

Available online at www.sciencedirect.com



Mechanics of Materials xxx (2003) xxx-xxx



www.elsevier.com/locate/mechmat

## Fatigue of polycrystalline silicon for microelectromechanical system applications: crack growth and stability under resonant loading conditions

C.L. Muhlstein<sup>a</sup>, R.T. Howe<sup>b</sup>, R.O. Ritchie<sup>c,\*</sup>

<sup>a</sup> Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA <sup>b</sup> Department of Electrical Engineering and Computer Science, The Berkeley Sensors and Actuators Center, University of California, Berkeley, CA 04720, USA

University of California, Berkeley, CA 94720, USA

<sup>c</sup> Materials Sciences Division, Lawrence Berkeley National Laboratory, Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA

Received 15 June 2002; received in revised form 27 July 2002

#### Abstract

Although bulk silicon is not known to exhibit susceptibility to cyclic fatigue, micron-scale structures made from silicon films are known to be vulnerable to degradation by fatigue in ambient air environments, a phenomenon that has been recently modeled in terms of a mechanism of sequential oxidation and stress-corrosion cracking of the native oxide layer. To date, most stress-life (S/N) fatigue tests on such silicon films have been conducted using resonant-loaded specimens. Consequently, there is a need to establish the interaction between the dynamic loading and the driving force for fatigue-crack growth. In this paper, finite element models are used to establish the relationship between natural frequency, specimen compliance, and linear-elastic stress-intensity factor for a commonly used micron-scale, micromechanical fatigue characterization structure. These results are then incorporated into a general, lumped parameter model to evaluate the stability of fatigue cracks in resonant-loaded structures. It is well known that the applied stress amplitude and corresponding driving force for crack advance depend on the system damping, as well as sample geometry. Consequently, changes in damping caused by cycling in different environments can have a significant mechanical effect on the stability of fatigue cracks. In the case of the fatigue characterization structure used by the authors, the models show that tests conducted at atmospheric pressure subject cracks to a monotonically increasing driving force for crack advance. However, when the damping in the system is reduced (e.g., by testing in vacuo) fatigue cracks may arrest, independent of environmental effects on crack growth. Therefore, testing of structures loaded in resonance at a fixed natural frequency in vacuum should not be considered equivalent to an "inert" atmosphere. Finally, the finite element models are applied to polycrystalline silicon structural films to determine the critical crack lengths ( $\sim 5.5-66$ nm) and an average fracture toughness (~0.85 MPa  $\sqrt{m}$ ) from specimens subjected to fatigue cycling at stress amplitudes ranging from  $\sim 2.2$  to 3.5 GPa.

© 2003 Published by Elsevier Science Ltd.

Keywords: Fatigue; MEMS; Resonance; Polycrystalline silicon; Crack stability

\*Corresponding author. Tel.: +1-814-865-1523; fax: +1-814-865-2917.

E-mail addresses: clm28@psu.edu (C.L. Muhlstein), howe@eecs.berkeley.edu (R.T. Howe), roritchie@lbl.gov (R.O. Ritchie).

0167-6636/03/\$ - see front matter @ 2003 Published by Elsevier Science Ltd. doi:10.1016/S0167-6636(03)00028-0

#### 1. Introduction

For the characterization of fatigue behavior with either total-life or fracture-mechanics methodologies, there is a need to simulate cyclic stresses, fatigue lifetimes (i.e., cycles to failure), and crack-growth rates in the laboratory. This requires the application of cyclic forces to test specimens at reasonably high frequencies. In actuality, the loading frequency sets practical limits on the maximum fatigue lives and minimum crackgrowth rates that can be measured (ASTM, 2001a; ASTM, 2001b; Saxena and Muhlstein, 1996). Where large numbers of cycles are required, electromechanical and resonant systems are often employed; indeed, with the developing emphasis on "gigacycle" fatigue (Stanzl-Tschegg and Mayer, 2001) and microelectromechanical systems (MEMS), there has been a renewed interest in such testing. Macroscale resonant fatigue testing systems utilize axial fatigue and fracture mechanicsstyle specimens, and have been used for both stress-life and crack-growth studies (e.g., Mayer, 1999). In contrast, the micromechanical fatigue systems used for micron-scale fatigue testing generally behave like simple harmonic oscillators consisting of an elastic specimen (i.e., a spring) attached to a mass. Indeed, the micromechanical resonant fatigue characterization structure shown in Fig. 1 has been widely used to evaluate the fatigue behavior of thin structural films of mono and polycrystalline silicon for MEMS applications (Allameh et al., 2000; Brown et al., 1997; Muhlstein et al., 2000, 2001a,b, 2002a,b; Van Arsdell, 1997; Van Arsdell and Brown, 1999).

