Method to analyze dislocation injection from sharp features in strained silicon structures

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(Received 30 September 2006; accepted 23 November 2006; published online 27 December 2006)

A microelectronic device usually contains sharp features (e.g., edges and corners) that may intensify stresses, inject dislocations into silicon, and fail the device. The authors describe a method to analyze dislocation injection on the basis of singular stress fields near the sharp features, and apply the method to interpret available experiments of nitride pads on silicon substrates. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2424665]

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 (see Ref. 1 for a review). A device usually contains sharp features such as edges and corners, which may intensify stresses, inject dislocations into silicon, and fail the device.[2,3] On the basis of singular stress fields near the sharp features, this letter describes a method to obtain conditions that avert dislocations.

We illustrate the method using an idealized structure shown in Fig. 1. A blanket film of silicon nitride (Si_3N_4), 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 (110) plane of silicon. The structure is similar to those used in Refs. [4–9]. Here we use a long stripe, rather than a square pad, so that we can focus on the essentials of the method without the complication of three-dimensional corners of the pad. The latter will be considered elsewhere.

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.

Early models of the stress field near an edge of a film have been reviewed in Refs. 5 and 6. One model, for example, replaces the edge with a concentrated force acting on the surface of the substrate.[5,7,8] Not surprisingly, the resulting stress field is inaccurate at a distance smaller than the film thickness, as demonstrated by a finite element analysis.[9]

We will study the stress field using a method developed by Williams,[10] Bogy,[11] and others. The method has also been used to analyze the nucleation of a misfit dislocation from the edge of an epitaxial island.[12] 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

$$\sigma_{ij}(r,\theta) = \frac{k}{(2\pi r)^{\lambda}} \Sigma_{ij}(\theta). \tag{1}$$

The exponent λ is between 0 and 1, and 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.

The quantity k is known as the stress intensity factor. Linearity and dimensional consideration dictate that k should take the form

$$k = \sigma h^{\lambda} f(L/h). \tag{2}$$

The stress intensity factor scales with the residual stress σ and with h^{λ}; the dimensionless function $f(L/h)$ will be determined by using a finite element method.

The actual stress field around the root deviates from Eq. (1) within a zone, known as the process zone, because materials deform inelastically and because the root is not perfectly sharp. We are interested in a conservative condition for

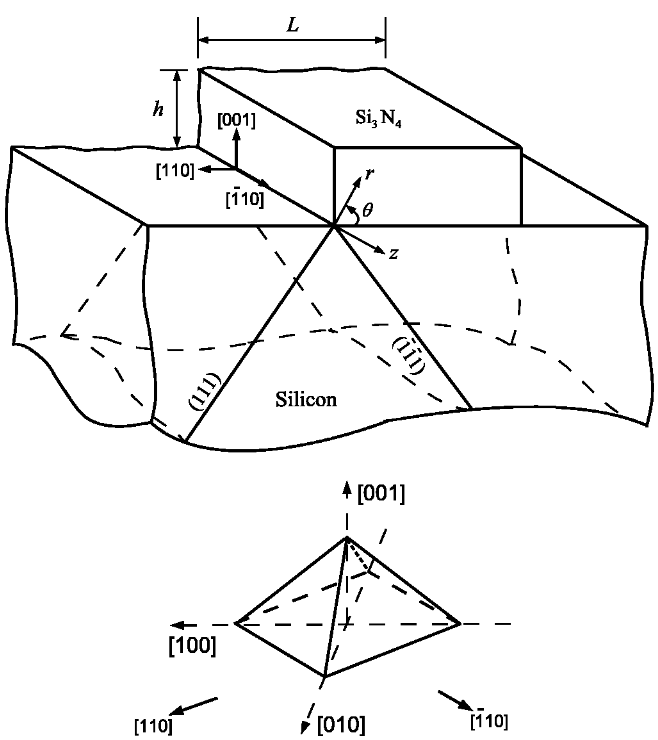

FIG. 1. SiN film, of thickness h and residual stress σ, is grown on the (001) surface of a single-crystal silicon substrate. The film is then patterned into a stripe of width L, with the side surfaces parallel to the (110) plane of silicon.

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dislocations to be emitted, 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 Eq. (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, $b \ll h$, the stress field [Eq. (1)] prevails within an annulus, known as the k annulus, of some radii bounded between b and h.

