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Non-Contact Technique for Determining the Mechanical Stress in thin Films on Wafers by Profiler

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Abstract. This paper presents an algorithm for analysis of relief for the purpose of calculating mechanical stresses in a selected direction on the plate in the form of software package Matlab. The method allows for the measurement sample in the local area. It provides a visual representation of the data and allows to get stress distribution on wafer surface. Automated analysis process reduces the likelihood of errors researcher. Achieved time saving during processing results. In carrying out several measurements possible drawing card plate to predict vield crystals. According to this technique done in measurement of mechanical stresses of thermal silicon oxide film on a silicon substrate. Analysis of the results showed objectivity and reliability calculations. This method can be used for selecting the optimal parameters of the material deposition conditions. In software of device-technological simulation TCAD defined process time, temperature and oxidation of the operation of the sample environment for receiving the set value of the dielectric film thickness. Calculated thermal stresses are in the system silicon-silicon oxide. There is a good correlation between numerical simulations and analytical calculation. It is shown that the nature of occurrence of mechanical stress is not limited to the difference of thermal expansion coefficients of materials.

1. Introduction

Technologies of micromechanics or microelectromechanical systems (MEMS) and integrated circuits (IC) develop quickly [1]. The mechanical stresses arising during manufacturing of IC and MEMS devices on Si plates have a strong impact on their reliability and dynamic characteristics [2–4].

Deformation occurs at temperature gradient in the structure, due to the difference between the coefficients of thermal linear expansion of different layers. Magnetostrictive effect, inverse piezoelectric effect or result of action of external forces are reason for strain. As a result, tensile stress in film structure typically results in film cracking or delamination. On the other hand, stress can increase the limit of the system of elasticity, fatigue strength, corrosion-mechanical stability, transistor performance. Therefore, it is important to evaluate and control the amount of stress, not only to avoid damage to device [2, 5], but also to improve product specifications.

The existing techniques for determination of mechanical stresses are based on wafer deformation (use of Newton rings, Stoney formula [2, 6]) or connected with measurement of lattice parameters (Raman spectroscopy [7], X–ray diffractometry [8, 9], transmission electron microscopy).

2. Problem statement

It is necessary to control the amount of stress to optimize the film deposition conditions. The authors calculated mechanical stresses on bending plate. The process of analyzing the surface of a relief on profilometer takes time. This is due to the fact that, to obtain a radius of curvature at the ends of two markers investigated interval must be put. If you move the marker using computer mouse errors may occur. Therefore, there is a need to develop a technique which includes a program with an algorithm relief analysis.

3. Research questions

The study was solved a number of problems. Calculate radius of curvature of the surface based on the model of the geometric representation. Visualize the data obtained. Select a programming language to design a program that implements the algorithm developed. Prove the objectivity and reliability of the presented techniques. Carry out numerical simulations to determine the parameters of the technological process of obtaining the required thickness of the film. Make an experiment. Compare the results of numerical modeling of thermal stress with the analytical calculation. Show different nature of occurrence of stress.

The main objective is to determine amount of stress in the local region of sample, reduction of relief analysis time and minimizing the probability of error.

4. Research methods

In this paper we used Stoney method [2, 6, 10]. Mechanical stresses are calculated by Equation (1) according to the bending wafer (the amount of change of the radius of curvature localized part of a surface of wafer):

$$\sigma_f = \frac{E_s \cdot d_s^2}{6(1-u_s)} \cdot \frac{1}{d_f} \cdot (\frac{1}{R_{after}} - \frac{1}{R_{before}}),\tag{1}$$

where σ_f are mechanical stresses; E_s is Young modulus of the substrate material; d_s is thickness of wafer; u_s is Poisson's ratio of the substrate material; d_f is thickness of film on wafer; R_{after} is curvature radius of surface after operation; R_{before} is curvature radius of surface before operation.

Scanning the surface of an optical profilometer is one way of determining the radius of curvature. The result is determined by relief of surface.

In the software for the modern devices are often incorporated in the calculation of the simplification of the stress. That is, the radius of curvature is much greater than the distance between adjacent points [3]. Therefore, by increasing the length of the scanning step error probability occurs. Also, the software of modern optical profilers usually does not provide the ability to automatically calculate the radius of curvature at all points of the surface profile. It became necessary to develop specialized techniques.

The technique involves performing measurements with the non-contact optical profiler and interpretation of the data obtained from it: calculation of the radius of curvature of the surface based on the model representation, and the subsequent calculation of the values of stress at selected area. It achieved a visual representation of the data. First, we analyzed geometry of surface operating plate. Scheme analysis of surface relief is shown in Figure 1.

We conducted geometric transformations, obtained an Equation (2) for calculating radius of curvature of surface of the local area:

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$$R = \frac{\{\frac{(x2-x1)\cdot(y3-y1)}{(x3-x1)\cdot\sin(arctg\frac{(x3-x1)}{(y3-y1)})}\}^2 + \{\{(y2-y1) - \frac{(x2-x1)\cdot(y3-y1)}{(x3-x1)}\} \cdot \sin\{arctg\frac{(x3-x1)}{(y3-y1)}\cdot\}\}^2}{2\cdot\{(y2-y1) - \frac{(x2-x1)\cdot(y3-y1)}{(x3-x1)}\} \cdot \sin\{arctg\frac{(x3-x1)}{(y3-y1)}\}}$$
(2)



Figure 1. The geometry of surface wafer to calculate radius of curvature.

The reliability of formula (2) tested in SolidWorks software environment.

