Mechanical stress design system for semiconductor devices

Hideo Miura, Naoto Saito, Hiroyuki Ohta, and Noriaki Okamoto
Mechanical Engineering Research Laboratory, Hitachi, Ltd.
Tsuchiura, Ibaraki 300, Japan

Hiroo Masuda
Device Development Center, Hitachi, Ltd.
Ome, Tokyo 167, Japan

1. Introduction

Recent trends in LSI integrations have resulted in extremely complicated device structures made of numerous thin-film materials. Since the thermal expansion coefficients of films differ from each other, thermal stress occurs during the manufacturing process. This sometimes causes mechanical failures, such as film delamination or cracking and dislocation formation in the silicon substrate [1], [2]. It can also cause electronic failure such as shifting a device electrical characteristics or shortening its life time [3], [4]. These failures degrade a device's yield and reliability while increasing its development cost. Conventionally, these problems were solved by trial and error. Since the manufacturing process has become more complicated, however, it sometimes takes several months to confirm the effectiveness of countermeasure.

As a result, stress simulation has been introduced to eliminate mechanical failures in the structural design and manufacturing of semiconductor devices [5]. Additionally, a new mechanical design system has been developed for semiconductor devices to reduce both the development period and the cost. The main feature of the system is to minimize or control stresses that develop in the device structure during manufacturing. This system helps eliminate careless mechanical failures and reduces the number of experimental trials. An outline of the system is shown in Fig. 1. The system consists of three main subsystems; a material database construction system, a stress simulation system using the finite element method, and a stress evaluation system.

