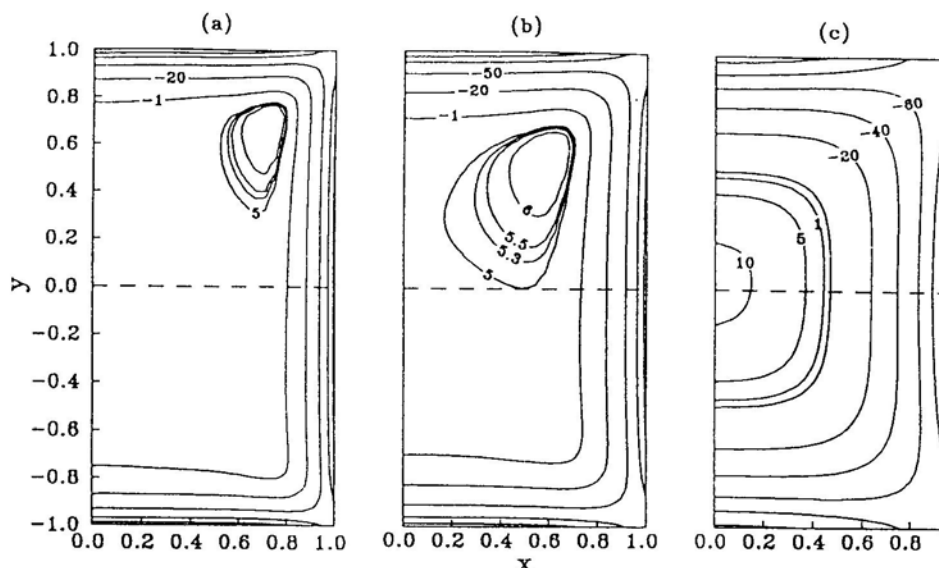


Figure 9. σ_{zz} contours for $p = 0.1$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

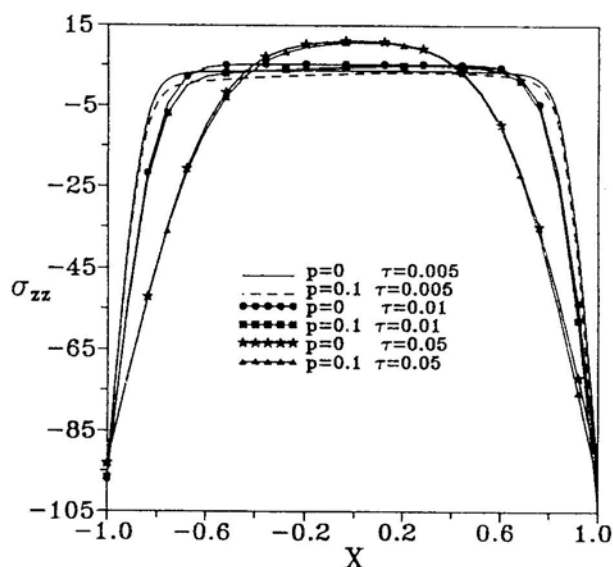


Figure 10. σ_{zz} distribution along the y axis.

solved, we then can combine equations (11)–(13) and (18) and (19) to obtain the diffusion-induced stress σ_{ij} .

4. Results

In calculations of this work, $N = M = 25$ is chosen. We show in figure 2 the σ_{yy} contours at different times for $p = 0$. Because the contours are symmetric about the y axis, we only show them in the half domain $0 \leq x \leq 1$. Comparing these results with those of Chu and Lee [7], one finds that they are identical. Actually, as $p = 0$, all the σ_{yy} contour is also symmetric about x axis. Two equal local maximum tensions are located near the corners at short times, then as time increases, they will move towards the x axis and get close to but not onto the centre. In addition, one local maximum