We now paraphrase a fundamental idea in fracture mechanics.[13] The overall loading is set by the residual stress and the geometry of the stripe, while the atomic process of emitting dislocations occurs within the process zone. The effect of the overall loading on the atomic process is characterized by a single parameter: the stress intensity factor k. Consequently, dislocations are emitted from the root when the stress intensity factor reaches a critical value, $k=k_c$. The value of k_c is a constant specific to the materials and the wedge angle (90° in this letter), but is independent of loading (e.g., the residual stress) and overall geometry (e.g., the thickness and the width of the stripe).

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 to be 68.1 GPa and 0.22, respectively. Both materials are taken to be isotropic since anisotropy in the elasticity of silicon plays little role in the singular stress field.[14]

We determine the exponent λ and the functions $\Sigma_{ij}(\theta)$ by solving an eigenvalue problem.[10,11] Two values of the exponent λ are found, i.e., 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. [15–17], we find that the weaker singular term makes about 5% contribution to the total stress field. Hence, the stronger singular field dominates the stress field, which is expressed by Eq. (1) with $\lambda=0.4514$. The corresponding angular functions in silicon are

$$\Sigma_{rr}(\theta) = -(\lambda-1)\{(\lambda-2)[A\sin(\lambda-2)\theta + B\cos(\lambda-2)\theta] + (\lambda+2)[C\sin\lambda\theta + D\cos\lambda\theta]\}, \tag{3a}$$

$$\Sigma_{\theta\theta}(\theta) = (\lambda-1)(\lambda-2)[A\sin(\lambda-2)\theta + B\cos(\lambda-2)\theta + C\sin\lambda\theta + D\cos\lambda\theta], \tag{3b}$$

$$\Sigma_{r\theta}(\theta) = (\lambda-1)\{(\lambda-2)[A\cos(\lambda-2)\theta - B\sin(\lambda-2)\theta] + \lambda[C\cos\lambda\theta - D\sin\lambda\theta]\}, \tag{3c}$$

$$\Sigma_{zz}(\theta) = -4\nu(\lambda-1)[C\sin\lambda\theta + D\cos\lambda\theta], \tag{3d}$$

$$\Sigma_{rz} = \Sigma_{\theta z} = 0. \tag{3e}$$

with $A=0.9874$, $B=0.3534$, $C=-0.6503$, and $D=1.8348$.

We calculate the full stress field in the structure 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. The resulting value of k is plotted in Fig. 2 as a function of the aspect ratio of the stripe. The trend in this figure is readily understood. Although the stress field intensifies at the root, the side surface of the stripe is traction-free. When the stripe is very narrow, $L/h \to 0$, the stress in the stripe is almost fully relaxed, and $k \to 0$. When the stripe is very wide, $L/h \to \infty$, the stress field near one edge of the stripe no longer feels the presence of the other edge, and k attains a plateau.

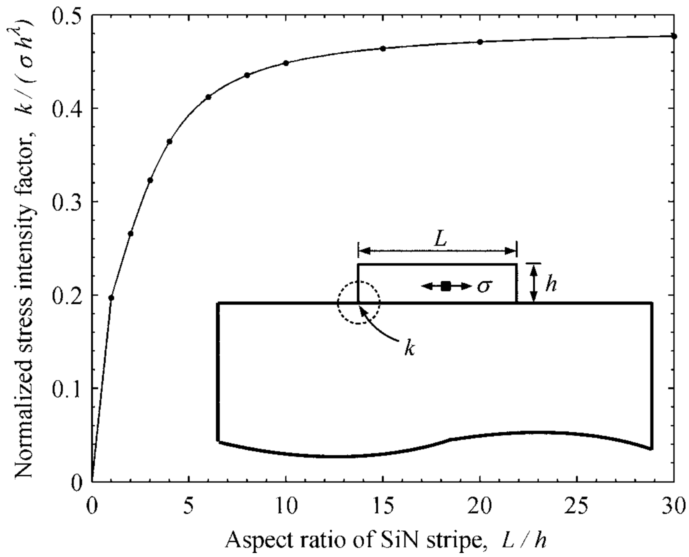

FIG. 2. Normalized stress intensity factor, $k/(\sigma h^{\lambda})$, calculated using a finite element method, is shown as a function of the aspect ratio, L/h, of the nitride stripe.

Upon setting $k=k_c$ in Eq. (2), we note that the critical condition for the root to emit dislocations depends on the residue stress σ and the feature sizes h and L. For a given deposition process, the magnitude of the residual stress in the blanket film σ is fixed. According to Eq. (2), it is more likely for the root to emit dislocations when the stripe is thicker and wider.