Despite its poor damage tolerance and low fracture toughness (~1 MPa  $\sqrt{m}$  (Ballarini et al., 1997; Chen and Leipold, 1980; Kahn et al., 2000; St. John, 1975; Wong and Holbrook, 1987)), silicon has emerged as the dominant structural material for MEMS. Given the absence of plasticity and crack-tip shielding phenomena at room temperature, one would not anticipate thin-film silicon to be vulnerable to failure via traditional ductile or brittle material fatigue mechanisms (Ritchie, 1999; Suresh, 1998). However, using micromechanical resonant fatigue characterization structures similar to that shown in Fig. 1, a number of investigations have demonstrated that micron-scale silicon exhibits "metal-like" stress-life (S/N) fatigue behavior in ambient air (Brown et al., 1997; Kahn et al., 1999; Kapels et al., 1999; Muhlstein et al., 2000, 2001a,b). Our recent studies have indicated that the fatigue degradation process occurs via mechanisms confined to the SiO<sub>2</sub> native oxide layer that forms upon exposure to the atmosphere (Muhlstein et al., 2002a,b); specifically, this reaction-layer fatigue process involves the sequential, stress-assisted oxidation and stress-corrosion cracking of the native oxide, as described in Muhlstein et al. (2002b). However, to understand how such fatigue damage accumulates in these S/N fatigue tests, it is necessary to fully characterize the micromechanical fatigue testing struc-



Fig. 1. SEM of the micron-scale fatigue characterization structure containing a notched cantilever-beam specimen. The (a) mass, (b) comb drive actuator, (c) capacitive displacement sensor, and (d) notched cantilever-beam specimen are shown. The nominal dimensions of the specimen are as indicated in the schematic.

<sup>2</sup> 

ture, and in particular to calculate the driving force for crack advance under resonant loading conditions.

During micromechanical fatigue characterization of silicon films, the compliance of the specimen increases as fatigue damage accumulates in the form of incipient crack growth. This degradation induces a corresponding decrease in the natural frequency of the structure. Much like macroscopic fracture-mechanics-based investigations (e.g., Chati et al., 1997; Chondros et al., 1998; Mahmoud et al., 1999; McGuire et al., 1995; Yokoyama and Chen, 1998), this change in specimen compliance can be correlated with crack growth through analytical or numerically based models. What is less obvious is that this change in natural frequency can lead to a rapid reduction in the stress amplitude, as depicted schematically in Fig. 2. Thus, the driving force for fatigue failure depends not only on the specimen geometry, but also on the damping in the system. Accordingly, the development of appropriate models of the fa-



Fig. 2. Schematic of the effect of increasing specimen compliance on the applied stress amplitude in a mass-spring system under loading at a fixed natural frequency. The dashed lines are the amplitude of stress (displacement) experienced by the simple harmonic oscillator as defined by Eq. (A.2) in the Appendix A. The system is excited at the initial natural frequency of the undamaged system,  $f_0$ , but as damage accumulates the compliance increases. If the damping in the system is sufficiently low, the resonant-loaded structure can experience a significant reduction in the driving force for damage accumulation and crack advance.

tigue characterization structure is a crucial step in understanding fatigue damage accumulation in polycrystalline silicon.

The primary objectives of this work were to evaluate the fatigue-crack growth behavior and fracture toughness of polycrystalline silicon thin films and to determine the stability of the cracks under resonant loading conditions used in the fatigue characterization structure shown in Fig. 1. First, finite element methods were used to evaluate the dynamic behavior and stress distribution of an uncracked structure. Similar models of a cracked structure were then developed to determine the natural frequency and linear-elastic crack-tip parameter, K. These models were then employed in a lumped, dynamic model of the micromechanical fatigue characterization structure to evaluate the stability of fatigue cracks. Finally, the finite element and lumped parameter numerical models of the structure were applied to experimental data from previous stress-life fatigue tests to evaluate the crack-growth rate and fracture toughness behavior of the n<sup>+</sup>-type, thin-film, polycrystalline silicon.

#### 2. Experimental and numerical methods

To determine the natural frequency, compliance, and stress distribution for the fatigue characterization structure shown in Fig. 1, dynamic and quasi-static finite element models were constructed for both uncracked and cracked structures. In the case of the cracked structure the relationships between the crack length and the natural frequency and the stress-intensity-factor, K, were also determined.

#### 2.1. Micromechanical fatigue testing

The fatigue characterization structure (Fig. 1) used for thin-film silicon S/N fatigue testing was originally developed by Van Arsdell (1997). This structure is square in overall shape (~300 µm on a side), and is analogous to a specimen, electromechanical load frame, and capacitive displacement transducer found in a conventional mechanical testing system. The specimen is a notched cantilever beam that is in turn attached to a large,