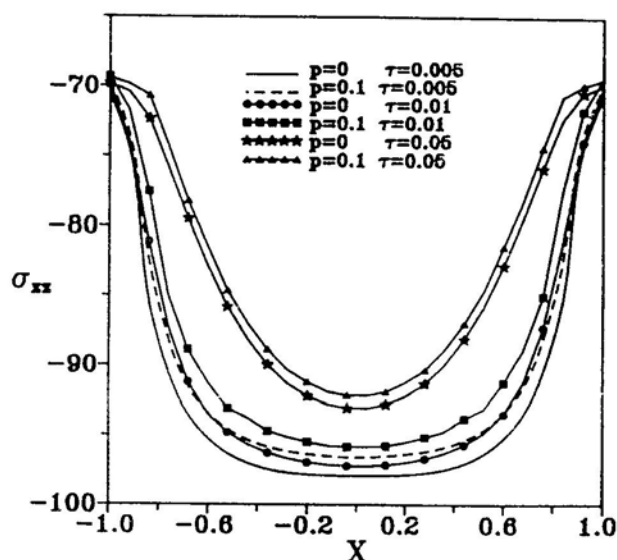


Figure 11. σ_{zz} distribution along $x = 1$.

compression is situated at the mid-edge ($x = 1, y = 0$) and remains at the same position with increasing time.

When the electric field is applied, the σ_{yy} contours at different times are plotted in figures 3 and 4 for $p = 0.05$ and $p = 0.1$ respectively. The results are as expected. As we can see, in each diagram of these figures the applied field causes stress distributions asymmetric about the x axis. In short times, the two local maximum tensions near the corners are not equal and, with increasing time, they move towards an axis deviating from the x axis. We show in figure 5 the distributions of σ_{yy} along the y axis to demonstrate the deviations caused by the field, although the local maximum tensions shown in this figure are not really those mentioned above. It is shown that the applied electric field can not only deviate the location of the local maximum tensions but can also depress the tensions

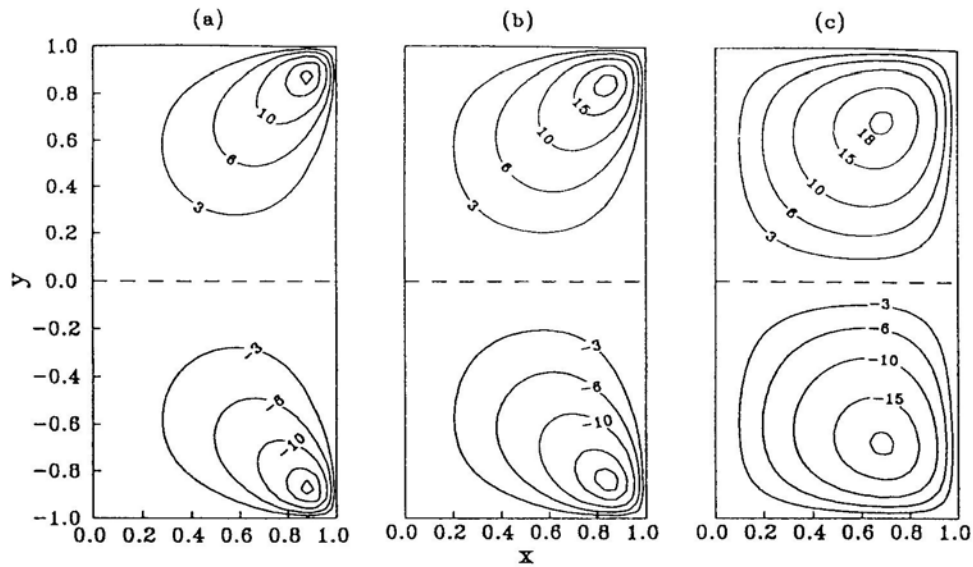


Figure 12. σ_{xy} contours for $p = 0$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