Emitting a dislocation is a thermally activated atomic process, an analysis of which is beyond the scope of this letter. A crude estimate of k_c, however, can be made by letting the resolved shear stress τ_{nb} at distance $r=b$, calculated from Eq. (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 12 slip systems in Fig. 1, the two systems $1/2(111)[01\bar{1}]$ and $1/2(111)[10\bar{1}]$ are found to have the largest resolved shear stress, given by

$$\tau_{nb}(r) = \frac{k}{(2\pi r)^{\lambda}}\Sigma_{r\theta}(\theta)\cos 30^{\circ}. \tag{4}$$

For the (111) plane, $\theta=-125.27°$, giving $\Sigma_{r\theta}=-1.0317$.

The theoretical shear strength can be estimated by $\tau_{th}=0.2\mu$, where μ is the shear modulus of silicon.[18] Setting $|\tau_{nb}(b)|=\tau_{th}$, we obtain that an estimate of the critical stress intensity factor,

$$k_c = 0.5\mu b^{\lambda}. \tag{5}$$

We may as well view Eq. (5) as a result of a dimensional analysis, leaving the prefactor adjustable by any specific atomic process of emitting a dislocation.

A combination of Eqs. (2) and (5) gives a scaling relation between the critical stress and the feature sizes,

$$\sigma_c = \frac{0.5\mu}{f(L/h)}\left(\frac{b}{h}\right)^{\lambda}. \tag{6}$$

From Fig. 2, when the aspect ratio of the Si_3N_4 stripe varies from 1 to ∞, the function $f(L/h)$ varies in the range $f=0.2\sim0.48$. Taking $\mu=68.1$ GPa, $b=3.83$ Å, and $h=1$ μm, the critical residue stress varies in the range $\sigma_c=4.9\sim2.03$ GPa. If $h=100$ nm, however, the critical stress varies in the range $\sigma_c=13.8\sim5.75$ GPa.

In an experiment by Kammler *et al.*,[4] a Si_3N_4 film, of thickness of 500 nm and residual stress of 6 GPa, was grown on a silicon substrate, and was then patterned into large $(10\times10\ \mu m^2)$ and small $(1\times1\ \mu m^2)$ square pads. Kammler *et al.* showed that dislocations emitted from the large pads, but not from the small ones. According to our Eq. (6), the critical stresses for the two cases are 2.8 and 5.0 GPa, respectively.

Isomae[7] reported that dislocations emitted from the edges of a 3×3 mm^2 Si_3N_4 pads of thickness of 200 nm under residual stress of 0.92 GPa. The critical residual stress predicted from Eq. (6) is 4.2 GPa. Isomae also observed that dislocations injected into the region of the substrate not covered by the pad, and noted that this observation was inconsistent with the concentrated-force model, which predicted that dislocations were equally likely to be emitted on both (111) and $(\bar{1}\bar{1}1)$ planes. We note that this experimental observation is consistent with the analysis our model. Indeed, according to Eq. (3c), the shear stress on the $(\bar{1}\bar{1}1)$ plane is only 0.26 times that on the (111) plane.

Our 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[19] and others. We also note two effects that can act in opposite directions: thermal activation will decrease the value of k_c, while blunt edge roots will increase the value of k_c.

We should also remark that, given the uncertainty in the sharpness of the edge root in an actual structure, the value of k_c may have a statistical distribution. One may as well forego the unreliable theoretical estimate of k_c, and simply use the experiments, such as those described above, as a means to determine the value of k_c and its statistical distribution. The approach is analogous to that of experimental determination of fracture toughness.[13] Once the statistical distribution of k_c is determined by using samples of one set of σ, h, and L, one can predict the statistical distribution of critical values of σ, h, and L by using Eq. (2). The procedure is analogous to a procedure to evaluate failure statistics of interconnects due to electromigration.[20]

In summary, we have described a method to analyze dislocations emission from sharp features in strained silicon structures. The method predicts the correct orders of magnitude of the critical stress, and gives a scaling relation between the stress level and feature sizes. These predictions call for more systematic comparison between the theory and experiments. Our approach can be applied to other crystallographic orientations, material combinations, and sharp features. The estimate of k_c may be improved significantly. The approach may ultimately contribute to the design of strained silicon devices.

This work is carried out when the authors are supported by Intel Corporation through a contract via the Semiconductor Research Corporation (Award No. 2005-KJ-1369) and by the National Science Foundation through the MRSEC at Harvard University. One of the author (J.Y.) acknowledges the support of a postdoctoral fellowship from the Canadian Government.

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