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## Nonlinear diffusion-induced stresses in a long bar of square cross section

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### Abstract

This paper is to investigate the nonlinear effect of the self-induced electric field on the diffusion-induced stresses in a long bar. We first approximate the nonlinear concentration-dependent diffusivity as a series of third-degree polynomials by the least-squares curve-fitting techniques, and then calculate the distributions of concentration by the Galerkin method. Afterwards, the diffusion-induced stresses inside the bar are determined analytically by introducing the Goodier displacement potential and Airy stress function. It is found that the nonlinear self-induced electric fields can depress both the concentration gradient and the maximum diffusion-induced stresses apparently, and these effects are more significant at short times than at long times. © 1998 Elsevier Science Ltd. All rights reserved.

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### 1. Introduction

Diffusion-induced stresses, during mass transfer, can change the mechanical properties in metal systems such as hardening (Reed-Hill, 1973; Hertzberg, 1983). The 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 (Bardsley, 1960). 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 (1961) was the first to analyze the transverse stresses developed in a thin plate during diffusion process. The diffusion-induced stresses related to the dislocation density was studied in detail by Tuck

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(1974). Li (1978) solved the diffusion-induced stresses in a single-phase elastic medium of various geometries and corrected an error made by Prussin (1961). Further, Lee and Li (1981) proposed that the most rapid diffusion processes occur without generation of dislocation. Lee and Ouyang (1987) derived a general solution for boundary stress as a function of time. Chu and Lee (1990) obtained diffusion-induced stresses in two-phase elastic media. Chu and Lee (1993) carried out a study of diffusion-induced stresses in a long bar of square cross section. Hwang et al. (1994) further investigated diffusion-induced stresses in a long bar under an electric field. However, the above calculations of diffusion-induced stresses only treated the simple linear systems with a constant diffusivity. Because the chemical stresses arising from diffusion are not only related to geometric shape but also related to the boundary conditions, Larché and Cahn (1982, 1985) studied the stress dependence of the local diffusion flux in crystalline solids. Chu and Lee (1994) investigated the effect of chemical stresses on diffusion. In order to accurately predict the electrical properties of the device, an accurate description of the final concentration distributions is necessary. In 1963, Weisberg and Blanc (1963) studied the nonlinear interstitial-substitutional equilibrium Zinc diffusion in GaAs. Hu and Schmidt (1968) introduced a concentration dependent diffusion model which included the effects of both the charged vacancy reaction and the impurity-induced electric fields. Warner and Wilson (1980) investigated the effect of the self-induced electric field on diffusion by numerical method. Kath and Cohen (1982) studied the waiting-time behavior in a nonlinear diffusion equation using singular-perturbation techniques. King (1988) obtained the approximate similarity solutions to a nonlinear diffusion equation in one and two dimensions. Schwendeman (1990) calculated the fully two-dimension nonlinear diffusion of impurities in semiconductors by numerical techniques. Moreover, Menon et al. (1993) studied the nonlinear diffusion in Cu–Au multilayer thin films.

Lin and Hwang (1995) investigated the nonlinear effect of self-induced electric field on diffusion-induced stresses in a thin plate. However, in practice, the application of mass transfer to manufacture is not confined to the generalized one-dimensional diffusion processes. It prompted us to investigate the nonlinear diffusion-induced stresses in a long bar of square cross section. In this work, we first approximate the nonlinear concentration-dependent diffusivity as a series of third-degree polynomials by the least-squares curve-fitting techniques, and then calculate the distributions of concentration by the Galerkin method. With these results, the diffusion-induced stresses inside the bar are determined analytically by introducing the Goodier displacement potential and Airy stress function. A comparison is made between the present results and the linear diffusivity model to investigate the nonlinear effect of self-induced electric field on the diffusion-induced stresses in a long bar.

## 2. Analysis of concentration distribution

Consider a long bar of isotropic material with square cross section in the region  $-a \leq X, Y \leq a$ , as shown in Fig. 1. Initially there is no charged impurity inside the bar, while as process begins, the concentration at the outer surface is maintained constant at  $C_s$  during diffusion. The diffusion with the nonlinear effect of the self-induced electric field can be modeled as in Warner and Wilson (1980). Hence, the concentration  $C(X, Y, t)$  for arsenic in silicon is described by the following equation:

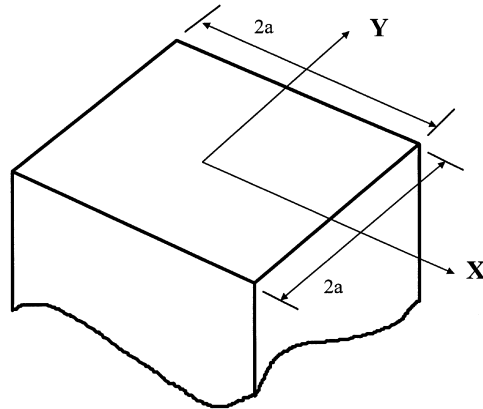


Fig. 1. Physical configuration of a long bar.

$$\frac{\partial \alpha}{\partial t} = \frac{\partial}{\partial X} \left[ D(\alpha) \frac{\partial \alpha}{\partial X} \right] + \frac{\partial}{\partial Y} \left[ D(\alpha) \frac{\partial \alpha}{\partial Y} \right] \quad (1)$$

where

$$\alpha = \frac{C}{2n_i}$$

and  $D(\alpha)$ , the concentration dependent diffusion coefficient, is defined by

$$D(\alpha) = D_0 \frac{1 + \beta[\alpha + \sqrt{\alpha^2 + 1}]}{1 + \beta} \left[ 1 + \frac{\alpha}{\sqrt{\alpha^2 + 1}} \right] \quad (2)$$

here  $n_i$  is the intrinsic carrier concentration,  $D_0$  is the phenomenological low concentration diffusion constant and  $\beta = 100$  for arsenic (Warner and Wilson, 1980).