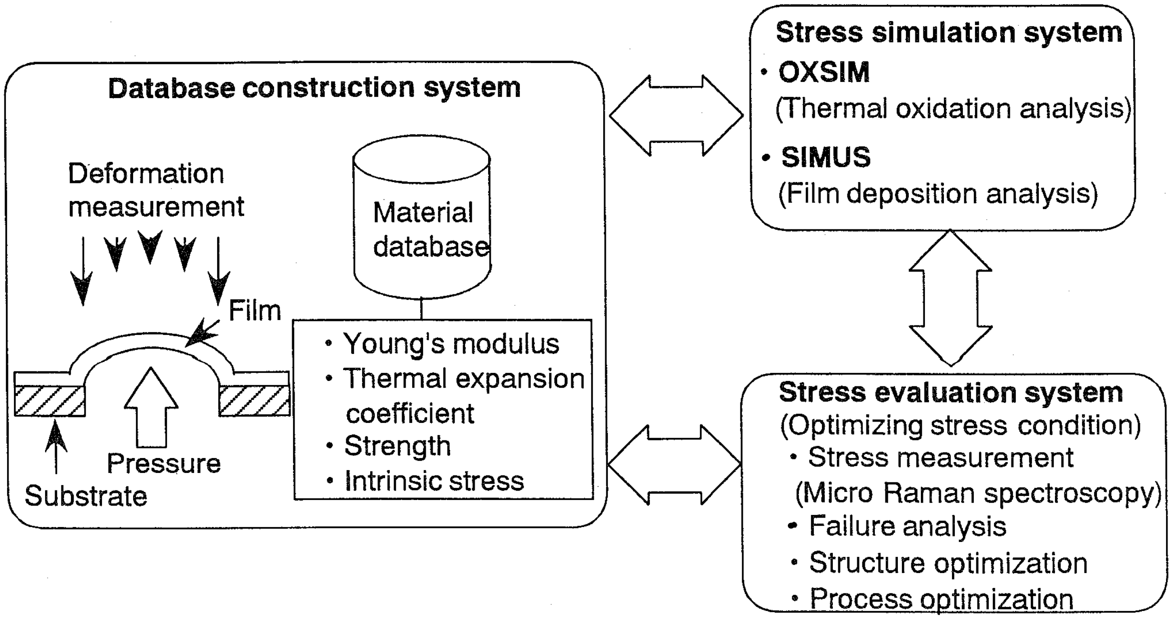

Fig.1 Outline of the mechanical design system for semiconductor devices

2. Database construction system

Mechanical properties, such as Young's modulus, the thermal expansion coefficient, and the intrinsic stress of thin films are important in performing a mechanical stress simulation. Since these properties are usually different from those of bulk materials, it is necessary to determine them experimentally. The authors have developed a suitable measurement system that applies the bulge method [6]. In this system, film deformation is measured using a scanning laser microscope at the minimum resolution of 0.1 μm. The mechanical properties are measured as a function of temperature between room temperature and 1000°C.

The intrinsic stress of thin films has become an increasingly important mechanical property because new materials being used, such as P-doped silicon thin film and WSIx film, have rather high intrinsic stress of about 1000 MPa. An example of measured stress change in P-doped silicon film during annealing is shown in Fig. 2 [7]. In this case, the deposited film is in an amorphous phase and crystallizes at about 600°C. During crystallization, a drastic internal stress change of about 1000 MPa occurs mainly due to film-volume shrinkage. Since the mismatch in the thermal expansion coefficients between the film and the substrate is very small, thermal stress is negligible during this annealing. In this case, the residual stress in the substrate is determined by the intrinsic stress of the deposited film. It is important, therefore, to have accurate mechanical properties of thin film materials for precise stress analysis.

Furthermore, the strength database of thin films and silicon substrates at high temperatures is necessary to evaluate mechanical failures, such as film cracking or dislocation formation in the substrate.

3. Stress simulation system

Stress simulation is performed using the finite element method. There are two main codes named OXSIM [8], [9] and SIMUS [10]. The code OXSIM was developed for analyzing the thermal oxidation process while considering effect of the stress on oxidation reaction [11]. The distribution of stress throughout the structure can be determined by considering the viscoelastic properties of materials. An example of the predicted stress distribution in the LOCOS structure is shown in Fig. 3. The reason for tensile stress development during thermal oxidation is the volume expansion of newly grown oxide film. Curved surface oxidation causes compressive stress and a complicated stress distribution near the oxide/substrate interface. The accuracy of the predicted stress distribution is confirmed using microscopic Raman spectroscopy [12].

