MECHANICAL MODELING OF OXYGEN-CONTAINING PRECIPITATES IN SILICON WAFERS

R.V. Goldstein, P.S. Shushpannikov, K.B. Ustinov
A.Yu. Ishlinsky Institute for Problems in Mechanics RAS, Moscow, Russia

Corresponding Author: K.B. Ustinov, A.Yu. Ishlinsky Institute for Problems in Mechanics RAS, prosp. Vernadskogo 101, block 1, 119526, Moscow, Russia; ustinov@ipmnet.ru

Abstract. The mechanical model of oxygen-containing precipitates in silicon wafers is proposed. The precipitate is modeled as an elastic isotropic inclusion in the shape of a spheroid buried in an anisotropic matrix. The stress-deformation state caused by the precipitate is obtained within the framework of the proposed precipitate model. A method for estimation of the precipitate eigenstrain based on an analysis of the precipitate-dislocation loops complexes is developed. The obtained eigenstrain estimate is used for calculation of the stress-deformation state in a silicon wafer with internal getter.

1 Introduction

The effective tool for eliminating of the negative influence of the defects within the silicon wafers is the formation of different sinks for point defects (including intrinsic and impurity defects) and dislocations. The internal sink for the defects is usually called getter and the process of the internal getter formation is called the gettering process. The silicon wafers with built-in internal getter are used in the modern VLSICs manufacturing technology. The getter is formed as a result of the controlled decomposition of the oversaturated solid oxygen solution in the silicon and it consists of the oxygen-containing precipitates. Depending on the precipitates sizes and the features of external loading the precipitates can be either sinks for the defects or sources of the defect nucleation. The modeling of the stress-deformation state in the silicon wafer containing precipitates is an actual problem since the mechanical strains and stresses caused by a precipitate strongly influence on its behavior.

2 The mechanical model of the oxygen-containing precipitate

The TEM image of the isolated oxygen-containing precipitate formed in the Czochralski single-crystal silicon as a result of multistage thermal treatments is given on Figure 1. According to experimental data the precipitates lie on the crystallographic plane {100} and have the plate-like shape. The precipitates edges coincide with crystallographic direction <110>.

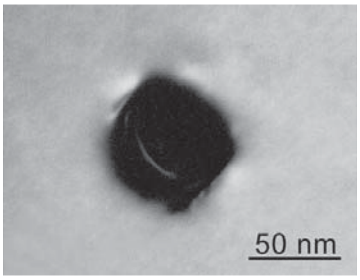


Figure 1. The TEM image of an isolated oxygen-containing precipitate.

Let us model a precipitate as an elastic inclusion in the shape of a spheroid buried in an infinite matrix. The matrix is supposed to be of cubic type anisotropy with the elastic constants corresponding to the single-crystal silicon. The inclusion is isotropic with the polycrystalline silicon dioxide elastic constants. The components of stiffness tensors of the matrix and inclusion will be referred to as C^0_{ijkl} and C^1_{ijkl}, respectively, and can be written in the following form

$$C^0_{ijkl} = \lambda_0 \delta_{ij}\delta_{kl} + \mu_0 \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \mu'_0 \sum_{p=1}^{3} \delta_{ip}\delta_{jp}\delta_{kp}\delta_{lp} \quad (1)$$

$$C^1_{ijkl} = \lambda_1 \delta_{ij}\delta_{kl} + \mu_1 \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) \quad (2)$$

Here δ_{ij} is the Kronecker delta. Elastic properties of the isotropic inclusion are characterized by two Lame constants λ_1 and μ_1 while for matrix due to the cubic type of anisotropy along with two Lame constants λ_0 and μ_0 there is additional independent elastic constant μ'_0.

Owing to the phase transformation during the precipitate formation the inclusion gains inelastic eigenstrains ε_{ij}^0 in the form of pure dilatation $\varepsilon^0\delta_{ij}$ [1]. The inclusion is supposed to be subjected to the uniform loading at infinity with the known strain tensor ε_{ij}^∞.