The corresponding initial and boundary conditions just mentioned are

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

where

$$\alpha_s = \frac{C_s}{2n_i}.$$

Then, if the dimensionless variables

$$x = \frac{X}{a}, \quad y = \frac{Y}{a}, \quad \tau = \frac{D_0 t}{a^2}, \quad 1 + \alpha^* = \frac{\alpha}{\alpha_s} = \frac{C}{C_s} \quad (4)$$

are introduced, eqns (1)–(3) will take the forms:

$$\frac{\partial \alpha^*}{\partial t} = \frac{\partial}{\partial x} \left[ D(\alpha^*) \frac{\partial \alpha^*}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D(\alpha^*) \frac{\partial \alpha^*}{\partial y} \right], \quad (5)$$

$$D(\alpha^*) = \frac{1 + \beta [\alpha_s (1 + \alpha^*) + \sqrt{\alpha_s^2 (1 + \alpha^*)^2 + 1}]}{1 + \beta} \left[ 1 + \frac{\alpha_s (1 + \alpha^*)}{\sqrt{\alpha_s^2 (1 + \alpha^*)^2 + 1}} \right] \quad (6)$$

and

$$\begin{aligned} \alpha^*(x, y, 0) &= -1, \\ \alpha^*(\pm 1, y, \tau) &= 0, \\ \alpha^*(x, \pm 1, \tau) &= 0. \end{aligned} \quad (7)$$

To be suitable for solving the nonlinear equation by the Galerkin method, eqn (6), which referred to the diffusion coefficient, may be approximated in a series of third-degree polynomials by the least-squares curve-fitting method as the following form:

$$D(\alpha^*) = B_0 + B_1 \alpha_s (1 + \alpha^*) + B_2 \alpha_s^2 (1 + \alpha^*)^2 + B_3 \alpha_s^3 (1 + \alpha^*)^3, \quad (8)$$

the coefficients can be regarded as phenomenological parameters.

Solving the above equations through the Galerkin method, we selected the solution

$$\alpha^*(x, y, \tau) = \sum_{j=0}^{\infty} \sum_{i=0}^{\infty} A_{ij}(\tau) \cos(\rho_j x) \cos(\omega_i y) \quad (9)$$

where

$$\rho_j = \frac{2j+1}{2} \pi, \omega_i = \frac{2i+1}{2} \pi, \quad (10)$$

and  $\cos(\rho_j x) \cos(\omega_i y)$  satisfied the boundary conditions, then  $A_{ij}(\tau)$  for  $i, j = 0, 1, 2, \dots, \infty$  can be determined from the set of the coupled nonlinear equations in Appendix A with the initial condition of  $A_{ij}(0) = -4(-1)^{i+j}/(\rho_j \omega_i)$ .

The infinite series in eqn (9) is truncated at  $j = J, i = I$  so as to obtain the results to four significant digits. For accuracy, in the present calculations, a choice of  $I = J = 30$  is made and  $A_{ij}(\tau)$  less than  $10^{-8}$  is deleted. Hence, the solution of the concentration can be expressed by

$$\frac{C}{C_s} = 1 + \sum_{j=0}^J \sum_{i=0}^I A_{ij}(\tau) \cos(\rho_j x) \cos(\omega_i y). \quad (11)$$

### 3. Diffusion-induced stresses

As the concentration distribution is obtained one can proceed to find the diffusion-induced stress distributions. The derivation of stress distribution arising from solute transfer is similar to that arising from heat transfer, if the thermal expansion coefficient and temperature are replaced by one-third of partial molal volume and concentration, respectively (Chu and Lee, 1993; Li, 1978).

In the present work, from the practical point of view, we assume that it is a quasistatic and uncoupled diffusion-induced-stress problem. Further, because of the long bar, we consider only the elastic plane strain states. In a similar way to Nowinski's work (1978), we introduce the dimensionless Goodier displacement potential  $\phi_0$  and the Airy stress function  $\phi_A$  which, respectively, have to satisfy

$$\Delta\phi_0 = C/C_s \quad (12)$$

$$\Delta\Delta\phi_A = 0 \quad (13)$$

where  $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$  and  $C/C_s$  is shown by eqn (11). Then, in similar procedures to the work of Iwaki and Kobayashi (1981), the diffusion-induced stresses are given by

$$\sigma_{ij} = \sigma_{0ij} + \sigma_{Aij}, \quad (14)$$

where

$$\begin{aligned} \sigma_{0xx} &= -\frac{\partial^2 \phi_0}{\partial y^2}, \\ \sigma_{0yy} &= -\frac{\partial^2 \phi_0}{\partial x^2}, \\ \sigma_{0zz} &= -\Delta\phi_0, \\ \sigma_{0xy} &= \frac{\partial^2 \phi_0}{\partial x \partial y}, \end{aligned} \quad (15)$$

