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Dislocation Injections by a Localized Stress Field in a Strained Silicon

Juil Yoon*

Department of Mechanical Systems Engineering, Hansung University, Seoul 136-792, Korea

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Abstract : In the 21st century, safety issues in the strained silicon industry, such as dislocation injection, should be carefully considered. This is because a microelectronic device usually contains sharp features (e.g., edges and corners) that may intensify stresses, inject dislocations into silicon, and ultimately cause the failure of the device. In this paper, critical residual stresses in various strained structures are calculated. It is confirmed that this model correctly predicts trends and the order of magnitude of critical residual stresses.

Key words: strained silicon, dislocation, critical residual stress, sharp features

1. Introduction

The steady reduction in the minimum feature size in integrated circuits (IC) has helped the microelectronic industry to produce products with spectacular increase in computational capability and integration density at lower cost. In the next decade, advances in semiconductor fabrication will lead to devices with gate lengths below 10 nanometers, as compared with current gate lengths in chips that are now about 50 nm [1]. This kind of scaling down in microelectronics, causes unexpected safety issue. One example is car sudden departure. It is suspected that the trend of increasing sudden departure accident may be correlated with increasing microprocessor in car. For example, 17 microprocessors are built in new model Sonata (Hyundai), since customer demands more functions, such as electronic stability control system. For other example, cell phone explosion has been numerously reported. Since it's been estimated that there'll be 1.3 billion cell phone users worldwide and that number will increase from there, with that many cell phones in use, cell phone safety is of importance.

After integration of billions of transistors, capacitors, resistors, inductors, etc. on its surface, the microelectronic devices are vulnerable to stresses. Stresses inevitably arise in a microelectronic device due to mismatch in coefficients of thermal expansion, mismatch in lattice constants, and growth of materials. Moreover, in the technology of strained silicon devices, stresses have been deliberately introduced to increase carrier mobility [1]. Strained-silicon technology has been successfully used in semiconductor industry to improve the performance of CMOS transistors while their feature size scaling below 100 nm. Stress induced electron/hole mobility change in silicon, known as piezoresistance effect, was first measured 50 years ago. The research on this topic has become very active since late 1980s. Manufacturable strained silicon technology was developed in 1990s. Nowadays, almost every semiconductor manufacturer is using this novel technology to improve the performance of their products. It is believed that this trend will continue and the stress in CMOS will be pushed to a much higher value since carry mobility is found to follow a superlinear relation with the stress. Imagine that hundred millions of transistors are squeezed in a centimeter-size IC chip, and each transistor needs to sustain considerable mechanical stresses and undergo severe process flow. Mechanical failures are conceivable.

As microelectronics becomes smaller and meets more customer friendly application, the safety issue may grow. Any failure mechanism, such as crack, wrinkle, and dislocation, cause mal-function in microelectronics devices [2,3]. In this paper, critical condition for dislocation injection in a localized stress filed is studied. The dislocations could fail the whole IC chip by electrical leakage if they appear near the channel area. This issue will become critical when higher and higher stresses are

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*Corresponding author: juilyoon@hansung.ac.kr

