

The Effect of Trench Corner Shapes on Local Stress Fields: A Three-Dimensional Finite-Element Modeling Study

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Abstract—Local stress fields associated with deep trench structures are modeled in three dimensions utilizing a finite-element method. A model consisting of a SiO₂-filled deep trench residing in a silicon substrate is utilized and stress is generated by differential thermal contraction. It is shown that corner regions, especially convex, “outside” corners dramatically enhance the elastic energy density and shear stresses locally compared to non-corner regions. The effects of the specific corner geometry on these local stress fields is then investigated and it is shown that subtle geometric changes can yield substantial decreases in the magnitude and lateral extent of the fields.

I. INTRODUCTION

THE pursuit for increased density in Si-based integrated circuits has led to the development of three-dimensional structures residing in or on the Si substrate. One such example is commonly referred to as “trench technology,” and involves anisotropic etching of patterns into the substrate to form trenches and subsequently filling them with a material which is, in general, different from the substrate. Trenches formed in this manner are used as storage capacitors in dynamic memory (DRAM) technologies [1], as well as isolation structures in CMOS, bipolar, and BiCMOS technologies. [2]–[4]. In addition to increasing density, trench structures can also lead to modest gains in circuit performance through the reduction in area-related parasitics.

While advantageous from a density perspective, trench structures have been shown to be a major contributing factor in the substrate defect generation during routine processing steps required for device/circuit fabrication [5], [6]. The sources of trench-related stress can be broadly categorized as follows: 1) intrinsic stress in the trench-fill material, 2) differential thermal expansion/contraction between the substrate and the trench-fill material, and 3) oxidation-induced stress generated by thermal oxidations after the trenches have been filled. The sources of stress can be minimized by optimizing processing con-

ditions (particularly oxidation, deposition, and annealing conditions) and a growing body of literature is devoted to this subject [5]–[9]. Very recently, local stress fields associated with isolation trenches subjected to realistic device processing conditions were analyzed (including visco-elastic behavior in SiO₂ regions, intrinsic film stresses, and thermal expansion mismatch); however, due to the extremely complex nature of the problem, the analysis was carried out in two dimensions: thus investigations into geometric subtleties (such as corner shapes) were not possible [10].

While processing details determine the exact “load” applied to the substrate along a long portion of trench, the geometry of the trench determines the local stress enhancement in regions such as corners or terminations. Experimental studies have shown that for identical processes, subtly different structures can show relatively large differences in their defect susceptibility [6] and our experience indicates that the specific geometry of trench corners is an especially important factor in processing-induced defect generation. In this work, a detailed three-dimensional analysis is performed for a conventional 90° corner to clarify the problems associated with such structures. We then examine the effects of modified corner geometries on the various stress fields for a fixed applied load.

Trench structures are pervasive in today’s semiconductor technologies; however, in the present work the bipolar isolation trench is examined in detail. A bipolar isolation trench is relatively deep (~5 μm) and provides collector-collector isolation between adjacent devices [3], [4]. To minimize parasitic capacitances, a low dielectric constant trench-fill material is desired and doped glasses [11] or pure SiO₂ [12] are being explored for this application. The present study concentrates on stress generated by differential thermal contraction between a Si substrate and a SiO₂-filled isolation trench as the temperature is decreased by 950°C. Stresses generated in this fashion are representative of the maximum thermal stress associated with a SiO₂-filled trench when cooled following a high-temperature annealing step. Due to the visco-elastic nature of SiO₂ [13], this is expected to be the case even if the annealing temperature is in excess of 950°C. Since the thermal expansion coefficient of SiO₂ is less than that

Manuscript received February 2, 1992; revised September 4, 1992. The review of this paper was arranged by Associate Editor Y. Nishi.

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IEEE Log Number 9206104.