and

$$\begin{aligned} \sigma_{Axx} &= \frac{1}{2\mu} \frac{\partial^2 \phi_A}{\partial y^2}, \\ \sigma_{Ayy} &= \frac{1}{2\mu} \frac{\partial^2 \phi_A}{\partial x^2}, \end{aligned}$$

$$\begin{aligned}\sigma_{Azz} &= \frac{\nu}{2\mu} \Delta \phi_A, \\ \sigma_{Axy} &= -\frac{1}{2\mu} \frac{\partial^2 \phi_A}{\partial x \partial y}.\end{aligned}\quad (16)$$

Here  $\mu$  is the Lamé constant and  $\nu$  is the Poisson's ratio. It should be noted that the dimensionless forms of  $\phi_0$ ,  $\phi_A$ , and  $\sigma_{ij}$  are given by

$$\phi_0 = \frac{\Phi_0}{a^2 \Lambda}, \quad \phi_A = \frac{\Phi_A}{a^2 \Lambda}, \quad \sigma_{ij} = \frac{\Sigma_{ij}}{2\mu \Lambda}, \quad (17)$$

where  $\Phi_0$ ,  $\Phi_A$ ,  $\Sigma_{ij}$  are the dimensional Goodier displacement potential, the Airy stress function and stresses, respectively, and  $\Lambda = (1 + \nu) \bar{V} C_s / 3(1 - \nu)$ . Here  $\bar{V}$  is the partial molal volume of solute and assumed to be constant (Li, 1978). The traction-free boundary conditions are adopted, i.e.,

$$\sigma_{xy}(x, \pm 1, \tau) = \sigma_{yy}(x, \pm 1, \tau) = 0, \quad (18a)$$

$$\sigma_{xx}(\pm 1, y, \tau) = \sigma_{xy}(\pm 1, y, \tau) = 0. \quad (18b)$$

Since the dimensionless concentration  $C/C_s$  has been found in the preceding section, by substituting eqn (11) into eqn (12), we have a particular solution:

$$\phi_0 = \sum_{j=0}^J \sum_{i=0}^I -\frac{1}{\rho_j^2 + w_i^2} A_{ij}(\tau) \cos(\rho_j x) \cos(\omega_i y) + \frac{1}{4}(x^2 + y^2). \quad (19)$$

The Airy stress function is constructed in the form

$$\phi_A = \phi_1 + \phi_2, \quad (20)$$

thus

$$\sigma_{Aij} = \sigma_{1ij} + \sigma_{2ij}, \quad (21)$$

where the stresses  $\sigma_{1ij}$  and  $\sigma_{2ij}$  are derived from  $\phi_1$  and  $\phi_2$ , respectively.

An admissible solution of the function  $\phi_1$ , suitable for the present problem, has the form (Nowinski, 1978)

$$\begin{aligned}\phi_1 = 2\mu \left\{ \sum_{j=0}^J [E_j \cosh(\rho_j y) + F_j \sinh(\rho_j y) + G_j y \cosh(\rho_j y) + H_j y \sinh(\rho_j y)] \cos(\rho_j x) \right. \\ \left. + \frac{1}{4}(x^2 + y^2) \right\}, \quad (22)\end{aligned}$$

where the unknowns  $E_j$ ,  $F_j$ ,  $G_j$  and  $H_j$  are determined so as to satisfy the boundary conditions of eqn (18a) at the edges along  $x = \pm 1$

$$\begin{aligned}\sigma_{0yy}(x, \pm 1, \tau) + \sigma_{1yy}(x, \pm 1, \tau) &= 0, \\ \sigma_{0xy}(x, \pm 1, \tau) + \sigma_{1xy}(x, \pm 1, \tau) &= 0.\end{aligned}\quad (23)$$

Consequently, one has

$$\begin{aligned}E_j &= \left\{ -\sinh \rho_j \sum_{i=0}^I \frac{(-1)^i \omega_i}{\rho_j^2 + \omega_i^2} A_{ij}(\tau) \right\} / \Delta_j, \\ F_j &= 0, \\ G_j &= 0, \\ H_j &= \left\{ \cosh \rho_j \sum_{i=0}^I \frac{(-1)^i \omega_i}{\rho_j^2 + \omega_i^2} A_{ij}(\tau) \right\} / \Delta_j,\end{aligned}\quad (24)$$

where

$$\Delta_j = \rho_j + \frac{\sinh(2\rho_j)}{2}.\quad (25)$$

To satisfy the boundary conditions of eqn (18b) at the edges along  $y = \pm 1$ , the function  $\phi_2$  is taken in the form (Nowinski, 1978)

$$\phi_2 = 2\mu \cos(\gamma x) [P \cosh(\gamma y) + Q \gamma y \sinh(\gamma y)],\quad (26)$$

which automatically satisfies eqn (13).