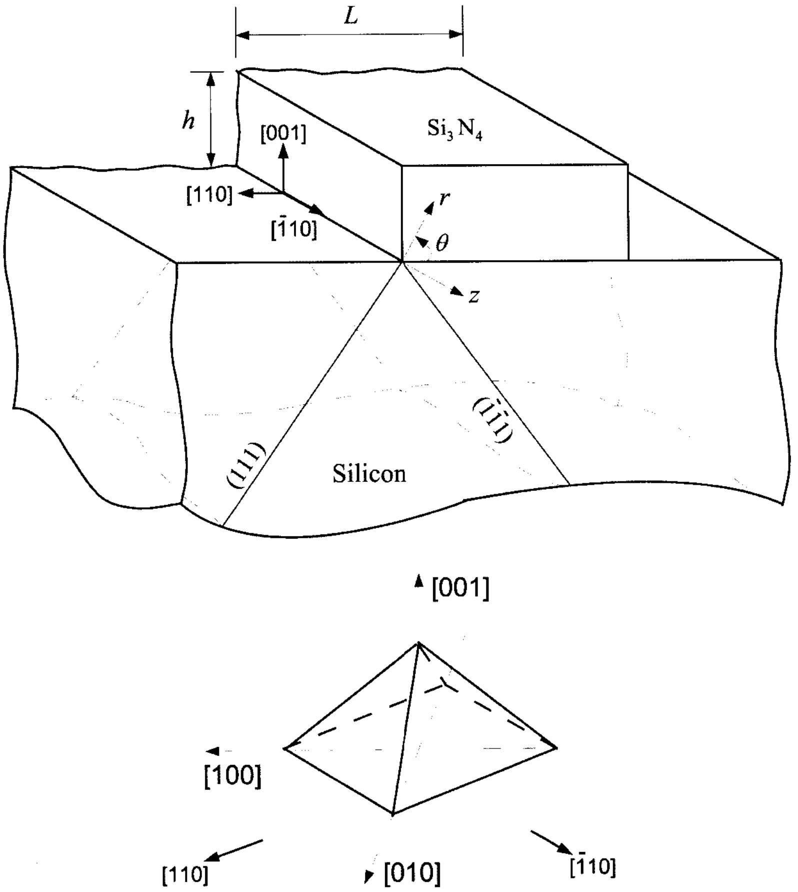

Fig. 1. A SiN film, of thickness h and residual stress σ, is grown on the (001) surface of a single-crystal silicon substrate. The film is then patterned into a stripe of width L, with the side surfaces parallel to the plane of silicon.

induced in the transistors. This is a good opportunity for mechanicians to make significant impacts on this multi-billion dollar industry.

2. Stress Field in Sharp Edges

A blanket film of silicon nitride (Si$_3$N$_4$), of thickness h and residual stress σ, is grown on the (001) surface of a single-crystal silicon substrate, as shown in Fig. 1. The film is then patterned into a stripe of width L, with the side surfaces parallel to the (110) plane of silicon. When the film covers the entire surface of the substrate, the film is under a uniform stress, and the substrate is stress free. When the film is patterned into a stripe, stress builds up in the substrate, and intensifies at the roots of the edges. It is this intensified stress that injects dislocations into the silicon substrate.

It is studied that the stress field using a method developed by Williams [4], Bogy [5] and others. In Fig. 1, a polar coordinate system (r,θ,z) is centered at the root of an edge. The stress field around the root is singular and takes the form

$$\sigma_{ij}(r,\theta) = \frac{k_1}{(2\pi r)^{\lambda_1}}\Sigma_{ij}^{1}(\theta) + \frac{k_2}{(2\pi r)^{\lambda_2}}\Sigma_{ij}^{2}(\theta) \qquad (1)$$

The exponent λ is between 0 and 1 and is shown in Fig 2. The angular distribution $\Sigma_{ij}(\theta)$ is normalized such that $\Sigma_{r\theta}(0) = 1$. Both λ and $\Sigma_{ij}(\theta)$ will be solved by an eigenvalue problem.

It is determined that the exponent λ and the functions $\Sigma_{ij}(\theta)$ by solving an eigenvalue problem [4,5]. Two values of the exponent λ are found, 0.4514 and 0.0752. Consequently, the stress field is a linear superposition of the two singular fields, one stronger and the other weaker. Following a similar discussion in Refs. [6-8], it is found that the weaker singular term makes about 5% contribution to the total stress field. Hence, the stronger singular field dominates the stress field, and weaker singularity can be neglected. Similarity, the corresponding angular functions in silicon can be obtained.

The quantity k, known as the stress intensity factor, scales with the loading. Linearity and dimensional con-

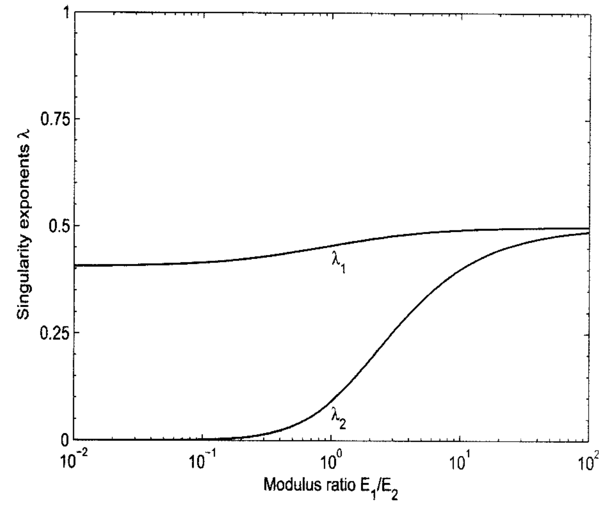

Fig. 2. Singular stress exponent λ is significantly varied by modulus ratio between pad (E_1) and substrate (E_2)

sideration dictate that k should take the form

$$k = \sigma h^{\lambda} f(L/h, S/h, E_f/E_s \ldots) \tag{2}$$

where $f(L/h, S/h, E_f/E_s \ldots)$ is a dimensionless function, to be determined by using a finite element method. It is noted that f is function of pad size (L/h), Spacing between pads (S/h), modulus ratio between pad (E_f) and Substrate (Es), and etc. Since the pad size is dominant factor, L/h is considered in following discussion.