To solve the problem of searching for the stress-deformation state caused by the precipitate within the stated above model let us consider an "equivalent inclusion" with the same elastic modulus C_{ijkl}^0 as a matrix but undergoing "equivalent eigenstrain" ε_{ij}^* differing from ε_{ij}^0. The necessary and sufficient condition for the equivalency of the strains and stresses induced by the precipitate and "equivalent inclusion" is the following [2]

$$C_{ijkl}^1\left(S_{klmn}\varepsilon_{mn}^* - \varepsilon_{kl}^0 + \varepsilon_{kl}^\infty\right) = C_{ijkl}^0\left(S_{klmn}\varepsilon_{mn}^* - \varepsilon_{kl}^* + \varepsilon_{kl}^\infty\right) \tag{3}$$

where S_{ijkl} are the components of the, so called, Eshelby tensor. Here and throughout the convention of summation for repeated indices is used. The components of the Eshelby tensor can be written in the following form [1,2]

$$S_{ijkl} = \frac{1}{8\pi}C_{pqkl}^0\int_{-1}^{1}\int_{0}^{2\pi}\left[G_{ipjq}\left(\frac{\zeta_1'}{a_1},\frac{\zeta_2'}{a_1},\frac{\zeta_3'}{a_3}\right)+G_{jpiq}\left(\frac{\zeta_1'}{a_1},\frac{\zeta_2'}{a_1},\frac{\zeta_3'}{a_3}\right)\right]d\theta d\zeta_3' \tag{4}$$

where $\zeta_1' = \left(1-\zeta_3'^2\right)^{1/2}\cos\theta$, $\zeta_2' = \left(1-\zeta_3'^2\right)^{1/2}\sin\theta$, a_1 and a_3 are the spheroid half-axis and

$$G_{ijkl}\left(\xi_1,\xi_2,\xi_3\right) = N_{ij}\left(\xi_1,\xi_2,\xi_3\right)D^{-1}\left(\xi_1,\xi_2,\xi_3\right)\xi_k\xi_l \tag{5}$$

$$\begin{aligned} D\left(\xi_1,\xi_2,\xi_3\right) = \mu_0^2\left(\lambda_0+2\mu_0+\mu_0'\right)\xi^6 + \mu_0\mu_0'\left(2\lambda_0+2\mu_0+\mu_0'\right)\xi^2\left(\xi_1^2\xi_2^2+\xi_1^2\xi_3^2+\xi_2^2\xi_3^2\right)+ \\ +\mu_0'^2\left(3\lambda_0+3\mu_0+\mu'\right)\xi_1^2\xi_2^2\xi_3^2 \end{aligned} \tag{6}$$

$$\begin{aligned} N_{11}\left(\xi_1,\xi_2,\xi_3\right) &= \mu_0^2\xi^4 + \beta\xi^2\left(\xi_2^2+\xi_3^2\right)+\gamma\xi_2^2\xi_3^2 \\ N_{12}\left(\xi_1,\xi_2,\xi_3\right) &= -\left(\lambda_0+\mu_0\right)\xi_1\xi_2\left(\mu_0\xi^2+\mu_0'\xi_3^2\right) \end{aligned} \tag{7}$$

Here β and γ are equal to $\mu_0\left(\lambda_0+\mu_0+\mu_0'\right)$ and $\mu_0'\left(2\lambda_0+2\mu_0+\mu_0'\right)$, respectively. The magnitude of the vector $\left(\xi_1,\xi_2,\xi_3\right)$ is denoted as ξ. Other components of the tensor N_{ij} can be obtained by cyclic permutation of indices 1, 2, 3. After solving Eqs(3) with respect to ε_{ij}^* the strains within the precipitate can be obtained as follows [2]

$$\varepsilon_{ij} = S_{ijkl}\varepsilon_{kl}^* \tag{8}$$

The strains outside the inclusion can be obtained by the similar formula [2]

$$\varepsilon_{ij}\left(\vec{r}\right) = D_{ijkl}\left(\vec{r}\right)\varepsilon_{kl}^* \tag{9}$$

with the following components of the tensor D_{ijkl} [1,2]