In determining  $\phi_2$ , the subsequent boundary conditions from the above calculation require

$$\sigma_{2yy}(x, \pm 1, \tau) = \sigma_{2xy}(x, \pm 1, \tau) = 0,\quad (27)$$

and

$$\begin{aligned}\sigma_{2xx}(\pm 1, y, \tau) &= -\sigma_{0xx}(\pm 1, y, \tau) - \sigma_{1xx}(\pm 1, y, \tau), \\ \sigma_{2xy}(\pm 1, y, \tau) &= -\sigma_{0xy}(\pm 1, y, \tau) - \sigma_{1xy}(\pm 1, y, \tau).\end{aligned}\quad (28)$$

By condition (27), one finds that  $\gamma$  must be the root of the transcendental relation

$$\sinh(2\gamma) + (2\gamma) = 0,\quad (29)$$

with

$$P = -\frac{\gamma \sinh \gamma}{\cosh \gamma} Q.\quad (30)$$

Equation (29) has infinitely many complex roots. Let  $\gamma_n$  by the  $n$ th root, thus  $\phi_2$  now can be expressed as the following series

$$\phi_2 = 2\mu \sum_{n=1}^N K_n f_n(x, y), \quad (31)$$

where

$$f_n(x, y) = \cos(\gamma_n x) [-\sinh \gamma_n \cosh(\gamma_n y) + y \cosh \gamma_n \sinh(\gamma_n y)], \quad (32)$$

and  $K_n$ 's are unknown complex coefficients. The remaining work of solving  $\phi_2$  is to determine  $K_n$ 's by using eqn (28). By using eqn (31), with eqn (32), for the left-hand side of (28) and by using the known functions  $\phi_0$  and  $\phi_1$  for the right-hand side of (28), 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, (28), 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

$$[S]_{2M \times 2N} [U]_{2N \times 1} = [V]_{2M \times 1}, \quad (33)$$

where the elements of each matrix in eqn (33) are shown in Appendix B. After  $\phi_0$ ,  $\phi_1$  and  $\phi_2$  have been solved, we then can combine eqns (14)–(16) and eqns (20)–(21) to obtain the dimensionless diffusion-induced stress  $\sigma_{ij}$ .

#### 4. Results and discussion

The diffusivity is approximately constant at low concentration levels (Warner and Wilson, 1980; King, 1988; Schwendeman, 1990). While, for arsenic diffusion in silicon, and as an example of high concentration levels, Warner and Wilson (1980) take  $\alpha_s = 20$  (this corresponds to a surface concentration at forty times the intrinsic carrier concentration), the diffusivity is concentration-dependent, and the nonlinear effect on concentration is increased with increasing  $\alpha_s$ . From our previous work (Lin and Hwang, 1995), the concentration-dependent coefficients  $B_0$ – $B_3$  of eqn (8) are calculated by the least-squares curve-fitting method. As we known, a higher-degree polynomials will reduce the deviations of the points from a curve, and one increases the degree of approximating polynomial as long as there is a statistically significant decrease in the variance. The criterion of choosing the optimum degree with good precision is that the sum of the deviations squared of the points from the curve should continually decrease as the degree of the polynomial is raised (Gerald and Wheatley, 1994). For simplicity, in the present study, the nonlinear case of  $\alpha_s = 10$  is considered. Then,  $B_0 = 5.44321 \times 10^{-1}$ ,  $B_1 = 3.62028$ ,  $B_2 = 6.32417 \times 10^{-2}$ ,  $B_3 = -3.53349 \times 10^{-3}$ , and the variance is  $4.89226 \times 10^{-3}$ . As shown in Fig. 2 of our previous study (Lin and Hwang, 1995), the least-squares approximation is one of good fits to eqn (6).

To investigate the nonlinear effect of the self-induced electric field, comparing these results of nonlinear  $D$  model with the solution to a linear case with a constant effective diffusivity of  $D(\alpha^*) = 1$  (linear  $D_0$  model). The contours of concentration  $C/C_s$  at  $\tau = 0.01$  in both nonlinear and linear models are plotted in Fig. 2. Because the contours are symmetric, we only show them in the one-eighths domain of  $0 \leq x \leq 1$ ,  $0 \leq y \leq 1$ . It is easy to see that the concentration gradient in the nonlinear diffusivity model is smaller than that in the linear one. The distribution of  $C/C_s$



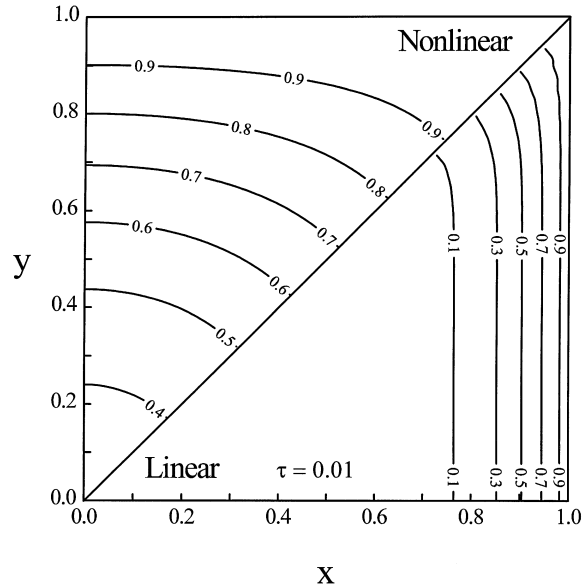


Fig. 2. Concentration  $C/C_s$  contours at  $\tau = 0.01$ .