Built ADB arc with arbitrary values of the coordinates of points (xi,yi). Further, the radius R is made calculation by formula (2). After that, done segments BP and AP with a length R. So that the length of the segment AP, DP, and BP of the same. The closed contour ADBP obtained proves the accuracy of the formula (2).

The second step was to make the algorithm calculating value of the local surface curvature radius by the formula (2) in the Matlab software.

The algorithm consists of several stages. In the first stage polynomial function was found that most correctly describes the relief. Next, we compared the value of the two nearest points of relief. If there is an increase function describing the relief of surface, calculation is made by Equation (2). If the function decreases, the sign of calculated values is reversed. At the end, values of radii are substituted in formula (1) to calculate the mechanical stresses.

5. Findings

The authors investigated a silicon wafer (diameter of 150 mm, thickness of 670 micrometers, orientation (100)) with thermal SiO_2 dielectric film. As is known, SiO_2 membrane is part of air flow sensors in [1]. Modeling was carried out in software of device–technological TCAD simulation. We determined process time, temperature and the operation of the sample oxidation environment for the necessary values of the dielectric film thickness.

The result of the simulation is shown in Figure 2.

In this way, at a temperature of 1000°C the active stage of the process of wet oxidation will be 220 minutes. Thickness of film on experimental sample was determined by Horiba ellipsometer and was 580 nm, which shows a good correlation between the results in TCAD environment and experiment.

Next, using plasma chemical etching without using a mask, silicon oxide film has been removed from back side wafer. A relief measurement in two directions: parallel and perpendicular to base shear before and after deposition. Measurement of relief of a surface was carried out using a non-contact optical profilometer Veeco Wyko NT9300. The results of measuring relief of a surface in perpendicular direction of base shear are shown in Figure 3. We analyzed the work area from 20 to 130 millimeters.



Figure 2. The dependence of film thickness of active stage of process time.

From these figure it can be concluded that after forming silicon oxide film on front side of plate became more curved. As is known, initial wafer of monocrystalline silicon with orientation (100) contains minor positive mechanical stresses. Hence, value of stress increased. For the equilibrium state of the substrate-film, resulting force compression-tension must be equal to zero. Therefore, thermal SiO_2 film negative compressive stresses are equal in magnitude stresses in silicon.



Figure 3. Surface profile in a perpendicular base shear direction.

With above-described algorithm in Matlab calculation performed curvature values before and after film deposition. Further, by formula (1) using the algorithm in Matlab determined magnitude of stress in the structure (Figure 4) after forming the SiO₂ film of 600 nm on the front side. Constant biaxial modulus ($E_s/(1-u_s)$) of the sample in the crystallographic plane (100) was $1.8 \cdot 10^{11}$ Pa [10, 11].



Figure 4. The distribution of mechanical stresses in the wafer

Figure 4 shows that at edges wafer increases the stresses. The average value mechanical stresses on the work area substrate is - 210 MPa, which corresponds to the order of magnitude [2, 3, 7, 10]. Comparing the values obtained by the maximum stress and the critical stress for the material, it is possible to prevent cracking of the structure. For example, by making structure of heat treatment the purpose of minimization stress [7, 12]. To determine nature of occurrence of mechanical stresses carried out comparative analysis of stress values and value of thermal stress calculated in TCAD software.

6. Numerical simulation of thermal stress in TCAD.

Presenting results of simulation of thermal stress in the silicon oxide film on a silicon substrate with crystallographic orientation (100) on the basis of device-technological TCAD simulation software package.

In TCAD software section process does not provide for setting value of Young's modulus E_f and Poisson's ratio u_f film. However, assigning a value of module substrate K_f and the shear modulus G_f of film material, it is possible to calculate the required values, determined system of Equations (3):

$$\begin{cases} K_f = \frac{E_f}{3(1 - 2 \cdot u_f)} \\ G_f = \frac{E_f}{2(1 + u_f)} \end{cases}$$
(3)

Material parameters used in TCAD library: value of substrate module K_f is $6.534 \cdot 10^{10}$ (Pa) and shear modulus $G_f 2.792 \cdot 10^{10}$ (Pa), respectively. Solving the system of Equations (3), received the Young's modulus E_f of SiO₂, equal to $8 \cdot 10^{10}$ (Pa). In the process of calculating difference in TCAD temperature coefficient of linear expansion of material $\Delta \alpha$ silicon and silicon oxide with a crystallographic orientation (100) was assumed to be - $1.5 \cdot 10^{-6}$ (1/°C) [3]. The magnitude of difference of film deposition temperature SiO₂ and measurement is ΔT 1000°C. As a result of simulation obtained stress value in the silicon oxide film -110 (MPa).

The purpose of analyzing correlation of numerical simulation results with analytical calculation, calculated the value σ_{term} thermal stress. In the analysis of one-dimensional problem with an absence of cross-compression Poisson ratio u_f tend to zero. Obtained Equation (4) to simplify the expression of the work [10]:

$$\sigma_{term} = E_f \cdot \Delta \alpha \cdot \Delta T \tag{4}$$

The calculated value of thermal stress in SiO₂ film was - 120 MPa.

Analyzing the results of numerical simulations and analytical calculations, we can conclude about good comparability of results. Thus obtained value of thermal stress is less than the mechanical stresses obtained experimentally using techniques described. The difference with experimental data indicates the multifaceted nature of stress, which includes the thermal stress, but not limited thereto.

7. Conclusion

Presented and implemented a technique that allows for analysis of surface relief for purpose of calculation stress. The method allows to obtain distribution of mechanical stresses on wafer surface. Analysis of the results showed objectivity and reliability calculations. This method can be used for selecting the optimal parameters of deposition material conditions.

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