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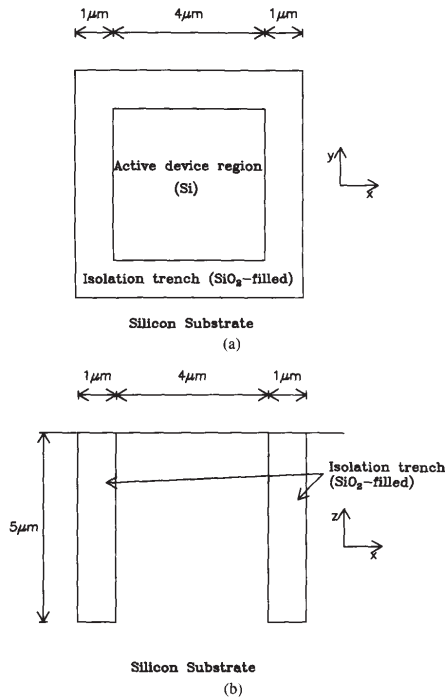


Fig. 1. (a) A top view and (b) cross-sectional view of the base-case structure.

of Si, the trench-fill material becomes relatively too large for the trench as the structure cools. Other relevant loading conditions, including the trench-fill material only expanding (relatively) in directions normal to the trench sidewalls, as well as a nonuniform trench sidewall load (decreasing with increasing distance from the surface) were also examined¹, however, all geometric trends were identical to the case of differential thermal contraction and discussion will be limited to this case.

In their simplest form, bipolar isolation trench patterns are rectangular or square when viewed from above and the active device is fabricated in the interior of the trench; however, more complex patterns are often utilized in cell structures [14]. The structure considered here is a 1-μm-wide, 5-μm-deep trench residing in a Si substrate. The trench is assumed to be far from other similar structures and hence the effects of other structures on the stress fields are not considered; however, an extension of this analysis to the problem of periodic structures is straightforward [15]. When viewed from above, the trench surrounds a 4 μm × 4 μm active device region and the dimensions of the structure were chosen to be representative of an isolation trench for a discrete device in a 0.5-μm bipolar

¹These loading conditions may be appropriate for oxidation-induced stresses [8].

technology [16]. Diagrams of the structure under consideration are shown in Fig. 1.

In the following, a brief review of elasticity and the stress tensor is presented. Then, modeled results for a conventional 90° corner are presented and the various problems associated with corners are highlighted. This geometry will be referred to as the base case. The effects of corner geometry on the lateral extent and magnitude of the various local stress fields are then examined. Corner geometries were systematically altered by beveling the outside corner with a 45° cut by various fractions of the trench width. It was found that an optimum amount of corner beveling exists and that subtle geometric modifications can have marked effects on the intensity and lateral extent of local stress fields.

II. A REVIEW OF ELASTICITY, THE STRESS TENSOR, AND PLASTIC DEFORMATION

While an exhaustive review of this subject is outside the scope of this work, the interested reader is referred to one of the classic texts devoted to this subject [17], [18]. The reader is also referred to Hu's recent review for a discussion on common conceptions and misconceptions about the stress tensor [7]. A very brief summary follows.

Under the action of external forces, a body will deform giving rise to internal forces or stresses (stresses are forces per unit area) as a result of the cohesive forces acting to hold the material together. For small strains, the deformation process is reversible and the deformations vanish when the load is removed. This is referred to as linear elasticity and is valid for applied loads below the yield strength or elastic limit of the material. While the elastic limit is rather easily defined for simple (one-dimensional) loading conditions, it is a more elusive quantity when complex, three-dimensional loads are applied.

For a three-dimensional body under a general load, the stress is described by a tensor, the stress tensor, which contains nine elements describing tractions and shears on the faces of a differential element of the body. The stress and strain tensors are related by the stiffness or compliance matrices which describe the elastic properties of the material as a function of direction. The case where the elastic properties are assumed to be independent of direction is referred to as isotropic elasticity. The present work assumes linear, isotropic elasticity using the bulk parameters given in Table I.