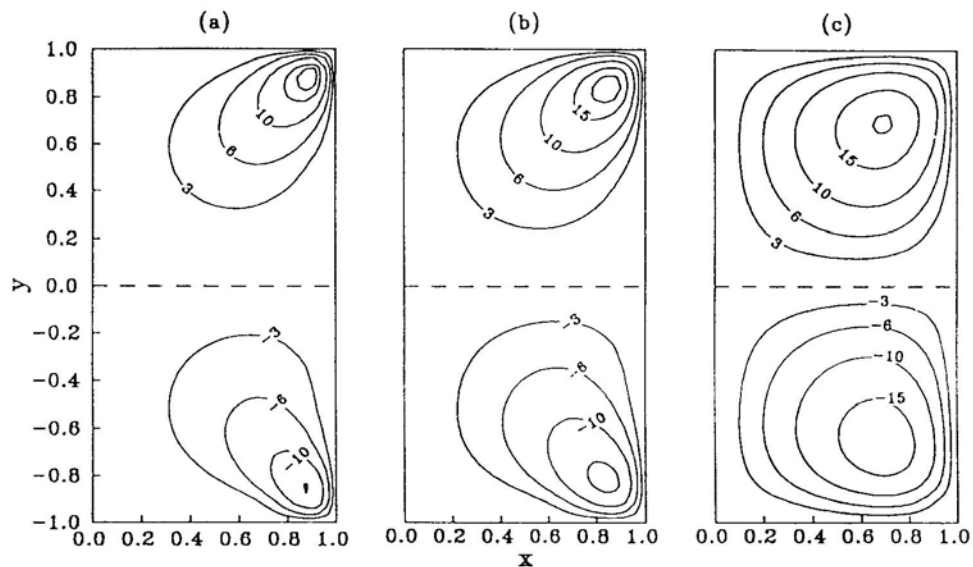


Figure 13. σ_{xy} contours for $p = 0.05$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

along the axis. The effects caused by the applied field are large at short times. As to the effects of the applied field on the compression along the edge $x = 1$, we show them in figure 6. It is shown that the applied field can also depress the compression, but the deviation of the location of the local maximum compression is very small and is negligible, even at short times. The stress component σ_{xx} is obtained from the stress component σ_{yy} , if the indices x and y are exchanged.

Figure 7 shows the contours of the stress component σ_{zz} for $p = 0$. Again, the result obtained from our calculation is identical to that obtained by Chu and Lee [7]. Two equal local maximum tensions are located near the corners and one local maximum compression is situated at the mid-edge at short times. With increasing time, the local maximum tension moves to

the centre along the diagonal, while the local maximum compression remains in the same position. Figures 8 and 9 show the results obtained when $p = 0.05$ and $p = 0.1$ respectively. Like the effects of the applied electric field on σ_{yy} , the effect on σ_{zz} also results in asymmetries about the x axis, the deviations of the local maxima, and the depressions of the stresses, as apparently observed in figures 10 and 11 which describe the σ_{zz} distributions along the y axis and the edge $x = 1$ respectively.

In addition to the normal stress, the contours of shear stress σ_{xy} are plotted in figures 12–14. Figure 12 shows the case of $p = 0$ and is identical to that shown by Chu and Lee [7]. Figures 13 and 14 show that the effect of the applied electric field on σ_{xy} is similar to those on the normal stresses.