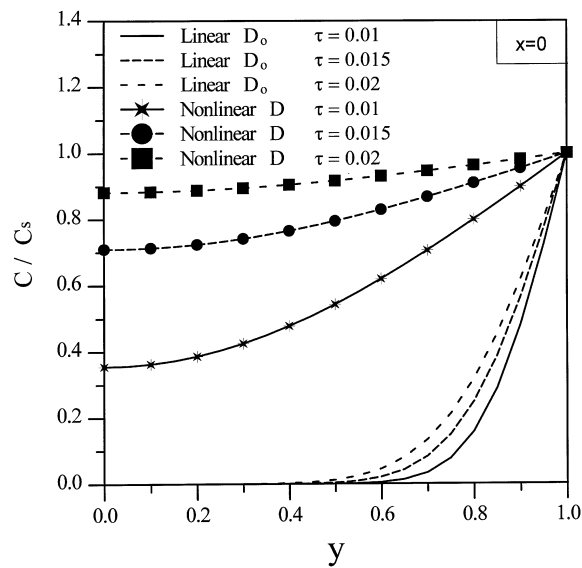


Fig. 3. Concentration  $C/C_s$  distribution along  $y$  axis.

along the  $y$  axis at different times is shown in Fig. 3. It is found that the nonlinear self-induced electric fields can depress the concentration apparently in a short time. Further, as the time is increased, the concentration gradient is decreased in both models. These results are in conformity

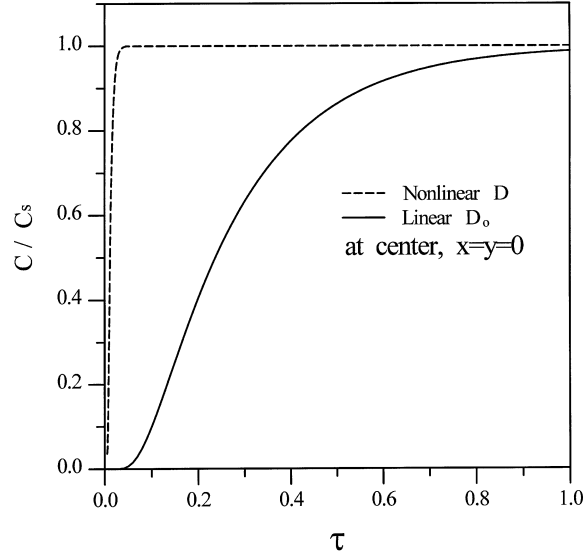


Fig. 4. The evolution of concentration  $C/C_s$  at  $x = 0, y = 0$ .

with the Warner and Wilson (1980) work. Also, in Fig. 4, the evolution of  $C/C_s$  at  $x = 0, y = 0$  is plotted. We find that the difference between the nonlinear model and the linear one is increased with increasing time extremely at short times ( $\tau < 0.025$ ). But, as the time is increased long enough (for example,  $\tau = 0.5$ ), i.e. at a long time diffusion, because the concentration distribution will approach uniform, the nonlinear effects at long times will be less apparent than at short times.

In this article, the stress that is calculated is the equivalent shear stress  $\Sigma_e$  which is defined by

$$\Sigma_e = \sqrt{S_{ij}S_{ij}/2}, \quad (34)$$

where  $S_{ij}$  is the stress deviator  $S_{ij} = \Sigma_{ij} - \Sigma_{kk}\delta_{ij}/3$ . We choose  $\Sigma_e$  to be calculated because it is a measure of that part of the stress tensor which causes plastic deformation by dislocation slip. Although, in the diffusion-induced stress analysis, we have obtained the analytical solutions of the stress tensor, only numerical results are in fact calculated (Hwang et al., 1993). If the local equivalent shear stress  $\Sigma_e$  exceeds the critical value, i.e. the yield stress, a dislocation occurs in the bar. Their presence may degrade both the mechanical and electronic properties of the material.

In the present calculations of the diffusion induced-stresses, a choice of  $N = 19$  and  $M = 21$  is made in order to provide better accuracy (Iwaki and Kobayashi, 1981, 1986) and the Poisson ratio is chosen as  $\nu = 0.3$ . The contours of non-dimensional  $\sigma_e = 100(\Sigma_e/2\mu\Lambda)$  at different times in both models are plotted in Fig. 5. As might be expected, the differences between the nonlinear model and the linear one are seen clearly. It is found that the maximum equivalent shear stress developed in the bar is located at the midedge in the beginning of diffusion. Further, the maximum  $\sigma_e$  is decreases with increasing time for both models. In Fig. 6, we show the distribution of  $\sigma_e$  along the  $y$  axis at different times. It is found that the  $\sigma_e$  distribution can be depressed by the nonlinear effect of the self-induced electric fields. In addition, for instance at the time of  $\tau = 0.01$ , we also find