Since the stress state of a three-dimensional body is given by the position-dependent tensor, lumped-parameters combining all, or some, of the tensor elements are generally used to characterize the deformation (elastic or plastic). In many polycrystalline and amorphous materials, the Von Mises stress has been shown to accurately describe departures from linearity. The Von Mises stress is a measure of the magnitude of the off-diagonal (or shear) elements of the stress tensor, and more specifically, is the maximum magnitude of a shear element attainable by rotation of a coordinate system [7]. In single-crystal mate-

TABLE I
MATERIALS PARAMETERS

Material	Elastic Modulus (dynes/cm ²)	Poisson's Ratio	Thermal Expansion Coefficient (/°C)
SiO ₂	0.7×10^{12}	0.17	0.5×10^{-6}
Si	1.3×10^{12}	0.28	2.6×10^{-6}

materials that contain dislocations, plastic deformation is accomplished by dislocation propagation and multiplication which is governed by the resolved shear stresses in specific slip systems. However, in a dislocation-free single-crystal material (such as a Si substrate), dislocation nucleation must precede plastic deformation. It is expected that the details of the dislocation nucleation problem are a convolution of the local elastic or strain energy density and crystallography, much like the crystal thickness phenomena in heteroepitaxial systems [19]. Simply stated, dislocations will not nucleate unless the process acts to lower the total energy of the system which, in turn, depends on the magnitude and lateral extent of the strain energy field as well as its orientation with respect to the crystal. In addition, the local pressure may be an important parameter controlling the kinetics of defect nucleation since point defect fluxes are driven by pressure gradients [7] and dislocations nucleate via condensation of intrinsic point defects [6], [20]. In this usage, pressure is defined as the negative of the average of the diagonal members of the tensor and indicates whether the local atomic density in the substrate is greater (positive pressure) or lesser (negative pressure) than in the unstrained condition.

In the present work, Von Mises stress, elastic energy density, and local pressure are utilized to describe the stress state in the substrate for the base case. It is believed that this combination of parameters is especially effective in presenting the stress analysis since the Von Mises stress describes the off-diagonal elements of tensor, while the pressure describes the diagonal elements and the elastic energy density describes the energy stored in the crystal as a result of the deformation associated with the entire tensor.

III. THE BASE CASE—A 90° CORNER

A. The Model

A perspective view of the modeled structure for the base case geometry is shown in Fig. 2. For computational efficiency, symmetric boundary conditions were utilized and hence only one quarter of the structure shown in Fig. 1 was considered. Stress analysis was performed with a three dimensional, finite-element approach using ABAQUS [21] and special care was taken to specifically elucidate behavior near the corner regions. The initial condition was a SiO₂-filled isolation trench residing in a silicon substrate with no stresses present. Stresses are generated in the structure by differential thermal contrac-

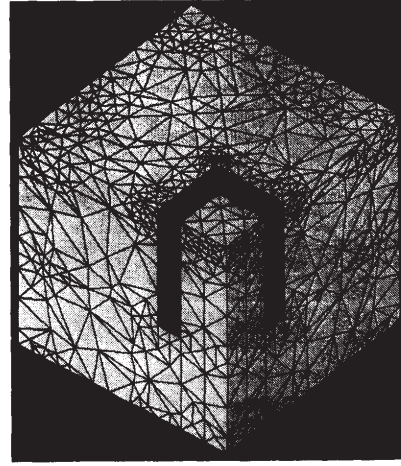


Fig. 2. The modeled structure for the base-case geometry. The model contains ~16 000 elements which is typical for all geometries investigated in the present work.

tion as the temperature is reduced by 950°C and the final (steady-state) stresses associated with this thermal excursion are presented. It was observed that the largest stresses and stress gradients are present in the near-surface region of the structure and particularly in the vicinity of the corner and hence finer meshes were utilized in these regions, as is apparent in Fig. 2. To balance the accuracy of the calculation with computing limitations, numerous simulations were performed to ascertain the effect of the element size (mesh generation parameters) on the resultant calculations. The size of the elements was decreased by a factor of two until further reductions in size yielded only differences of ~2% in the calculated stresses. Simulations were also performed to ascertain the effects of the "substrate" size on the resultant calculations and it was found that as long as the modeled structure was several times larger than the trench structure, the results were constant and in all of the following a volume of $9 \mu\text{m} \times 9 \mu\text{m} \times 9 \mu\text{m}$ was simulated. The model shown in Fig. 2 contains ~16 000 elements which is typical for all structures considered in the present work. On the outer boundaries of the structure, free surface boundary conditions are utilized, consistent with an isolated structure. In addition, the position of a single point of the structure is fixed to prevent rigid body motion (which would not contribute to the stress fields).

