FRACTURE PREDICTION OF SINGLE CRYSTAL SILICON MEMS UNDER MULTI-AXIAL LOADING

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ABSTRACT

We describe and validate a new failure prediction methodology specifically designed for single-crystal MEMS devices under general service loadings. The methodology uses experimental data efficiently generated from fracture testing of simple test specimens to calculate a series of Weibull parameters descriptive of specific surface conditions. These data, combined with finite element modeling, are used to predict the fracture load distribution for any MEMS device fabricated by the same process, under any type of loading. We demonstrate the accuracy of our method by comparing predicted fracture probabilities against actual fracture test results for a micro-mirror in two distinct multi-axial loading configurations.

INTRODUCTION

The reliability of a MEMS design, even with state-of-the-art simulation tools, can only be determined through destructive tests on finished devices. Determination of reliability therefore occurs very late in the development cycle, after significant time and funds have already been expended. This predicament occurs because traditional finite element (FE) simulations are incapable of calculating failure predictions for MEMS devices, due to the nature of the brittle materials from which they are made.

Brittle materials fail when the applied stress at a critically-sized flaw exceeds the fracture toughness of the material. If every flaw in and on a MEMS device could be measured and mapped, the principles of fracture mechanics would allow for a deterministic calculation of the fracture strength. However, while such a metrology-oriented approach is theoretically possible using tools such as Scanning Electron Microscopy (SEM) or Atomic Force Microscopy (AFM), from a practical standpoint it would be prohibitively time-consuming and expensive.

Statistical characterization of flaw populations provides a practical solution for brittle structure analysis. The material volume in a single-crystal silicon MEMS structure is, conveniently, essentially flaw-free due to the high purity and crystallinity of the silicon wafer. The etch processing used to machine silicon, by its nature, creates significant surface flaws, and the remaining flaw shapes and sizes are sensitive to process recipe [1,2]. Test-driven, statistical characterization of the process-specific surface flaw distributions is therefore a cornerstone of this prediction method.

Our methodology employs FE simulation, calibrated by experimental data, to predict fracture in MEMS devices under service conditions. First, simple four-point bend test specimens are used to generate fracture stress distribution data descriptive of the specific etch processes used to manufacture the MEMS device under study [3]. Next, a computational model of the MEMS device is created using commercial FE software. Our algorithm then merges the experimental data and the FE model results to calculate the fracture probability of the device under a range of given applied loads.

Although other researchers have explored similar methods, all previous studies are limited to fracture prediction of beams in uniaxial stress [4-6]. We believe this is the first demonstration of accurate fracture prediction for a MEMS device with realistically complex geometries, loadings, and stress fields. As an additional

benefit, our approach does not require time-consuming fractographic inspection or modeling of individual test specimens to generate accurate results.

METHODOLOGY

Our method assumes that fracture initiation in single-crystal MEMS devices depends only on the following: (i) the condition of the device surface areas, and (ii) the stress distributions on those areas. These assumptions are well supported in the literature [1,7]. While applied stresses can be calculated in a straightforward manner using FE, a quantitative description of the surface conditions is more challenging.

Weibull Statistics

The only practical approach to characterizing the surface conditions is to use a statistical description. We use the Weibull probability function to describe the fracture stress distribution of a population of test specimens fabricated by a specific process, which in turn provides a relevant, quantitative description of the surface characteristics of that process [2,8].

The Weibull probability density function is commonly employed to characterize failure in brittle materials at the macro- and micro-scales, for both single-crystal and polycrystalline materials [4,9]. A two-parameter Weibull fit to a sample population of fracture stresses provides a characteristic strength, σ_0 , defined as the stress at which 63.2% of the specimens fail, and the Weibull modulus, m , which describes the scatter in the distribution (lower values of m correspond to greater scatter.) Independent Weibull parameters are required to describe each different type of surface condition present in a MEMS device to be analyzed, including the polished surface of the wafer.

Four-Point Bend Beam

Test specimens are required to determine the Weibull parameters that characterize the various surface conditions. Although any type of test specimen geometry may be used, the four-point bend beam has a simple geometry and loading which is particularly advantageous. In this type of test specimen, the maximum stress develops uniformly on the surface of the beam within a well-defined area [3]. As a result, the fracture stress, σ_f , is calculated analytically according to Eqn. (1).

$$\sigma_f = 3PL/4bd^2 \quad (1)$$

Where P is the applied load at fracture, L is the support span, b is the width of the beam, and d is the beam depth.

In order to generalize the Weibull parameters to multi-axial loading conditions, a reference area from the test specimen, A_0 , is required. The reference area is defined as the entire area upon which the maximum stress (and therefore the fracture stress) develops and by definition includes the region in which the fracture initiates. The reference area is used to area-normalize the test specimen results and allow their application to MEMS devices with more complex geometries.

In the four-point bend beam, the parameter A_0 is simply the product of the distance between the inner two load points and the

width of the beam, b .

