Diffusion Induced Stresses in Microstructures of MEMS

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ABSTRACT

The diffusion-induced stresses in silicon wafers were studied. The effect of local electric field on dopant diffusion was considered in the diffusion equation. Only one-dimension problem with a constant surface dopant concentration was investigated. The closed form solutions of stresses and expansion of the wafer arising from dopant diffusion are obtained on the basis of linear elastic theory. The results show that the wafer surface is always under compression, while at the wafer center the stress is tensile. The maximum compressive stress is at the surface of the wafer at the initial time, which is independent of the local electric field. The stress at the wafer surface decreases with time. It increases with local electric field and gradually approach to zero with time.

Keywords: one-dimensional diffusion, stresses, electric field, wafers, and MEMS.

INTRODUCTION

Fabrication of microsystems starts with the same techniques used in silicon integrated-circuit chips in microelectronic industries. The techniques make it possible to fabricate many functional chips in a single silicon wafer, which dramatically reduce the cost of production. A variety of microelectromechanical devices have been constructed from combinations of flexible elements. The fabrication techniques include photolithography, surface micro-machining, and bulk micromachining.

In the fabrication of Microsystems, diffusion is a frequently used technique for the incorporation of dopant atoms into silicon substrate. The diffusion of impurity atoms into a semiconductor wafer leads to the formation of p-n junctions, conduction channels. The performance of the microelectronic devices and MEMS devices depends critically on the impurity concentration and the impurity profile. Therefore, the diffusion of various impurities in semiconductors has been studied extensively.

Diffusion-induced stresses essentially affect the performance and reliability of MEMS devices, which during anomalous mass transfer degrade electrical properties of semiconductor systems [1]. Diffusion-induced stresses in semiconductor materials were originally proposed by Prussin [2]. Li [3] analyzed the diffusion-induced stresses in an elastic medium of simple geometry. Lee and coworkers [4, 5] studied the effect in composite materials. Larche and Cahn [6, 7] investigated the stresses arising from material inhomogeneities. However there is little study on the effect of diffusion on the stress evolution in microstructures used in MEMS devices and microelectronic devices. This promotes us to study the diffusion-induced stresses in a wafer. Here the wafer is simplified as a one-dimensional thin slab, from which the dopant concentration with constant injection concentration at surfaces is solved analytically. Then the stresses generated by the dopant diffusion are calculated.

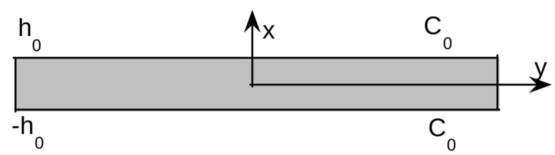

Fig. 1 Schematic diagram of a semiconductor wafer

CONCENTRATION DISTRIBUTION

Consider a semiconductor wafer of width $2h_0$, which is simplified as a thin slab as shown in Fig. 1. The diffusion is treated as one dimension in x direction. The diffusion equation [8] taking the effect of electric field into account is

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{eE}{kT}\frac{\partial C}{\partial x}\right) \tag{1}$$

where D is the diffusivity of impurity, C is concentration, e is the absolute magnitude of the charge on electron, T is the absolute temperature, k is the Boltzmann constant. Equation (1) was solved by using the Laplace transformation. For impurity concentration being constant C_0 for all $t > 0$ at both surfaces and initially the wafer being dopant free, the concentration of the dopant in the wafer for $h_0 > x \geq 0$ is

$$C = C_0\left\{1 - 2\exp\left[\frac{eE}{2kT}(h_0 - x)\right]\right.$$
$$\left.\sum_{n=1}^{\infty}\frac{\lambda_n \sin[\lambda_n (h_0 - x)/h_0]}{\beta_n^2 (1 - 2kT\cos^2\lambda_n / eE)}\exp(-\beta_n^2 Dt/h_0^2)\right\} \tag{2}$$

where

$$\lambda_n = h_0\frac{eE}{2kT}\tan\lambda_n \tag{3}$$

$$\beta_n = h_0^2\left[\left(\frac{eE}{2kT}\right)^2 + \lambda_n^2\right] \tag{4}$$

If the effect of electric field is negligible, the dopant concentration in the wafer becomes

$$C = C_0\left\{1 - \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^n}{2n+1}\cos\left[\frac{(2n+1)\pi x}{2h_0}\right]\exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4h_0^2}\right]\right\} \tag{5}$$

Figure 2 shows the dopant concentration in the wafer with no electric field. The gradient of the dopant concentration at the center of the wafer is zero. The dopant gradually penetrates into the wafer with time and the its concentration at the center of the wafer increases with time and eventually reaches the same concentration as in the wafer surface. Figure 3 shows the dopant concentration in the wafer in electric field. As expected, the local electric field created internally under high dopant-concentration concentration enhances the diffusion of dopants.