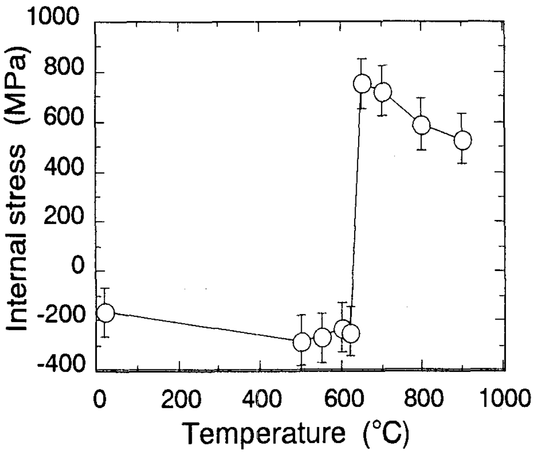

Fig. 2 An example of the internal stress change of amorphous silicon film

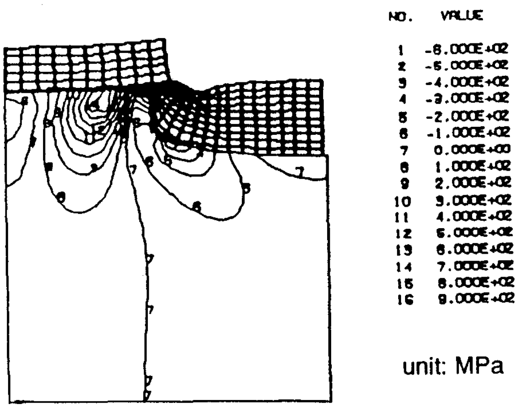

Fig. 3 Predicted resolved shear stress distribution in a LOCOS structure

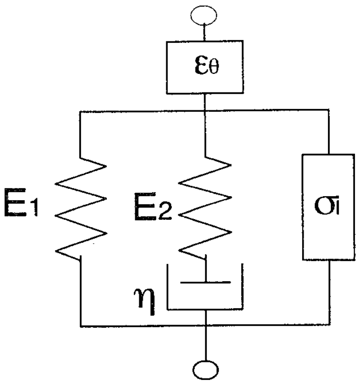

Fig. 4 Viscoelastic analysis model for films with intrinsic stress

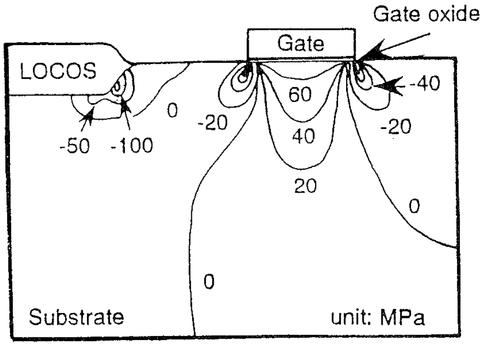

Fig. 5 Predicted resolved shear stress distribution in a MOS structure

The code SIMUS was developed for analyzing stress distribution in the device structure during thin-film deposition. The analysis can be performed step by step i.e., every film deposition step or etching step can be determined. As mentioned above, it is very important to consider the existence of intrinsic stress of deposited films. For an example, in the case of viscoelastic stress analysis, the intrinsic stress of the deposited film is taken into account by applying the Maxwell model as shown in Fig. 4. In this model, the stress-strain relationship is expressed as,

$$\Delta\sigma=(D+\Delta D)(\Delta\varepsilon-\Delta\varepsilon_\theta-\beta\Delta\varepsilon_v)+\Delta D\cdot D^{-1}(\sigma-\sigma_i).$$

Here, σ is the stress, σ_i is the intrinsic stress of the film, ε is the total strain, ε_θ and ε_v are the thermal and viscous strains, respectively, D is the material moduli matrix and D^{-1} is its inverse matrix. Also, β is the elastic ratio of Young's modulus, E1 and E2. An example of a predicted stress distribution for a MOS structure is shown in Fig. 5. In this analysis, P-doped silicon film is used for gate electrode material. It is clearly seen that a stress concentration occurs at the edges of the LOCOS structure and the gate electrode. These stress concentrations sometimes cause dislocation in the substrate. Therefore, it is important to design an optimum film-deposition process that reduces these stresses to at least a level below the substrate strength at temperatures of interest.

4. Stress evaluation system

To apply the predicted stress distributions to actual product design, it is necessary to construct design criteria for each mechanical failure. In film-cracking analysis, strength data of the thin film materials are indispensable for comparing the predicted maximum stress with the database. If the predicted stress exceeds the film strength, film cracking should be eliminated by lowering the stress condition of the film deposition process. The process can be optimized by changing conditions such as the temperature, structure or shape of the deposited film, and the atomic composition of the film. In film-delamination analysis, it is important to consider fracture mechanics because delamination usually starts at the film edge where stress is concentrated. The stress intensity factor at the film edge is a useful evaluation parameter for delamination analysis.

An example of an evaluation system for dislocation analysis during thermal oxidation is modeled in Fig. 6. The maximum stress value that develops at the LOCOS edge depends on several independent process parameters such as pattern size, thicknesses of the SiNx film, the pad-oxide film, and the grown oxide film, and oxidation conditions such as temperature and ambient gas. Stress analysis is first performed based on a proposed process, then the predicted stress is compared with the critical stress for dislocation formation at temperatures