B. Results

Fig. 3(a) and (b) shows the Von Mises stress and elastic energy density, respectively, as a result of the thermal excursion outlined previously. Note the qualitative similarity of the figures. In both cases, the most intense part of the field is located at the surface of the substrate at the corner of the trench pattern. It should be noted that this

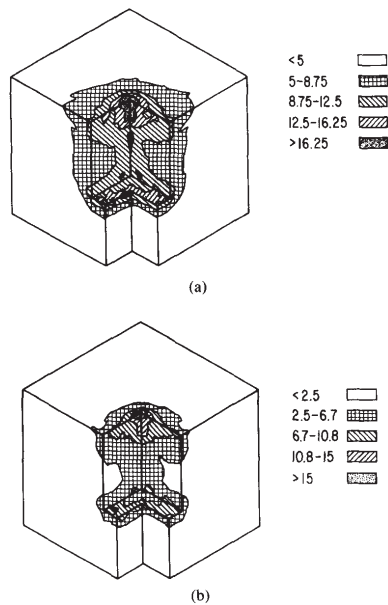


Fig. 3. (a) The Von Mises stress and (b) the elastic energy density resulting from the temperature excursion discussed in the text. These views are analogous to Fig. 2; however, the active device region and trench-fill material have been removed revealing the field contours on the trench sidewall and exterior surfaces. Note the maximum intensity in both fields occurs in the corner region at the substrate surface. Contour values are given in units of 10^8 dynes/cm² for the Von Mises stress and in units of 10^5 dynes/cm² for the elastic energy density.

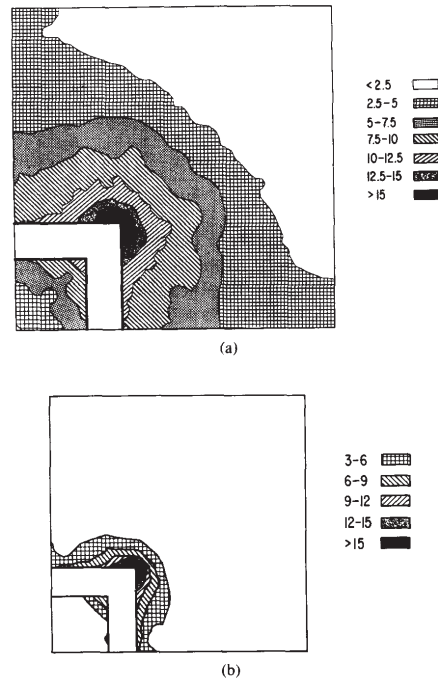


Fig. 4. (a) The Von Mises stress and (b) the elastic energy density on the substrate surface resulting from the temperature excursion discussed in the text. The trench-fill material has been removed for clarity. Contour values are given in units of 10^8 dynes/cm² for the Von Mises stress and in units of 10^5 dynes/cm² for the elastic energy density.

same behavior is noted for the resolved shear stresses in various diamond-cubic slip systems. The magnitude of the fields along the trench sidewalls decreases as the distance from the surface increases and remains nearly constant in the middle region of the trench. The intensity of the fields again increases along the bottom of the trench reaching levels comparable to those at the corner in the near-surface region. The figure also clearly illustrates the value of the three-dimensional analysis. A two-dimensional analysis in the xy plane is equivalent to simulating a thin slice of an infinitely deep trench and hence, the large magnitudes observed in the near-surface regions would not be apparent. On the other hand, if a two-dimensional analysis were carried out in the xz or yz planes, it would not be possible to consider a corner and the associated stress enhancements. Thus a full three-dimensional analysis is required to capture the full flavor of this problem.

Fig. 4(a) and (b) shows the Von Mises stress and the elastic energy density, respectively, at the substrate surface. Again, the Von Mises stress and elastic energy fields are qualitatively similar reaching a maximum value at the outside, convex corner. It should also be noted that the magnitude of the fields in the inside, concave corner of the trench are slightly higher than those present along the straight portion removed from the corner region.