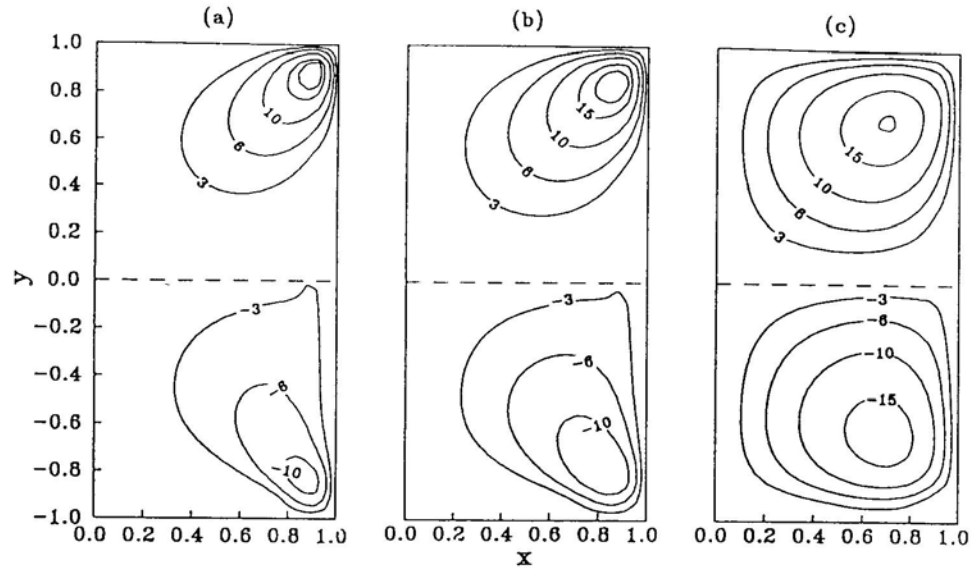


Figure 14. σ_{xy} contours for $p = 0.1$, (a) $\tau = 0.005$, (b) 0.01 , (c) 0.05 .

5. Conclusion

In this work we have investigated the effects of an applied electric field on the diffusion-induced stresses in a long bar of square cross section. The mass transfer process of constant surface concentration is considered. We first calculate the distributions of solute concentration analytically then, by introducing the displacement potential and the Airy stress function, we also obtain analytically the diffusion-induced stresses. Some important results are observed.

(1) When an electric field is applied the solute is forced to diffuse along the field direction, consequently causing asymmetry about the axis perpendicular to the field direction.

(2) The electric field can depress the stresses.

(3) The electric field can also deviate the positions of local maximum stresses along the field direction, more apparently in the interior than on the outer surface.

(4) The effects of the electric field are more apparent at short times than at long times.

Appendix

The elements of $[\mathbf{S}]_{2M \times 2N}$, $[\mathbf{U}]_{2N \times 1}$ and $[\mathbf{V}]_{2M \times 1}$ in equation (30) are:

$$V_m = 0$$

$$\begin{aligned} V_{M+m} = & 2\mu \sum_i \sum_j \dot{B}_{ij} y_m \alpha_i (-1)^j e^{-\lambda_{ij} \tau} \\ & - \sum_j \alpha_j^2 (-1)^j [E_j \sinh \alpha_j y_m - F_j \cosh \alpha_j y_m \\ & + G_j y_m \sinh \alpha_j y_m - H_j y_m \sinh \alpha_j y_m \\ & + (G_j \cosh \alpha_j y_m + H_j \sinh \alpha_j y_m) / \alpha_j] \end{aligned}$$

$$U_n = \text{Re } K_n$$

$$U_{N+n} = \text{Im } K_n$$

$$S_{m,n} = \text{Re } f_n(1, y_m)$$

$$S_{m,N+n} = \text{Im } f_n(1, y_m)$$

$$S_{M+m,n} = \text{Re } f_n(1, y_m)$$

$$S_{M+m,N+n} = \text{Im } f_n(1, y_m).$$

where Re and Im denote the real and imaginary part of a complex number respectively, and m, n are integers, $0 \leq n \leq N$, $1 \leq m \leq M$.

References

- [1] Bardsley W 1960 *Progress in Semiconductors* vol 4, ed A F Gibson (New York: Wiley) p 155
- [2] Prussin S 1961 *J. Appl. Phys.* **32** 1876–81
- [3] Tuck B 1974 *Introduction to Diffusion in Semiconductors* (London: Peter Peregrinus)
- [4] Li J C M 1978 *Metall. Trans. A* **9** 1353–80
- [5] Lee S and Li J C M 1981 *J. Appl. Phys.* **52** 1336–46
- [6] Chu J L and Lee S 1990 *Int. J. Eng. Sci.* **28** 1085–109
- [7] Chu J L and Lee S 1993 *J. Appl. Phys.* **73** 3211–9
- [8] Iwaki T and Kobayashi N 1981 *ASME J. Appl. Mech.* **48** 866–70
- [9] Hwang C C, Wu C S and Hsieh J Y 1993 *J. Crystal Growth* **132** 523–32