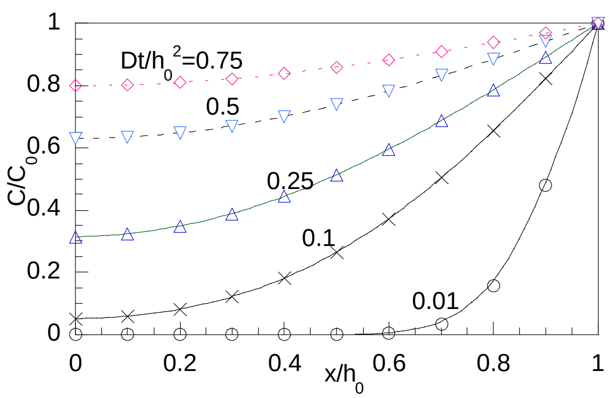

Fig. 2. Dopant distribution in the wafer (E=0)

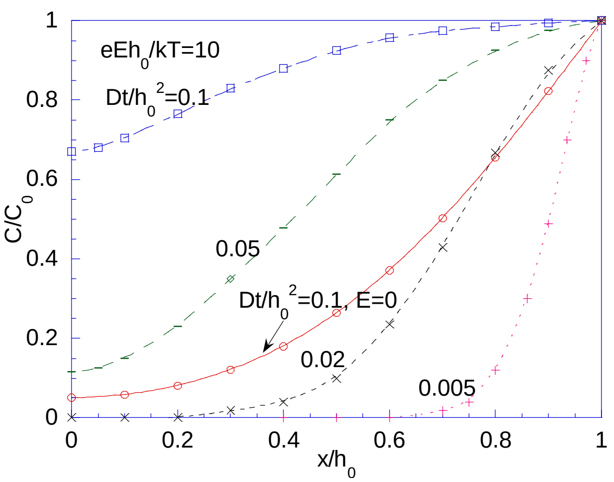

Fig. 3 Dopant distribution in the wafer at different time ($eEh_0 / kT = 10$)

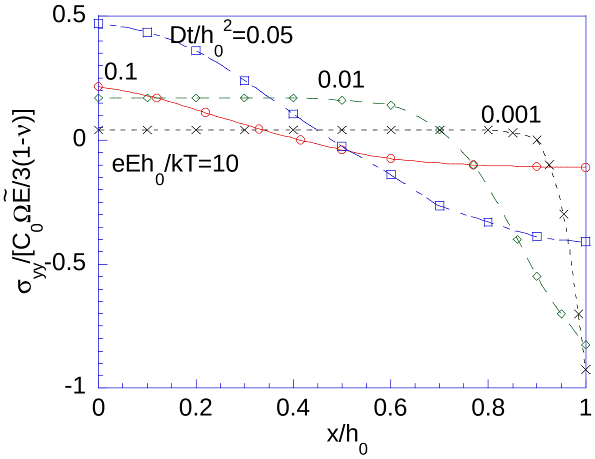

Fig. 4 Stress distribution in the wafer at different time ($eEh_0 / kT = 10$)

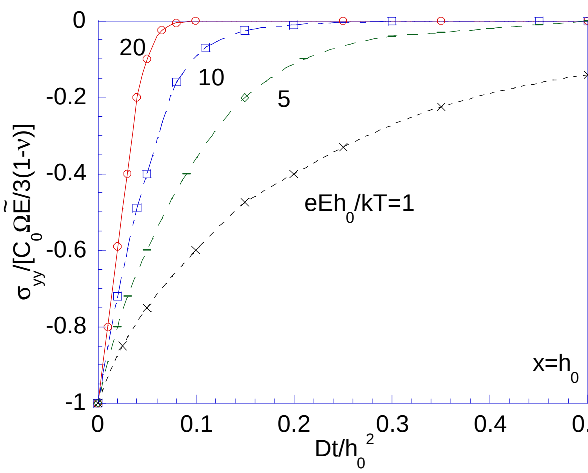

Fig. 5 Time dependence of stress at the wafer surface

STRESS DISTRIBUTION

For the present purpose, only linear elastic deformation of the wafer is considered. The equilibrium equation is

$$\nabla \cdot \vec{\sigma} = 0 \tag{6}$$

where $\vec{\sigma}$ is the stress tensor. The relationships between the strain tensor (ε_{ij}) and the displacement components (u_i) is

