Elasto-Plastic Modeling of Microelectronics Materials for Accurate Prediction of the Mechanical Stresses in Advanced Silicon Technologies

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Abstract

This paper reports the implementation of an elasto-plastic model in advanced stress simulation system within the process simulator IMPACT to predict the mechanical behavior of (poly)crystalline materials used in the microelectronic technologies. The benefits of this new model are a better prediction of the stresses magnitude in elasto-plastic materials, the capability to calculate the location and size of plastic area in silicon substrate and the possibility to analyze very accurately stresses evolution in (un)passivated metal interconnects networks, a serious reliability issue for the IC industry in the recent years.

This work has been partly carried out within the STREAM project funded by the EC as IST-1999-10341.

1. Introduction

Stresses develop in integrated circuit (IC) structure during processing as a result of a variety of different effects. These stresses can lead to process modifications as well as change in the electrical behavior of the final device. More seriously, they can induce plastic flow, cracking, void formation and mechanical failure. That is why the knowledge of both the locations and magnitudes of such stresses is important. The finite element method is a powerful tool for solving problems of this nature. However, an accurate simulation of the stresses evolution requires informations on the materials, on the geometries of the structures and on the stresses sources. Only process simulation can provide all of these data at the same time and that is why we started few years ago the development of an homogenous and advanced stress simulation system in IMPACT, allowing the evaluation of the cumulative mechanical stresses at each process steps [1]. Our last work concerns the introduction of a complex rheological behavior for (poly)crystalline microelectronics materials which exhibit elasto-plastic properties under large stress sollicitations. To our knowledge, there is very few works reporting the implementation of an elasto-plastic algorithm in a process simulator [2]. Furthermore, they only focuse on the silicon behavior and do not take into account several complex mechanical behaviors such as stress-dependent viscoelasticity and elastoplasticity in the same numerical calculations. The benefits of this new model are a better prediction of the stresses magnitude in elasto-plastic materials, the capability to calculate the location and size of plastic area in silicon substrate and the possibility to analyze very accurately stresses evolution in (un)passivated metal interconnects networks, a serious reliability issue for the IC industry in the recent years.

2. Numerical implementation

The numerical "Return Mapping" algorithm is based on the works of Zienkiewicz [3] and Simo [4] and corresponds to an elastic perfectly plastic behavior. It is schematically summarized in Fig.

1a: from a residual stress σ_0 in the elastic domain, a new elastic trial stress σ'_1 is computed. If the resulting state defined by σ'_1 lies outside of the elastic region enclosed by the yield surface (F=0), one defines the final state as the "closest-point-projection" of σ'_1 onto the yield surface. The yield surface is defined with the von-Mises stress at the end of the time step. Then the new elastic residual stress σ_1 is calculated and $\Delta\sigma_1$ is converted into an un-balanced deviatoric stress, which by definition, is tangent to the yield surface. A new mechanical equilibrium is computed which leads to the residual stress σ'_2. This non-linear algorithm is accomplished by a Newton-Raphson procedure and is considered converged when all displacements are smaller than 10^{-9}cm. For problems requiring to solve both non-linear viscoelasticity and elastoplasticity, we use a decoupled approach given in Fig. 1b. First, we solve the non-linear (Eyring) viscoelasticity using SOR technique where poly(crystalline) materials are considered elastic. If, the elastic limit is reached,

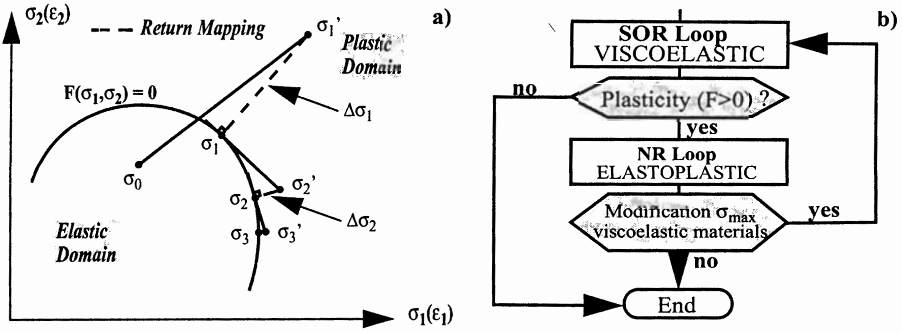

Fig. 1. a) Graphic interpretation of the numerical treatment of elasto-plasticity. b) Schematic algorithm of the decoupled treatment of elasto-plasticity and of viscoelasticity.