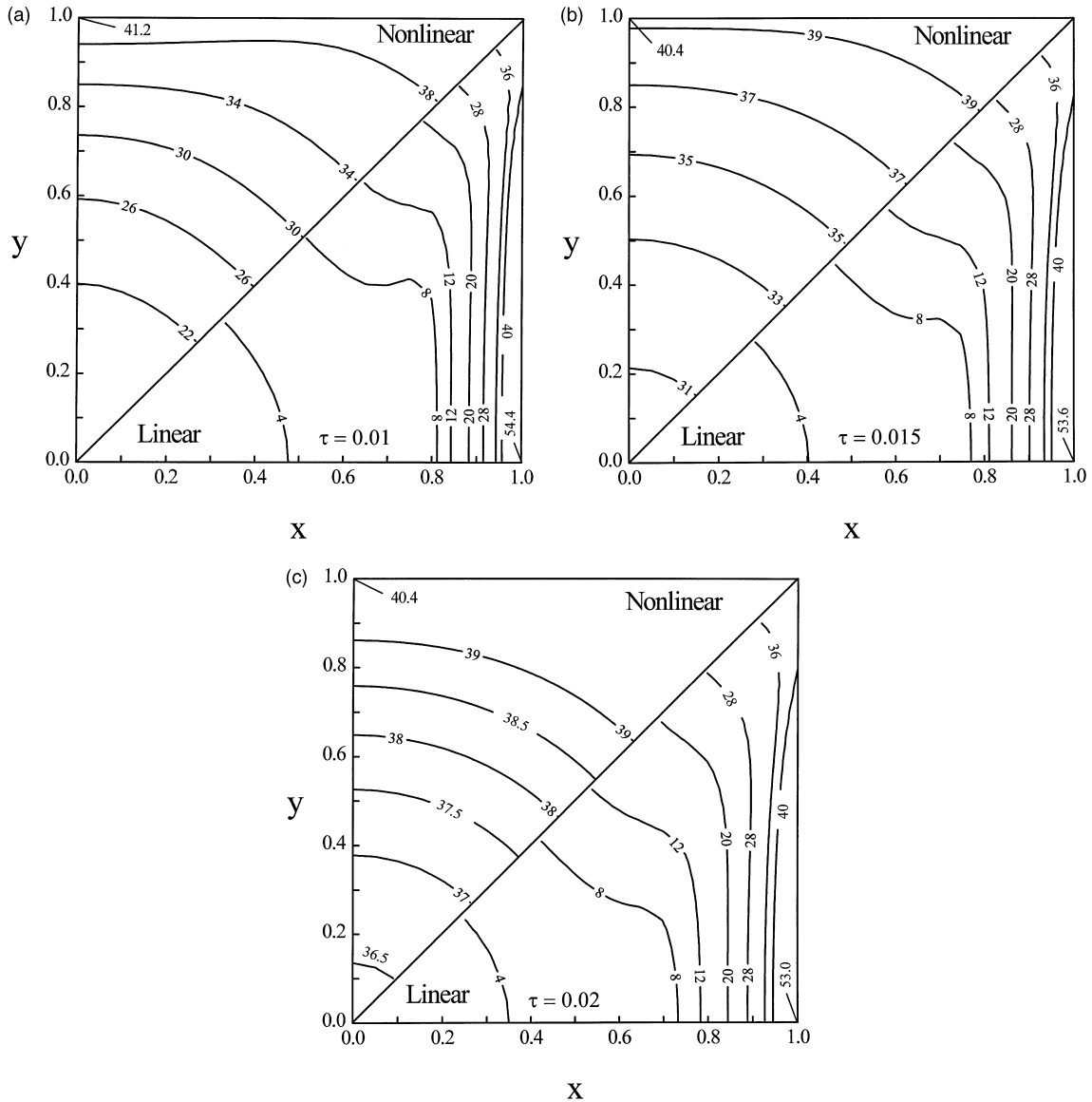


Fig. 5. Non-dimensional equivalent shear stress  $\sigma_e = 100(\Sigma_e/2\mu\Lambda)$  contours (a):  $\tau = 0.01$ , (b): 0.015, (c): 0.02.

from Fig. 5(a), the maximum equivalent shear stress of the nonlinear model may be less than 20% that of the linear one.

Finally, in Fig. 7, the evolutions of the maximum  $\sigma_e$  developed at the midedge ( $x = 0, y = 1$ ) of the bar for both models are demonstrated. With increasing time, the maximum  $\sigma_e$  in both models will approach  $100|\sigma_{zz}|/\sqrt{3}$  which is the value of  $\sigma_e$  when  $\sigma_{xx} = 0 = \sigma_{yy} = \sigma_{xy}$ , i.e. the concentration distribution is approximately uniform in the  $x$ - $y$  plane of the bar. So, the dimensionless value of  $100|\sigma_{zz}|/\sqrt{3}$  is equal to  $100(1-\nu)/\sqrt{3}$  which is the same as the value in a thin slab. We also find

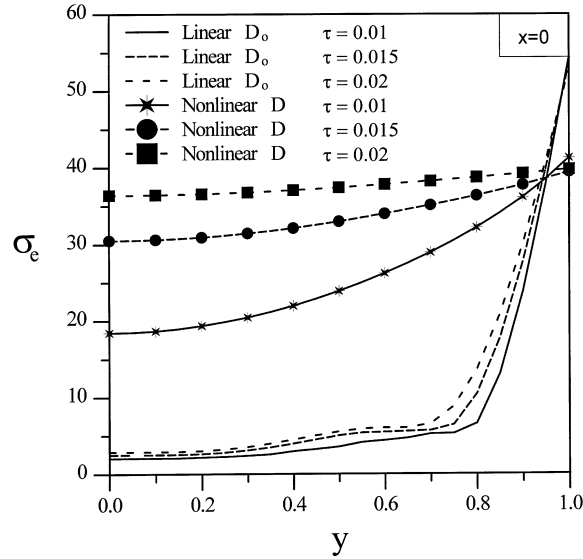


Fig. 6. Non-dimensional equivalent shear stress  $\sigma_e = 100(\Sigma_e/2\mu\Lambda)$  distribution along  $y$  axis.