The use of a four-point bend beam eliminates the need for FE analysis to calculate maximum stresses and reference areas, which complicated previous analyses of cantilever specimens [10], and for detailed inspection of every sample to determine the location of fracture initiation [11]. The elegance of the four-point bend beam simplifies gathering experimental data and enables cost-effective surface characterization.

Probability Calculation

Once the surfaces of the test specimens have been characterized, a FE model of the MEMS device to be analyzed is constructed. To capture the mechanical response of the device, orthotropic material properties are defined for the silicon volume. In cases where solution speed is critical, such as parametric design optimization, isotropic material properties for silicon may be substituted. This assumption leads to an error in the stress distribution of approximately 3% or less [1].

Standard FE modeling practice is used to calculate the stress distribution in the entire MEMS device under service loading. After solution, the first, second and third principal stresses (S_1 , S_2 , S_3) are readily available at each surface node of the entire device. The tensile principal stresses ($\hat{S}_1$, $\hat{S}_2$, $\hat{S}_3$) at each node of interest are then calculated according to Eqn. (2). As is common in the reliability analysis of brittle materials, compressive stresses are ignored [12,13].

$$\hat{S}_i = \begin{cases} S_i & \text{if } S_i \geq 0, \text{ for } i=1,2,3 \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

To facilitate further discussion, it is necessary to define some terms. First, let $ntype$ be the total number of surface types associated with a particular MEMS device to be analyzed, where $k = 1$ to $ntype$. Hence, the analysis requires $ntype$ sets of Weibull parameters (σ_{0k} , m_k , A_{0k}). Next, let $narea$ be the total number of areas associated with a particular surface type (specific etch), where $j = 1$ to $narea$. Finally, let $nnode$ be the total number of nodes associated with a single surface area, where $i = 1$ to $nnode$. The value of $nnode$ will vary from area to area, according to the size of the area and the density of the FE mesh.

To continue, the scalar failure probability per unit area, ψ_i , at each surface node, is calculated from the tensile principal stresses using an isotropic failure probability function as shown in Eqn. (3) [1,12,13]. Although the fracture toughness, K_{IC} , varies with crystal axis orientation, the difference is small, and thus the use of an isotropic failure probability function is justified for single-crystal silicon [1].

$$\psi_i = \frac{1}{A_{0k}} \left[\left(\frac{\hat{S}_1}{\sigma_{0k}} \right)^{m_k} + \left(\frac{\hat{S}_2}{\sigma_{0k}} \right)^{m_k} + \left(\frac{\hat{S}_3}{\sigma_{0k}} \right)^{m_k} \right] \quad (3)$$

Once the nodal values of the failure probabilities are determined per unit area, these values are multiplied by the total area contribution per node, ΔA , the area increment. This yields the scalar failure probability, f_i , at each surface node, as shown in Eqn. (4).

$$f_i = \psi_i \Delta A_i \quad (4)$$

Next, the total probability of failure for the device under

service conditions, P_s , is estimated as shown in Eqn. (5).

$$P_s(A) = \exp \left[- \int_A \psi dA \right] \approx \exp \left[- \sum_{k=1}^{ntype} \sum_{j=1}^{narea} \left[\sum_{i=1}^{nnode} \psi_i \Delta A_i \right]_{j,k} \right] \quad (5)$$

Finally, the total device survivability, or reliability, R , is related to the total failure probability as shown in Eqn. (6).

$$R = 1 - P_s \quad (6)$$

VERIFICATION EXPERIMENT

We demonstrate our methodology and its accuracy by predicting the reliability of a representative MEMS device. A doubly-suspended MEMS micro-mirror was chosen because it can be loaded in two distinct states, tension and torsion, that produce different complex stress fields in the device.

Following the outlined methodology, four-point bend beam specimens were fabricated and fractured to gather data for both the polished and etched surfaces of the beam, thereby capturing the specific surface conditions that would be present on the micro-mirror. The data were used to make a prediction of the fracture load distributions for the micro-mirror in both load states. Finally, we fractured actual micro-mirror samples in both tension and torsion in order to verify the accuracy of our predictions.

Specimen Fabrication

Test specimen four-point bend beams and micro-mirrors were fabricated using oxidized, double-polished (100)-orientation silicon wafers (310 μm thickness) as a starting material. The specimen patterns were defined in a single contact lithography step, followed by a plasma etch to remove oxide in the areas to be trenched (the remaining field oxide served as a hard mask during the long silicon etch). Next, a Surface Technology Systems (STS) Multiplex ICP etcher was used to deep reactive ion etch entirely through the silicon wafer to define the specimens. The oxide was stripped in buffered oxide etch, and the wafer was sawed to separate the individual specimens. Special precautions were taken during sawing to protect the etched sidewalls from damage.

The four-point bend beams used to calibrate the micro-mirror analysis were designed to fracture in a load range that was easily measured using a macro-scale apparatus. Handling lugs at each end of the beam prevent accidental contact with the etched surface areas (and hence possible damage) during specimen handling, and also facilitate alignment in the test fixture (Fig. 1).

Figure 1: The silicon four-point bend test specimen used for calibration (length = 11.7 mm, width = 300 μm , height = 310 μm , gage length = 8 mm).