we treat the elastoplasticity considering that the viscosity of viscoelastic materials is constant. When we have converged on the elastoplastic problem, if the maximum shear stress σ_{max} of each viscoelastic materials has been modified by more than 1% after the NR loops, we go back to the viscoelastic problem. To evaluate the performances of this algorithm, we have simulated the "fictive" annealing from 25 to 1200°C of an AlCu line patterned on an oxidized silicon wafer (Fig. 2a). On can see that the plasticity of AlCu is activated around 100°C and the viscoelasticity of SiO_2 around 975°C. During the simulation, there is no iterations between the elastoplastic and the viscoelastic problems, the higher variation of σ_{max} being 0.6 MPa at 1100°C. If we now analyse

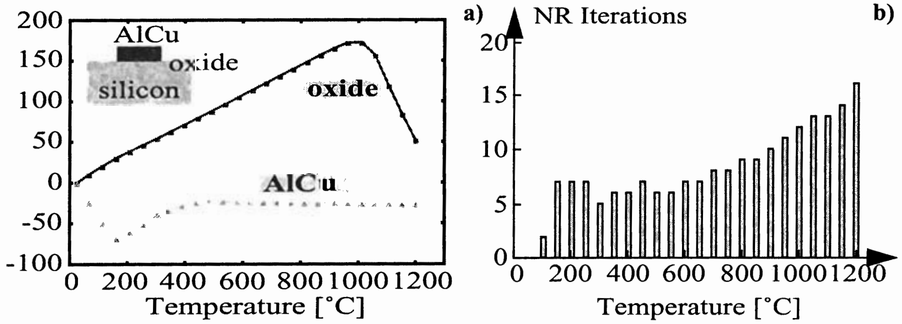

Fig. 2. a) Average stress in AlCu and oxide versus annealing temperature for a structure given in the insert. b) Histogram of the number of Newton-Raphson iterations versus temperature for the mechanical simulation reported in fig. 2a.

the elastoplastic treatment (Fig. 2b), a very good convergence rate is reached which slighlty decreases at high temperatures due to the purely viscous behavior of SiO_2. To validate this modeling, we have chosen the experiment of Vanhellemont [5] where a very thick LOCOS is grown in wet ambient. It leads to the creation of a dislocation in silicon in the bird's beak region (Fig. 3c). The simulations of this process, using either an elastic behavior for silicon (Fig. 3a) or an elastoplastic behavior (Fig. 3b) have been performed considering a rather high elastic limit (σ_Y) equal to 1GPa. Figs 3a-b gives the 2D distributions of the von-Mises stress and show the appearance of a plastic area in the bird's beak region in agreement with the experiment. The use of the elastoplastic algorithm increases the computing time by 6% only.

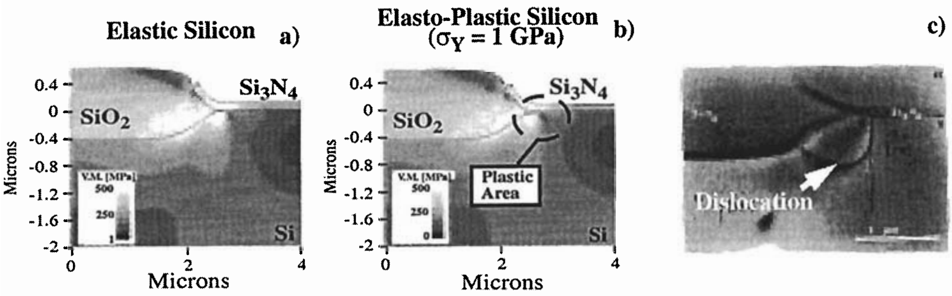

Fig. 3. Growth of a LOCOS isolation considering either a) an elastic or b) an elasto-plastic silicon, c) corresponding SEM picture showing the presence of a dislocation [5].