The full stress field in the structure is calculated by using the finite element package ABAQUS, then fit the interfacial shear stress close to the root, say $10^{-3}<r/h<10^{-2}$, to the equation $\sigma_{r\theta} = k/(2\pi r)^{\lambda}$, with k as the fitting parameter. When the aspect ratio of the Si_3N_4 stripe varies from 1 to ∞, the function $f(L/h)$ varies in the range $f = 0.2$-0.48.

The actual stress field around the root deviates from equation (1) within a zone, known as the process zone, because materials deform inelastically and because the root is not perfectly sharp. Researchers are interested in a conservative condition for dislocations to emit, and assume that the root is atomistically sharp. Consequently, the size of the process zone should be on the order of the Burgers vector b. The actual stress field also deviates from (1) at size scale $r \sim h$ and beyond, where the boundary conditions affect the stress distribution. Provided the process zone is significantly smaller than the film thickness, $b << h$, the stress field (1) prevails within an annulus, known as the k-annulus, of some radii bounded between b and h.

3. Critical Stress for Dislocation Injection

Emitting a dislocation is a thermally-activated atomic process, an analysis of which is beyond the scope of this paper. A crude estimate of k_c, however, can be made by letting the resolved shear stress τ_{nb} at distance $r = b$, calculated from equation (1), equal the theoretical shear strength τ_{th}. For a given slip system with the Burgers vector b_i and the unit normal vector n_i of the slip plane, under a general state of stress σ_{ij}, the resolved shear stress is $\tau_{nb} = \sigma_{ij} n_i b_j / b$. Of the twelve slip systems in Fig. 1, the two systems $\frac{1}{2}(111)[01\bar{1}]$ and $\frac{1}{2}(111)[10\bar{1}]$ are found to be most critical. Consequently, the resolved shear stress is

$$\tau_{nb}(r) = \frac{k}{(2\pi r)^{\lambda}} \sum_{r\theta}(\theta) \cos 30^{\circ} \tag{3}$$

For the (111) plane, $\theta = -125.27^{\circ}$, giving $\Sigma_{r\theta} = -1.0317$. The theoretical shear strength can be estimated by $\tau_{rh} = 0.2\mu$, where μ is the shear modulus of silicon [9]. Setting $|\tau_{nb}(b)| = \tau_{th}$, an estimate of the critical stress intensity factor can be obtained :

$$k_c = \frac{\mu}{5\sum_{r\theta}} \times \frac{2}{\sqrt{3}} \times (2\pi b)^{\lambda} \approx 0.5\mu b^{\lambda} \tag{4}$$

We may as well view equation (4) as a result of dimensional analysis, leaving the pre-factor adjustable by any specific atomic process of emitting a dislocation.

A combination of equation (2) and (4) gives a scaling relation between the critical stress and the feature sizes:

$$\sigma_c = \frac{0.5\mu}{f}\left(\frac{b}{h}\right)^{\lambda} \tag{5}$$

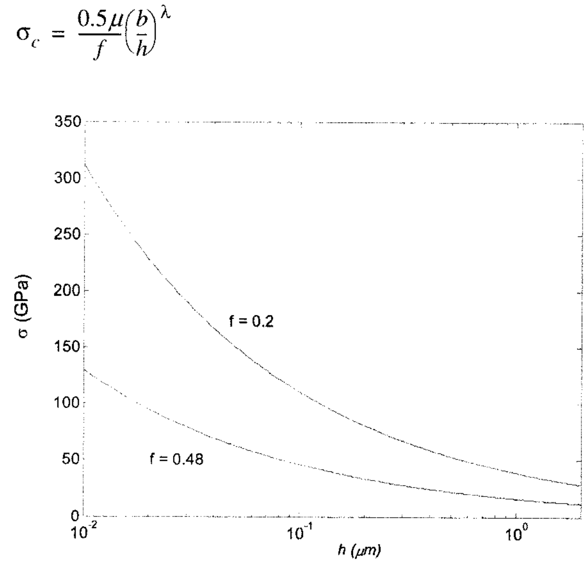

Fig. 3. The critical stress decreases as pad thickness increases when shear modulus and Poisson's ratio of Si_3N_4 to be 54.3 GPa and 0.27, and those of silicon 68.1GPa and 0.22.