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{7}$$

The constitutive relations are

$$\varepsilon_{ij} = \frac{1}{\tilde{E}}[(1+\nu)\sigma_{ij} - \nu\sigma_{kk}\delta_{ij}] + \frac{C\Omega}{3} \tag{8}$$

where Ω is the partial molar volume of the dopant, $\tilde{E}$ and ν are the Young's modulus and Poisson ratio of the semiconductor wafer.

Considering the one-dimension problem as shown in Fig.1, assume both y and z directions of the wafer are constrained with no variation in their dimensions. The stresses generated in the wafer by the dopant diffusion are $\sigma_{xx} = 0$ and $\sigma_{yy} = \sigma_{zz} = -\Omega C\tilde{E}/3(1-\nu)$. These stresses create both axial forces and moments in both y and z directions. Release of these axial forces and moments will remove the dimensional constraints in both y and z directions. This gives

$$\sigma_{yy} = \sigma_{zz} = \Omega\tilde{E}/3(1-\nu)\left\{-C + \frac{1}{2h_0}\int_{-h_0}^{h_0} C dx + \frac{3x}{2h_0^3}\int_{-h_0}^{h_0} Cx dx\right\}$$

$$= -C_0^2\Omega\tilde{E}/3(1-\nu)\left\{1 - 2\exp[\frac{eE}{2kT}(h_0 - x)]\cdot \sum_{n=1}^{\infty}\frac{\lambda_n \sin[\lambda_n (h_0 - x)/h_0]}{\beta_n^2(1-2kT\cos^2\lambda_n/eE)}\exp(-\beta_n^2 Dt/h_0^2)\right\}$$

$$+C_0^2\Omega\tilde{E}/3(1-\nu)\cdot \left\{1 - 4\sum_{n=1}^{\infty}\frac{\exp(-\beta_n^2 Dt/h_0^2)}{\beta_n^2(1-2kT\cos^2\lambda_n/eE)e^2E^2h_0^2 + 4\lambda_n^2k^2T^2}\cdot \left[2\lambda_n k^2T^2 + 2\exp[\frac{eEh_0}{2kT}]kT(-2\lambda_n kT\cos\lambda_n + eEh_0\sin\lambda_n)\right]\right\} \quad (9)$$

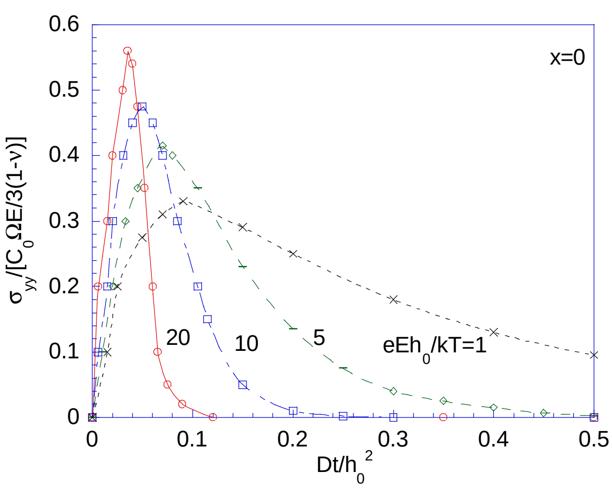

Fig. 6 time dependence of stress at the wafer center

Figures 4-6 show the stress evolution in the wafer with time. The wafer is under compression near the surface while it is under tension at the center. The maximum magnitude of the stresses is $-C_0\Omega\tilde{E}/3(1-\nu)$ at the surface at the initial time, which is independent of electric field. The stress at the wafer surface decreases with time. As shown in Fig. 5, the surface stresses increases with decreasing local electric field and gradually approach to zero with time. The time derivative of the surface stresses increases with local electric field. The stresses developed at the wafer center first increases with time and reaches a maximum, then decreases with time as shown in Fig. 6. The maximum stress at the center of the wafer increases with local electric field.