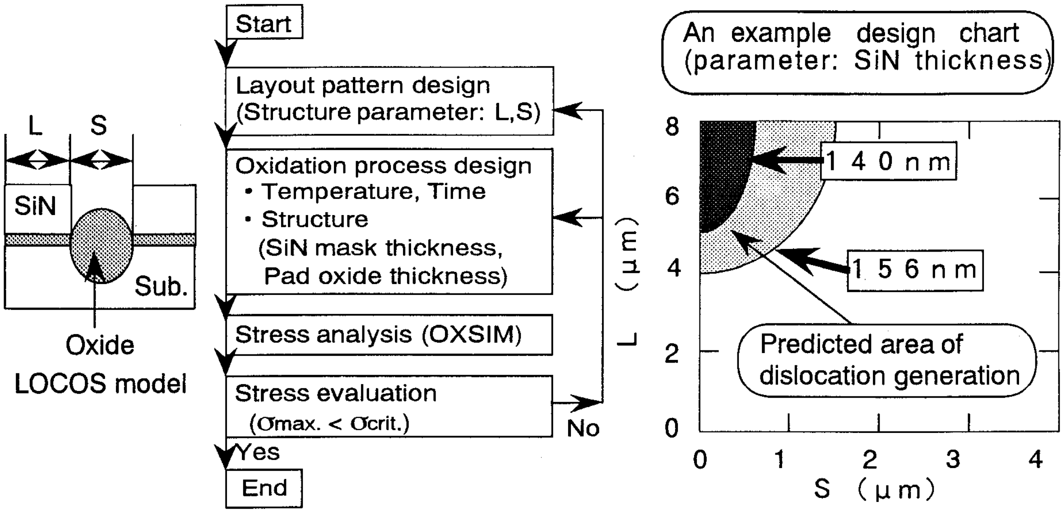

Fig. 6 An example of a LOCOS process design model

of interest. If the predicted stress is higher than the critical stress, the proposed process is revised by changing the process parameters until the maximum stress goes below the critical stress. Design charts for the LOCOS structure can be drawn as shown in Fig. 6. Using this chart, engineers can design LOCOS structures and processes without dislocation.

Stress optimization of device structures and fabrication processes can be performed using this step-by-step stress evaluation system. Though the critical stress at each step has not yet been obtained fully, most primitive mechanical failures can be eliminated at the analytical design stage. Stress control without mechanical failures will be achieved by further challenging studies.

5. Summary

A new, mechanical stress design system for semiconductor manufacturing has been developed to reduce or minimize mechanical failures and development costs. By applying this system, it is possible to eliminate most mechanical failures at the analytical design stage.

Acknowledgements

The authors would like to thank Dr. E. Takeda , Dr. S. Isomae, Dr. S. Ihara, Mr. S. Kiyota, Dr. H. Sakata, and Dr. S. Sakata for their helpful discussions.

References

[1] J. Vanhellemont and C. Claeys, *J. Electrochem. Soc.* **135**, 1509 (1988).
[2] S. M. Hu, *J. Appl. Phys.* **70**, R53 (1991).
[3] Y. Ohno, et al., *Proc. of IRPS*, 34(1989).
[4] A. Hamada, et al., *IEEE Trans. Electron Devices*, **38**, 895 (1991).
[5] P. M. Fahey, et al., *IBM J. Res. Develop.*, **36**, 158 (1992).
[6] H. Ohta, et al., *Proc. of the 69th JSME spring annual meeting (in Japanese)*, **A**, 510 (1992).
[7] H. Miura, et al., *Appl. Phys. Lett.* **60**, 2764 (1992).
[8] N. Saito, et al., *IEDM Tech. Digest*, 695 (1989).
[9] H. Miura, et al., *Proc. of Int. Workshop on VLSI Process and Device Modeling*, 48 (1991).
[10] N. Saito, et al., *Proc. of the Int. Conf. on Computational Engineering Science*, 880 (1991).
[11] D. B. Kao, et al., *IEEE Trans. Electron Devices*, **35**, 25 (1988).
[12] H. Miura, et al., *Mat. Res. Soc. Symp. Proc.*, **226**, 345 (1991).