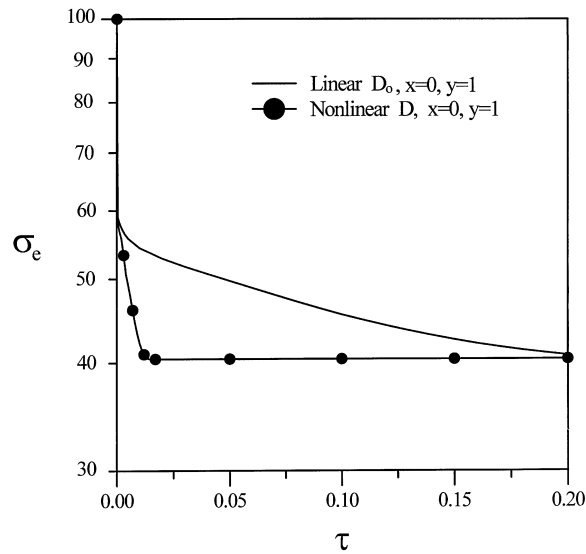


Fig. 7. The evolution of non-dimensional equivalent shear stress  $\sigma_e = 100(\Sigma_e/2\mu\Lambda)$  developed at the midedge of the bar.

that the difference of  $\sigma_e$  between the nonlinear model and the linear one is increased with increasing time at short times, but is decreased with increasing time at long times. As the time is increased long enough, there will be significant difference in  $\sigma_e$  between the nonlinear model and the linear one. This means that the nonlinear effects on the induced-stress  $\sigma_e$  are more apparent at short times than at long times.

For an example of boron diffusion in silicon, the elastic constant of silicon at 1225°C for diffusion into a {100} surface,  $2\mu(1+\nu)/(1-\nu)$ , is a value of  $2.156 \times 10^{12}$  dynes/cm<sup>2</sup> (215.6 GPa). And, the values of  $\bar{V}$  and  $C_s$  for boron at 1225°C are, respectively,  $5.6 \times 10^{-24}$  cm<sup>3</sup>/atoms and  $5 \times 10^{20}$  atoms/cm<sup>3</sup> (Prussin, 1961). Then, a value of  $2\mu\Lambda$  in eqn (17) is calculated to be  $2.01 \times 10^9$  dynes/cm<sup>2</sup> (201 MPa), which is the maximum  $\Sigma_e$  in both models at the beginning of diffusion. Further, if we assumed the value of  $\beta$  in eqn (2) is also equal to 100 in this case, the maximum  $\Sigma_e$  in both nonlinear and linear models are, respectively,  $0.83 \times 10^9$  dynes/cm<sup>2</sup> (83 MPa) ( $\sigma_e = 41.2$ ) and  $1.1 \times 10^9$  dynes/cm<sup>2</sup> (110 MPa) ( $\sigma_e = 54.4$ ) at  $\tau = 0.01$ . The yield stress in silicon whiskers is given by  $5.5 \times 10^9$  dynes/cm<sup>2</sup> (550 MPa) at 800°C, and extrapolating the data to 1225°C reduced the value of the yield stress by an order of magnitude. With a comparison between the maximum  $\Sigma_e$  and the yield stress, it is found that the diffusion-induced stresses may not be ignored in semiconductor materials during diffusion processes especially at short times.

## 5. Conclusions

In this paper, we have investigated the nonlinear effect of the self-induced 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 approximate the nonlinear concentration-dependent diffusivity as a series of third-degree polynomials by the least-squares curve-fitting techniques, and then calculate the distributions of concentration by the Galerkin method. Afterwards with these results, the diffusion-induced stresses inside the bar are determined analytically by introducing the Goodier displacement potential and Airy stress function. It is found that the maximum equivalent shear stress developed in the bar is located at the midedge in the beginning of diffusion. With increasing time, both the concentration gradient and the maximum induced-stresses are decreased. Further, the nonlinear self-induced electric fields can depress the concentration gradient and the maximum diffusion-induced stresses, and these effects are more apparent at short times than at long times.