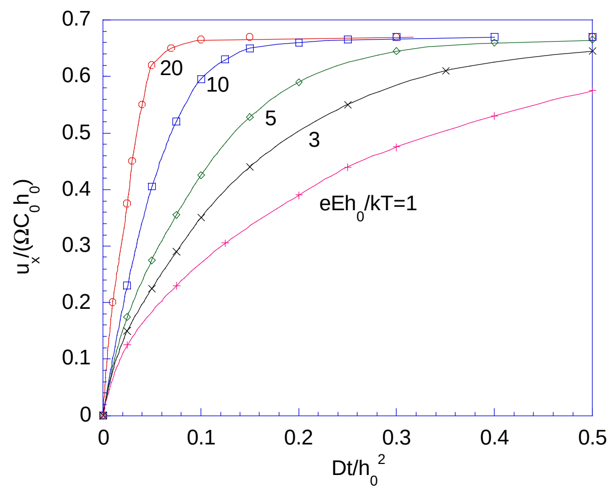

Fig. 7 Time dependence of wafer expansion

EXPANSION OF WAFER

Based on the constitutive relation (8), the transverse strain of the wafer due to dopant diffusion is

$$\varepsilon_{xx} = \frac{1}{\tilde{E}}[\sigma_{xx} - \nu(\sigma_{yy} + \sigma_{zz})] + \frac{C\Omega}{3} \quad (10)$$

$$= -\frac{2\nu\sigma_{yy}}{\tilde{E}} + \frac{C\Omega}{3}$$

Substituting Eq. (9) into Eq. (10), there is

$$\varepsilon_{xx} = \frac{C\Omega}{3}\left(1 + \frac{2\nu}{1-\nu}\right) - \frac{2\nu\Omega}{3(1-\nu)}\frac{1}{h_0}\int_0^{h_0} Cdx$$

$$= \frac{C_0^2\Omega}{3}\left(1 + \frac{2\nu}{1-\nu}\right)\left\{1 - 2\exp[\frac{eE}{2kT}(h_0 - x)]\cdot \sum_{n=1}^{\infty}\frac{\lambda_n \sin[\lambda_n(h_0 - x)/h_0]}{\beta_n^2(1-2kT\cos^2\lambda_n/eE)}\exp(-\beta_n^2 Dt/h_0^2)\right\}$$

$$-\frac{2\nu C_0^2\Omega}{3(1-\nu)} \left\{1 - 4\sum_{n=1}^{\infty}\frac{\exp(-\beta_n^2 Dt/h_0^2)}{\beta_n^2(1-2kT\cos^2\lambda_n/eE)e^2E^2h_0^2 + 4\lambda_n^2k^2T^2}\cdot \left[2\lambda_n k^2T^2 + 2\exp[\frac{eEh_0}{2kT}]kT(-2\lambda_n kT\cos\lambda_n + eEh_0\sin\lambda_n)\right]\right\} \quad (11)$$

Integrating Eq. (11), the transverse expansion of the wafer due to dopant diffusion is

$$u_x = \frac{2\Omega}{3}\int_0^{h_0} Cdx \quad (12)$$

$$= \frac{2C_0^2\Omega}{3}\left\{1 - 4\sum_{n=1}^{\infty}\frac{\exp(-\beta_n^2 Dt/h_0^2)}{\beta_n^2(1-2kT\cos^2\lambda_n/eE)e^2E^2h_0^2 + 4\lambda_n^2k^2T^2}\cdot\right.$$
$$\left.\left[2\lambda_n k^2T^2 + 2\exp[\frac{eEh_0}{2kT}]kT(-2\lambda_n kT\cos\lambda_n + eEh_0\sin\lambda_n)\right]\right\}$$

The effect of the dopant diffusion the transverse expansion of the wafer is shown in Fig. 7. The expansion increases with the local electric field and time, which reaches the maximum $2C_0\Omega h_0/3$ when the dopants uniformly distribute in the wafer. The wafer expands much faster at the initial time than that at long time, because of the gradient of dopant concentration as shown in Fig. 2.

SUMMARY

The diffusion-induced stresses in silicon wafers created in the doping processes have been studied by considering diffusion problem in a thin layer of wafer. The local electric field created by the ionic dopant diffusion has been incorporated into the analysis of dopant diffusion and its effect of diffusion-induced stresses. One dimensional diffusion problem with constant surface dopant concentration was solved by using the Laplace transforms. The results show that the electric field enhances the dopant diffusion. Using the relationship between strain tensor and dopant concentration, the closed form solutions of stress fields developed during the dopant diffusion in the wafer were obtained. The maximum magnitude of the stresses is at the surface at the initial time, which is independent of electric field. The wafer surface is always under compression, while at the wafer center the stress is tensile.

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