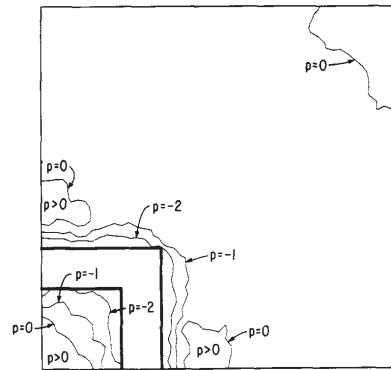


Fig. 5. The local pressure on the substrate surface resulting from the temperature excursion described in the text. Note the differences between this figure and Fig. 4(a) and (b). Also note the qualitatively different behavior in the corner region from the noncorner region. Contour values are given in units of 10^8 dynes/cm².

Fig. 5 shows the pressure present at the substrate surface as a result of the trench-related load. It is obvious that this figure is qualitatively different than Fig. 4(a) and (b) and indeed, shows much more complex behavior.

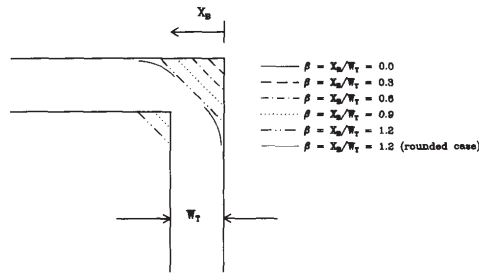


Fig. 6. The various corner geometries examined in the present work. The fine, unbroken line illustrates the "rounded corner" geometry examined for the $\beta = 1.2$ case.

Along the outer surface of the trench, minimum pressures are located along the trench sidewall and, in general, the pressure increases with increasing distance from the trench sidewall. However, note the qualitatively different behavior between the corner and non-corner regions. In the non-corner regions the pressure reaches a local maximum a short distance from the trench and falls with further increasing distance. This behavior is not apparent in the corner region. Whether the pressure gradients present in close proximity to the trench sidewalls are sufficient to bias point defect migration, and hence effect dislocation nucleation, is not clear. While a wealth of information exists in the literature on diffusion processes in the Group IV semiconductors [22], [23], we are unaware of investigations into the pressure/stress dependencies for self-diffusion in these materials. In any case, the pressure contours are intensely interesting and attest to the many non-intuitive features of the problem under consideration.

IV. MODIFIED CORNER GEOMETRIES

The multitude of problems associated with outside, convex-corner regions has now been clarified and we now ask the question whether the corner geometry can be altered in some technologically meaningful fashion to reduce the magnitude and lateral extent of the various stress fields in this region. Corner geometries were systematically altered by beveling the outside corner with a 45° cut by various fractions of the trench width and the geometries considered are shown in Fig. 6. Corner beveling is characterized by the dimensionless parameter $\beta = X_B / W_T$, where X_B is the distance beveled and W_T is the width of the trench, as shown in Fig. 6. Simulations were performed for $0.0 \leq \beta \leq 1.2$ and in cases where the beveling reduced the trench width at the corner to less than the nominal width ($\beta > 0.6$) the inside corner was also beveled to maintain the nominal width across the corner, consistent with process constraints. Note that for $\beta \leq 0.6$, the dimensions of the active device regions are unchanged, and hence a redesign of this region would not be required; however, this is not the case for greater values of β .