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## Appendix A

$$\begin{aligned} \frac{dA_{ij}}{d\tau} = & -B(\rho_j^2 + \omega_i^2)A_{ij} - \bar{C} \sum_{l=0}^j \sum_{k=0}^i A_{i-k,j-l} A_{kl} [(\rho_l^2 + \omega_k^2)F - \rho_{j-l}\rho_l \bar{G} - \omega_{i-k}\omega_k \bar{H}] \\ & - \bar{D} \sum_{l=0}^j \sum_{k=0}^i \sum_{q=0}^l \sum_{p=0}^k A_{i-k,j-l} A_{k-p,l-q} A_{pq} [(\rho_q^2 + \omega_p^2)\bar{I} - 2\rho_{l-q}\rho_q \bar{J} - 2\omega_{k-p}\omega_p \bar{K}] \end{aligned}$$

$$\begin{aligned}
& -\bar{E} \sum_{l=0}^j \sum_{k=0}^i \sum_{q=0}^l \sum_{p=0}^k \sum_{s=0}^q \sum_{r=0}^p A_{i-k,j-l} A_{k-p,l-q} A_{p-r,q-s} A_{rs} \\
& \times [(\rho_s^2 + \omega_r^2) \bar{L} - 3\rho_{q-s} \rho_s \bar{M} - 3\omega_{p-r} \omega_r \bar{N}] \quad \text{for } i, j = 0, 1, 2, \dots, \infty
\end{aligned}$$

where

$$\bar{B} = B_0 + B_1 \alpha_s^2 + B_2 \alpha_s^2 + B_3 \alpha_s^3,$$

$$\bar{C} = B_1 \alpha_s + 2B_2 \alpha_s^2 + 3B_3 \alpha_s^3,$$

$$\bar{D} = B_2 \alpha_s^2 + 3B_3 \alpha_s^3,$$

$$\bar{E} = B_3 \alpha_s^3,$$

$$\bar{F} = \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \cos(\rho_l x) \cos(\omega_i y) \cos(\omega_{i-k} y) \cos(\omega_k y) \, dx \, dy,$$

$$\bar{G} = \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \sin(\rho_l x) \cos(\omega_i y) \cos(\omega_{i-k} y) \cos(\omega_k y) \, dx \, dy,$$

$$\bar{H} = \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \cos(\rho_l x) \cos(\omega_i y) \sin(\omega_{i-k} y) \sin(\omega_k y) \, dx \, dy,$$

$$\begin{aligned}
\bar{I} &= \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \cos(\rho_{l-q} x) \cos(\rho_q x) \\
&\quad \times \cos(\omega_i y) \cos(\omega_{i-k} y) \cos(\omega_{k-p} y) \cos(\omega_p y) \, dx \, dy,
\end{aligned}$$

$$\begin{aligned}
\bar{J} &= \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \sin(\rho_{l-q} x) \sin(\rho_q x) \\
&\quad \times \cos(\omega_i y) \cos(\omega_{i-k} y) \cos(\omega_{k-p} y) \cos(\omega_p y) \, dx \, dy,
\end{aligned}$$

$$\begin{aligned}
\bar{K} &= \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \cos(\rho_{l-q} x) \cos(\rho_q x) \\
&\quad \times \cos(\omega_i y) \cos(\omega_{i-k} y) \sin(\omega_{k-p} y) \sin(\omega_p y) \, dx \, dy,
\end{aligned}$$

$$\begin{aligned}
\bar{L} &= \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \cos(\rho_{l-q} x) \cos(\rho_{q-s} x) \cos(\rho_s x) \\
&\quad \times \cos(\omega_i y) \cos(\omega_{i-k} y) \cos(\omega_{k-p} y) \cos(\omega_{p-r} y) \cos(\omega_r y) \, dx \, dy,
\end{aligned}$$

$$\begin{aligned}
\bar{M} &= \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \cos(\rho_{l-q} x) \sin(\rho_{q-s} x) \sin(\rho_s x) \\
&\quad \times \cos(\omega_i y) \cos(\omega_{i-k} y) \cos(\omega_{k-p} y) \cos(\omega_{p-r} y) \cos(\omega_r y) \, dx \, dy,
\end{aligned}$$

$$\begin{aligned}
\bar{N} &= \int_{-1}^1 \int_{-1}^1 \cos(\rho_j x) \cos(\rho_{j-l} x) \cos(\rho_{l-q} x) \cos(\rho_{q-s} x) \cos(\rho_s x) \\
&\quad \times \cos(\omega_i y) \cos(\omega_{i-k} y) \cos(\omega_{k-p} y) \sin(\omega_{p-r} y) \sin(\omega_r y) \, dx \, dy.
\end{aligned}$$

## Appendix B

The element  $[S]_{2M \times 2N}$ ,  $[U]_{2N \times 1}$ , and  $[V]_{2M \times 1}$  in eqn (33) are:

$$V_m = 0,$$

$$V_{M+m} = \sum_j \sum_i (-1)^j \frac{\rho_j \omega_i}{\rho_j^2 + \omega_i^2} A_{ij}(\tau) \sin(\omega_i y_m) - \sum_j \rho_j (-1)^j [\rho_j E_j \sinh(w_i y_m) + \rho_j H_j y_m \cosh(\rho_j y_m) + H_j \sinh(\rho_j y_m)],$$

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

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

$$S_{m,n} = \text{Re} \frac{\partial^2 f_n}{\partial y^2}(1, y_m),$$

$$S_{m,N+n} = -\text{Im} \frac{\partial^2 f_n}{\partial y^2}(1, y_m),$$

$$S_{M+m,n} = \text{Re} \frac{\partial^2 f_n}{\partial x \partial y}(-1, y_m),$$

$$S_{M+m,N+n} = -\text{Im} \frac{\partial^2 f_n}{\partial x \partial y}(-1, y_m),$$

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

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