3. Applications to the behavior of aluminum-copper interconnects

For this material, it is known that σ_Y is function of the thickness of the film as well as the temperature. The experimental variations of the average stress in different films versus the temperature are given in Fig. 4 [6-7]. They reveal a complex mechanical elasto-plastic behavior which can be reproduced by the calibrated model. This calibration, performed for seven temperatures, is compared (Fig. 5a) with other works [8-9] and shows a good agreement. The full set of calibrated data is plotted in Fig. 5b and one can observe that at low temperature σ_Y is less sensitive to the film thickness than at high temperature. To validate this modeling, we have chosen the experiments of Yeo [10] where a network of AlCu lines (0.8μm thick) are patterned with different widths on an

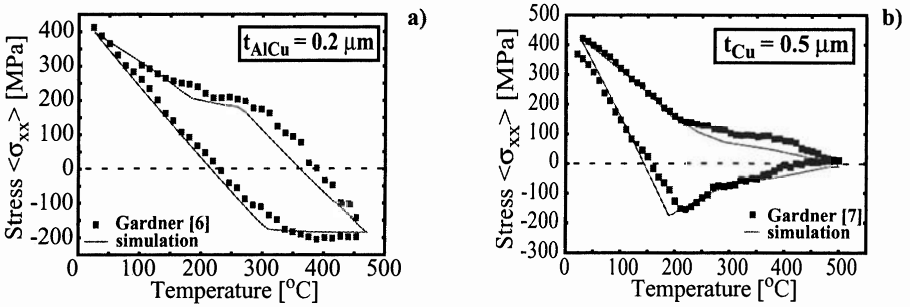

Fig. 4. Validation of the elasto-plastic modeling of aluminum-copper and of copper films for various thicknesses: a) 0.2μm, b) 0.5μm.

oxidized silicon wafer. The variations of the average stress versus temperature are given in Fig. 6a and, without any additional calibration, one can see they are well predicted by the model (Fig. 6b). One can notice that the magnitude of the hysteresis becomes smaller when the width is smaller. If we now analyze the effect of the passivation (Fig. 6c), one can see that the confinement increases the magnitude of the stress and that the aspect ratio of the line is an important factor in the activation of plasticity. If we study more specifically this parameter, one can show that the optimization of the geometry of the line is not only dependent of its aspect ratio as concluded by Yeo but also of its thickness. This later aspect will be developed in details in our oral presentation.

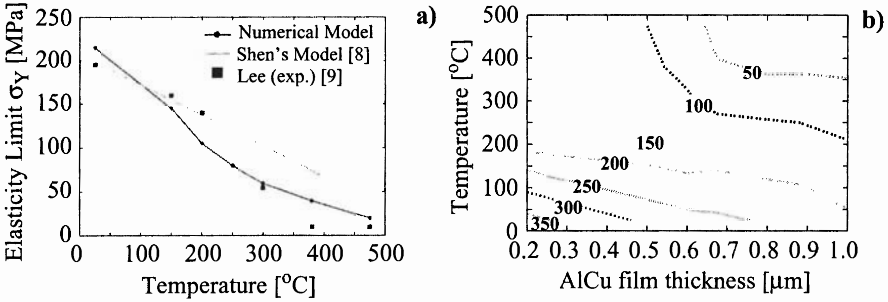

Fig. 5. Calibration of the elasto-plastic model for AlCu films: a) comparison of the elasticity limits for a 1μm thick film, b) variation of the elasticity limit versus temperature and thickness.

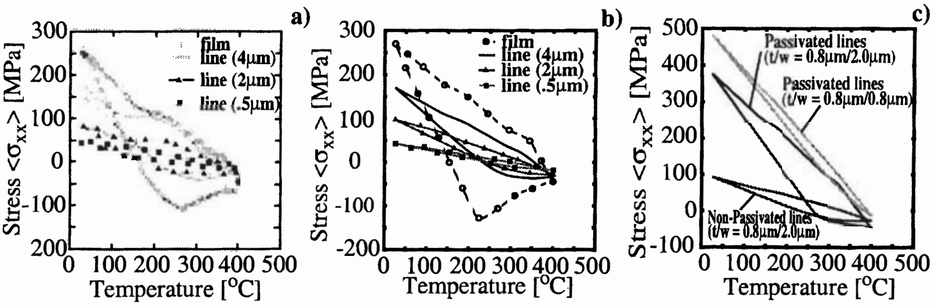

Fig. 6. a) Experimental variations of the average stress in AlCu lines (0.8μm thick) having different widths versus temperature [10], b) corresponding simulation results, c) influence of the passivation on the stresses in the AlCu lines.

4. References

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