$$\begin{aligned} D_{ijkl}\left(\vec{r}\right) = \frac{1}{8\pi}C_{pqkl}^0\Bigg\{\int_{-1/y}^{1/y}\int_{0}^{2\pi}\left[G_{ipjq}\left(\frac{\zeta_1}{a_1},\frac{\zeta_2}{a_1},\frac{\zeta_3}{a_3}\right)+G_{jpiq}\left(\frac{\zeta_1}{a_1},\frac{\zeta_2}{a_1},\frac{\zeta_3}{a_3}\right)\right]d\theta d\zeta_3' - \\ -\frac{2}{y}\int_{0}^{2\pi}\left[G_{ipjq}\left(\frac{\zeta_1}{a_1},\frac{\zeta_2}{a_1},\frac{\zeta_3}{a_3}\right)+G_{jpiq}\left(\frac{\zeta_1}{a_1},\frac{\zeta_2}{a_1},\frac{\zeta_3}{a_3}\right)\right]_{\zeta_3'=1/y}d\theta\Bigg\} \end{aligned} \tag{10}$$

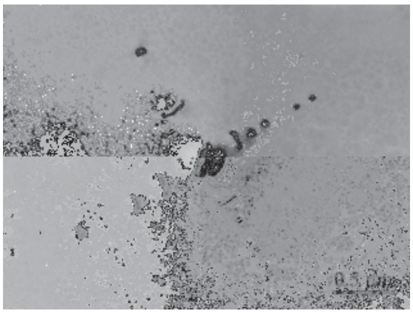
Here y is the magnitude of vector $\vec{y} = \left(x_1/a_1, x_2/a_1, x_3/a_3\right)$, ζ_i is equal to $A_{ij}\zeta_j'$ with the following transition matrix

$$A = \begin{pmatrix} -\cos\alpha_1\cos\alpha_2 & \sin\alpha_2 & \sin\alpha_1\cos\alpha_2 \\ -\cos\alpha_1\sin\alpha_2 & -\cos\alpha_2 & \sin\alpha_1\sin\alpha_2 \\ \sin\alpha_1 & 0 & \cos\alpha_1 \end{pmatrix} \tag{11}$$

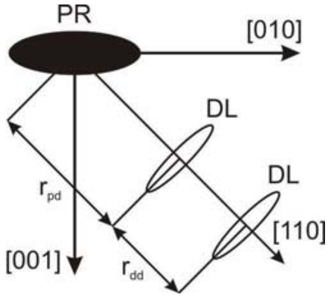
where α_1 and α_2 are the zenith and azimuth angels of vector $\vec{y}$. Eqs(3),(8),(9) give the solution of the problem of searching for the strain caused by precipitate within the framework of the proposed precipitate model.

To perform model calculation of the stress-deformation state caused by the precipitate one should know the precipitate eigenstrain ε^0. Therefore, the next section is devoted to eigenstrain estimation.

3 The estimation of the oxygen-containing precipitate eigenstrain



a)



b)

Figure 2. a) The TEM image of precipitate-dislocation loops complex;
b) The geometrical characteristics of precipitate-dislocation loops complex (PR – precipitate, DL – dislocation loop).

To estimate precipitate eigenstrain ε^0 let us consider the precipitate-dislocation loops complex (Figure 2a) arising on later stages of multistage silicon wafers thermal treatments. Since the investigated complexes have a stable configuration it is reasonable to assume that the force F_{pd} acting on the first dislocation loop in the complex from the precipitate is opposite and equal to the force F_{dd} acting on it from the nearest dislocation loop [3], namely

$$F_{pd} = F_{dd} \tag{12}$$

Since both F_{pd} and F_{dd} are rapidly decreasing functions of the distance the following asymptotic estimates are valid [2,3]

$$F_{pd} \approx \frac{m_p m_d}{r_{pd}^4}, \qquad F_{dd} \approx \frac{m_d^2}{r_{dd}^4} \tag{13}$$

Here m_p and m_d are coefficients of proportionality depending on the precipitate and dislocation loops characteristics, r_{pd} and r_{dd} are the distances between the precipitate and dislocation and between two dislocations (Figure 2b). The simple dimensional analysis [3] allows to obtain the following estimates of m_p and m_d

$$m_p \approx S_p 2a_3\varepsilon^*, \qquad m_d \approx S_d b \tag{14}$$

where S_p is the precipitate sectional area in the plane (001), S_d is the area of the dislocation loop and b is the Burgers vector of the dislocation loop. The estimate of "equivalent eigenstrain" ε^* can be obtained from Eq.(4) and has the following form

$$\varepsilon^* \approx \frac{E_1}{E_0}\varepsilon^0 \tag{15}$$

where E_0, E_1 are the Young modulii of matrix and inclusion, respectively.
Finally, substituting Eqs(13),(14),(15) into Eq.(12) one obtains