Fig. 7(a)–(d) shows the elastic energy density at the

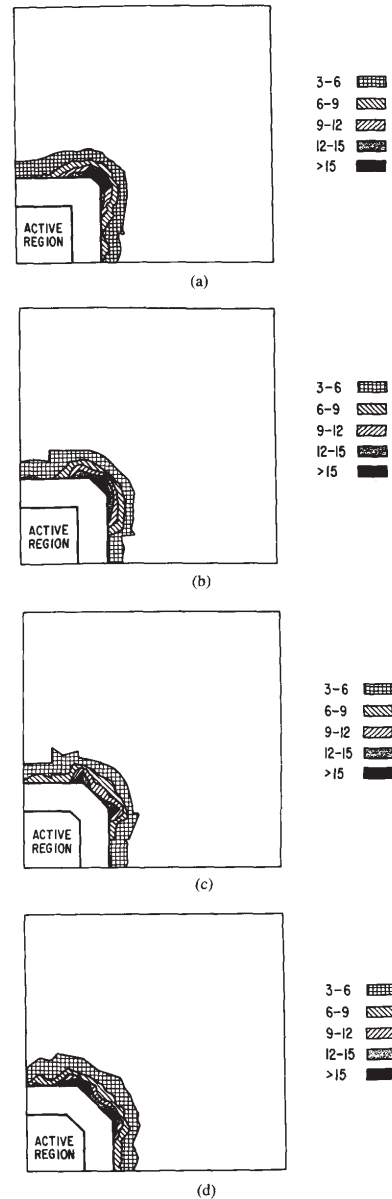


Fig. 7. The elastic energy density present at the substrate surface for the various corner geometries: (a) $\beta = 0.3$, (b) $\beta = 0.6$, (c) $\beta = 0.9$, (d) $\beta = 1.2$. The $\beta = 0.0$ case is shown in Fig. 4(b). Note the qualitative change in behavior as β increases from 0.6 to 0.9. Contour values are given in units of 10^5 dynes/cm².

substrate surface as β is increased from 0.3 to 1.2 in increments of 0.3. The $\beta = 0.0$ case is shown in Fig. 4(b). The $\beta = 0.3$ case is quite similar to the base case; how-

ever, the most intense part of the elastic energy field is actually slightly larger. As β is increased to 0.6, a clear reduction in the lateral extent of the most intense portion of the strain energy field is noted compared to $\beta = 0.0$ or 0.3 with the maximum intensity occurring at the same relative position. As β is increased to 0.9, the most intense part of the field actually moves away from the original corner and two symmetric "hot spots" are noted at the 45° corner regions. As β is further increased to 1.2, the results are qualitatively similar to the $\beta = 0.9$ case, except the lateral extent of the hot-spots is greater. The qualitatively different nature of the elastic energy fields for the $\beta = 0.6$ and 0.9 cases suggests that some optimum amount of corner beveling exists between these two values.

Finally, due to corner rounding normally associated with lithographic printing, the precise trench patterns studied here would be practically unachievable. However, simulations were performed to ascertain the effects of corner rounding on the resultant stress fields. It was found that if a constant radius of curvature equal to the trench width was utilized to round the corners for the $\beta = 0.6, 0.9$, and 1.2 cases, the same geometric trends were observed—that is, a single "hot spot" is present for low values of β while two are present for larger values. A diagram of the simulated structure for the $\beta = 1.2$ case with rounded corners is shown in Fig. 6. Another possibility would be to round the corner such that a simple circular arc exists between the two straight portions of the trench. In this case, the magnitude of the stress fields are reduced as the radius of curvature of the corner increases, as intuitively expected. While effective from a stress reduction perspective, corners with a large radii of curvature are quite costly from a density perspective as they severely limit the packing density of the individual transistors.

V. CONCLUSIONS

In conclusion, a three-dimensional finite-element analysis was performed to elucidate the various stress fields associated with deep-trench structures. In all cases, stress was generated by differential thermal contraction between the SiO_2 -filled trench and the surrounding Si substrate as the temperature was reduced by 950°C . It was observed that the highest elastic energy density and shear stresses are present at outside, convex corners of the trench pattern making these regions especially dangerous from a defect nucleation and propagation perspective. The magnitude of these fields is also greater in inside, concave-corner regions than along long, straight portions of the trench. Various corner geometries were examined to ascertain the effect of corner shape on the resultant stress fields. It was found that the nature of the stress fields changes from having a single "hot spot" for amounts of corner beveling ($\beta \leq 0.6$) to having two separate "hot spots" for larger amounts of beveling ($\beta \geq 0.9$). Beveling by $\beta = 0.6$ yields beneficial effects from a stress per-

spective and does not require redesign of subsequent lithographic levels required for device/circuit fabrication.

Finally, the present study has only considered one aspect in the complex problem of processing-induced defect generation associated with deep-trench structures—the trench geometry. Clearly, many other factors are also extremely important—namely, the actual processing conditions used in device/circuit fabrication. Detailed process modeling [10] in conjunction with geometric modeling of the present sort should allow the design of structures and processes which minimize the risk of dislocation generation, and increasingly important consideration in the fabrication of high-density integrated circuits.

ACKNOWLEDGMENT

The authors wish to acknowledge the technical assistance of A. Kalbag as well as the support of Dr. Y. C. Sun and Dr. V. Srinivasan.

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