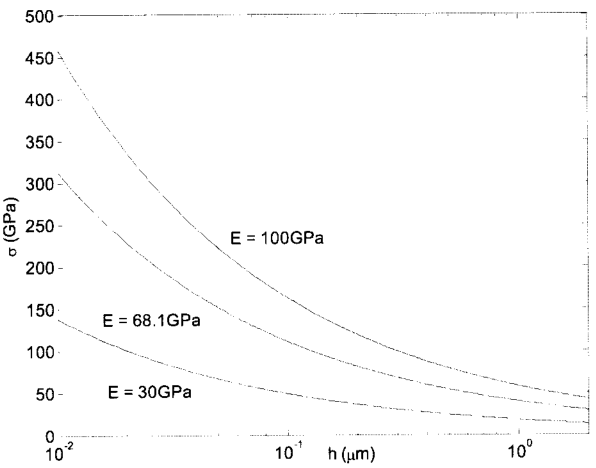

Fig. 4. The critical stress is sensitive to the modulus ratio of pad and substrate

In the numerical examples below, we take shear modulus and Poisson's ratio of Si_3N_4 to be 54.3 GPa and 0.27, and those of silicon 68.1GPa and 0.22. Both materials are taken to be isotropic since anisotropy in the elasticity of silicon plays little role in the singular stress field. It is found that critical stress increases significantly as pad thickness h decreases (Fig. 3). For example, $h = 1\mu m$, the critical residue stress varies in the range σ_c =4.9Gpa–2.03Gpa, depending on value f. This factor f can be adjusted by experiments procedure. For studying the effect of material properties, modulus of substrate varies from 30 GPa to 100 GPa. It is found from Fig 4. that hard substrate can effectively retard the critical stress.

This model can be confirmed by experiment by Kammler et al [10]. A Si_3N_4 film, of thickness 500 nm and residual stress 6 GPa, was grown on a silicon substrate, and was then patterned into large ($10\mu m \times 10\mu m$) and small ($1\mu m \times 1\mu m$) square pads. Kammler et al showed that dislocations emitted from the large pads, but not from the small ones. According to our equation (6), the critical stresses for the two cases are 2.8 GPa and 5.0 GPa, respectively.

This model predicts correct trends and orders of magnitude. However, we recognize that the good agreement with some of the experimental observations may be fortuitous. Our procedure to estimate k_c is crude, and can be improved by using more advanced model such as those due to Rice[11] and others.

4. Summary

As microelectronic devices get smaller to satisfy more application needs of customers, the safety issues have become more critical. The failure of microelectronics may be critical for numerous applications and their customers. In this paper, critical condition for dislocation injection in a localized stress filed is investigated. This problem is expected to be more critical when greater stresses are induced in transistors.

Acknowledgement

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References

[1] M. Ieong, B Doris, J. Kedzierski, K. Rim, and M. Yang, Science 306, 2057 (2004).

[2] M. Dellith, G.R. Booker, B.O. Kolbesen, W. Bergholz, and F. Gelsdorf, J. Electrochem. Soc. 143, 210 (1996).

[3] M. Miyake and M. Takahashi, J. Electrochem. Soc. 144, 1020 (1997).

[4] M.L. Williams, J. Appl. Mech. 19(4), 526 (1952).

[5] D. B. Bogy, J. Appl. Mech. 38, 377 (1971).

[6] X. H. Liu, Z. Suo, and Q. Ma, Acta Mater. 47(1), 67 (1999).

[7] P.E.W. Labossiere, M.L. Dunn, and S.J. Cunningham, J. Mech. Phys. Solids 50, 405 (2002).

[8] Z. Zhang and Z. Suo, Int. J. Solids Struct. (submitted)

[9] J. P. Hirth and J. Lothe, *Theory of dislocation*, 2nd ed. (Krieger Publishing Company, Malabar, Florida, 1992), p. 6.

[10] M. Kammler, D. Chidambarrao, K.W. Schwarz, C.T. Black, and F.M. Ross, Appl. Phys. Lett. 87, 133116 (2005).

[11] J. R. Rice, J. Mech. Phys. Solids, 40(2), 239 (1992).