The silicon micro-mirrors used to verify the prediction methodology were designed with a support frame which facilitated handling and clamping in the test fixture (Fig. 2). Two alignment holes in the frame allow the sample to be accurately positioned via locating pins in the test fixture.

Figure 2: The silicon micro-mirror used for verification (the mirror: 8 x 8 mm, and the flexures: length = 2 mm, width = 300 μ m, height = 310 μ m).

Test Apparatus

A specially designed load fixture was installed on an Instron® 5542 mechanical tester. The fixture was designed specifically to accurately locate the samples, to allow easy placement and removal of the samples, and to remove any mechanical play in the tester and load cell (Fig. 3). Careful design of the test fixture allowed for repeatable and efficient collection of the necessary fracture data. All loads were measured using a Transducer Techniques GS0-1K (10N) piezoresistive load cell. The Instron® was operated under load control and all specimens were loaded at a rate of 300 μ m/min until fracture.

Figure 3: Schematic of loading apparatus and specimen fixtures. Top: Four-point bend fixture. The four-point support design was based on ASTM D-6272-02. Bottom: Fixture plate for edge-loading of micro-mirror. The silicon specimens are in orange.

Four-Point Bend Beam Calibration Data

Two groups of test specimen beams ($N = 50$ for each group) were created by randomly sampling twenty-five beams from each of two wafers. One group of beams was loaded in four-point bend to fracture with the polished surface in tension, while the second group was loaded with the etched surface in tension. The fracture stress of each beam was calculated from the fracture load, according to Eqn. (1). A two-parameter Weibull fit was used to characterize the fracture stress distribution of each set of beams, and hence $n_{type} = 2$, due to the two types of surfaces (Fig. 4).

As shown in Fig. 4, the polished surface of the beam has a characteristic strength of 636 MPa, which is 15% greater than the

etched surface characteristic strength of 555 MPa. These data provide an illustration of the sensitivity of fracture strength to surface condition.

Figure 4: Probability plot of fracture stress data from test specimens ($Shape = m$, $Scale = \sigma_0$).

Reliability Prediction

Following the outlined methodology, a FE model of the MEMS micro-mirror was created in ANSYS® Multiphysics v. 11.0 (Fig. 5). The model employs half-symmetry and a varying mesh density (highest in anticipated high stress-gradient areas) to reduce computational cost. Displacement boundary conditions are applied to the model such that the range of reaction forces in the loading direction spanned the experimentally-measured applied load.

Figure 5: Finite element half-symmetry model of the MEMS micro-mirror constructed in ANSYS®.

Equations (2)-(6) were implemented in a numerical algorithm scripted in APDL, the ANSYS® scripting language. The experimentally-determined Weibull parameters from the two groups of test beams (polish and etch surfaces) were used to predict the micro-mirror failure probabilities under a range of loads in both center (tension) and edge (torsion) loading configurations.

MEMS Micro-Mirror Verification Data

Two groups of micro-mirrors were created by random sampling from two wafers. Employing the same test apparatus, one group of mirrors was loaded in the center, to create a tension load/stress distribution in the flexure ($N = 20$). The second test group was loaded at the edge of the mirror, thus generating a torsion load/stress distribution in the flexure ($N = 18$). The micro-mirrors were loaded to failure under load control. The reliability

data from this testing were compared to the results of the reliability prediction.

RESULTS AND DISCUSSION

The predicted and experimental failure probabilities (versus applied load) matched with reasonable accuracy (Figs. 6 and 7). The difference in characteristic load (defined at 63.2% probability of failure) between the actual data and the prediction is -12% for tension and 6.9% for torsion.

Figure 6: Predicted failure probability for mirrors loaded in tension compared with actual data ($N=20$).

Figure 7: Predicted failure probability for mirrors loaded in torsion compared with actual data ($N=18$).

The method appears to be quite robust. Despite variations in the four-point bend beam dimensions due to manufacturing variability, and the analytical determination of both the fracture stress, σ_f , and of the area-normalization parameter, A_0 , the method predicted the true device reliability with acceptable accuracy.

Furthermore, despite the relatively large device size, we contend that the method is valid at any length scale provided that: (i) the single-crystal material acts as a continuum, and (ii) the etching processes used to build the four-point beam specimens (and hence generate the surface-specific data) is representative of the etching processes used to manufacture the devices to be analyzed.

CONCLUSION

We have demonstrated accurate fracture prediction in single-crystal silicon MEMS subjected to realistically complex, multi-

axial loadings. Importantly, the experimental methods are efficient, cost effective, and repeatable. Once a particular set of manufacturing processes is characterized using simple beam specimens, accurate reliability estimates can be made for future devices of any complexity to be fabricated using the same processes. Failure probability estimates for any subset of specific device features or types of surfaces (and hence their impact on overall device reliability), as well as parametric design optimization, are also possibilities. Our method and algorithm stand to improve predictive design of brittle microstructures, enabling reduction of development time, and of the cost, size, and complexity of the resulting MEMS devices.

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