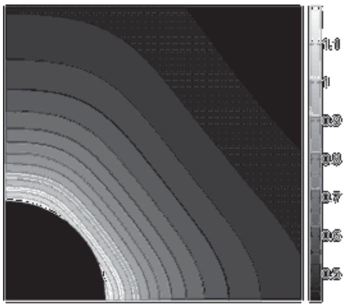
$$\varepsilon^0 \approx \frac{E_0}{E_1}\frac{b}{2a_3}\frac{S_p}{S_d}\left(\frac{r_{pd}}{r_{dd}}\right)^4 \approx \frac{E_0}{E_1}\frac{b}{2a_3}\left(\frac{r_{pd}}{r_{dd}}\right)^4 \tag{16}$$

where we take into account that the area S_p is approximately equal to the area S_d.

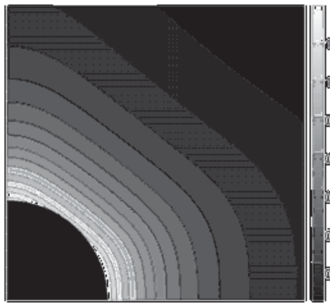
Eq.(16) gives the estimate of the precipitate eigenstrain. The estimate of oxygen-containing precipitates eigenstrains obtained from Eq.(16) after performed an analysis of a set of precipitate-dislocation loops complexes is equal to 6% [3]. This estimation is used in the next section to perform calculations of the stress-deformation state caused by a precipitate.

4 The results of the calculations

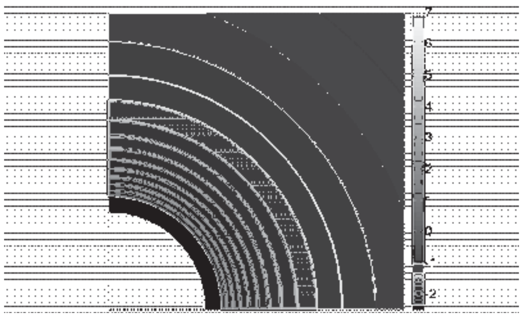
Since the dislocation loops nucleated by the precipitate lie at the crystallographic plane (001) the stress-deformation state at this plane are of interest. The results of the calculations of the normal strain tensor components at the plane (001) are given in Figure 3. Figure 3 shows that the strains caused by an oxygen-containing precipitate are highly non-uniform and have maximal value at the external surface of the precipitate. Therefore the most probable place for dislocation loop nucleation is the vicinity of the precipitate surface.



a)



b)



c)

Figure 3. The isolines of strains caused by the precipitate at the plane (001) a) ε_{11} (%); b) ε_{22} (%); c) ε_{33} (%). In the figures due to the symmetry the quarter of the precipitate is presented.

5 Conclusion

The model of the oxygen-containing precipitate buried in a silicon wafer accounting for the anisotropy of the silicon matrix, external loading and the difference of the precipitate and silicon wafer elastic constants is proposed. A method for estimation of the precipitate eigenstrains based on analysis of the precipitate-dislocation loops complexes arising on the later stages of the silicon wafers thermal treatments is developed. The proposed precipitate model and method for eigenstrain estimation are used for calculation of the stress-deformation state caused by an oxygen containing precipitate.

This study was supported by the Russian Foundation for Basic Research (Project No.08-02-01080).

6 References

[1] Goldstein R.V., Mezhennyi M.V., Milvidskii M.G., Reznik V.Y., Shushpannikov P.S. and Ustinov K.B.: *The experimental and theoretical investigation of the oxygen-containing precipitate – dislocation loops complex formation process (in Russian).* Preprint IPMech RAS, 808 (2007).

[2] Mura T.: *Micromechanics of defects in solids.* Martinus Nijhoff Publishers, Dordrecht, 1987.

[3] Goldstein R.V., Mezhennyi M.V., Milvidskii M.G., Reznik V.Y., Shushpannikov P.S. and Ustinov K.B.: *Evaluating intrinsic deformations in oxygen-containing precipitates.* Technical Physics Letters, 34 (2008), 106-108.