perforated plate that serves as a resonant mass. The mass and beam are electrostatically forced to resonate and the resulting motion is measured capacitively. On opposite sides of the resonant mass are interdigitated "fingers" commonly referred to as "comb drives". One side of these drives is for electrostatic actuation; the other side provides capacitive sensing of motion. The resonance generates fully reversed, constant amplitude, sinusoidal stresses at the notch, i.e., a load ratio, R(ratio of minimum to maximum load), of -1. The structure is designed for testing at  $\sim$ 40 kHz and is excited at a fixed frequency that is updated periodically during the test. The notched beam specimens are  $\sim 40 \ \mu m$  long, 19.5  $\mu m$  wide, and 2  $\mu m$ thick. A 13 µm deep notch is located 9.8 µm from the base and has a root radius of about 1 µm based on scanning electron micrographs (SEM) of the structures. The toroidal plate spanning 60° (inner radius,  $r_{inner} = 30 \ \mu m$ , outer radius,  $r_{outer} = 300$ µm) rotates about the midpoint of the remaining ligament of the notched beam and serves as a mass to lower the natural frequency of the structure. The specimens are tested at a constant applied electrostatic force amplitude until failure occurs by complete separation of the beam at the notch. During the test, the natural frequency of the structure decreases as fatigue damage accumulates at the notch. The natural frequency of the structure is periodically characterized (about every 60 s) throughout the fatigue test by measuring the amplitude of the resonance as the excitation frequency is varied by  $\pm 50$  Hz around the resonant frequency of the structure, f. The dynamic response of the structure is fit with a second-order polynomial and the maximum is taken as an estimate of the resonant frequency. The fatigue characterization structure is then excited at this frequency with a constant force amplitude until the frequency sweep and curve fit are repeated (Muhlstein et al., 2001a). The motion is measured via the rate of change of capacitance, calibrated using the method detailed in Muhlstein et al. (2001a), and is monitored during every test. Thus, the natural frequency as a function of time data are a record of damage accumulation and a loss of resonance indicates specimen failure. The applied stress amplitude and crack-growth behavior are

determined from the finite element methods described herein.

In total, 28 specimens of n<sup>+</sup>-type polycrystalline silicon,  $\sim$ 2-µm thick films were tested to failure and the natural frequency as a function of time monitored. In previous studies, the fracture surfaces, crack paths, and microstructure were examined in detail (Muhlstein et al., 2001a). In this study, the focus of the work is on the interpretation of the change in natural frequency and the stability of cracks in the specimen.

The design of the micromechanical fatigue characterization structure is amenable to a wide range of processing techniques and material systems, and has been used for studies of both silicon and silicon-germanium structural films. During a recent fabrication run of a polycrystalline SiGe surface micromachining process (Franke et al., 2000), in addition to the "standard" notched cantilever beam geometry, a new specimen variant was introduced for characterization of the fatigue properties of brittle structural films. A  $\sim$ 3 µm square hole was added to the center of the remaining ligament of a notched cantilever beam in order to blunt the crack and, under resonant loading, to halt motion of the structure. Fig. 3 shows SEM of single- and double-notched specimens with centrally located holes. The polycrystalline SiGe was an alloy of approximately 33 atomic percent silicon and 66 atomic percent germanium. The film was in situ doped, p<sup>+</sup>-type and was used in the as-deposited condition with a polycrystalline germanium sacrificial layer. The sacrificial layer was removed using 50% H<sub>2</sub>O<sub>2</sub> for 1.5 h followed by drying at 110 °C in air for 2 min. The structures were excited near the natural frequency of the uncracked structure and the amplitude of the electrostatic excitation was rapidly increased until the structure ceased to resonate. After testing, the structures were examined in the SEM, without the use of conductive coatings typically employed to improve image contrast of low conductivity materials.

#### 2.2. Numerical modeling

A series of planar, finite element models were evaluated using a commercial software package





Fig. 3. SEM of (a) single ( $f_0 = 16.88$  kHz) and (b) double-notched ( $f_0 = 23.17$  kHz) cantilever-beam specimens with centrally located holes in fatigue characterization structures fabricated using a polycrystalline SiGe surface micromachining process (Franke et al., 2000). The specimens were excited at a fixed natural frequency and the amplitude rapidly increased until motion of the structure ceased. Cracks initiated at the notch root and were arrested by the hole, preventing complete separation of the beam (insets), illustrating the interaction between the resonant loading conditions and crack advance in the structure.

(ANSYS v. 5.7). Modal and quasi-static structural analyses of the uncracked structure were used to determine the dynamic response of the structure and the applied stress amplitude for a given displacement. The fatigue characterization structure was modeled as an elastically isotropic, notched, cantilever beam and mass, with the geometry determined by SEM of released devices, as summarized in Fig. 1. Six-node, triangular, plane-stress, solid elements with constant thickness were used in the model and small elastic deformations were assumed. The displacements of nodes located at the base of the notched cantilever beam were set to zero to achieve the "built-in" boundary conditions of the structure. The mesh in the vicinity of the notch was refined until solutions converged. An average of the Voigt and Reuss bounds for a random, polycrystalline silicon aggregate (Young's modulus, E = 163 GPa, Poisson's ratio, v = 0.23(Simmons and Wang, 1971)) was used for the elastic properties of the elements. The density of the polycrystalline silicon in the modal analysis was assumed to be the same as the bulk, single crystal form ( $\rho = 2329 \text{ kg/m}^3$  (Tatsumi and Ohsake, 1988)). A subspace extraction method was used to determine the eigenvalues and eigenvectors for the system, establishing the first in-plane natural frequency of the structure. An identical, plane-stress model with unit thickness was used to establish the degree of nonideality (i.e., the deviation from a mass-spring system) of the structure. The maximum principal stress at the notch root,  $\sigma_1$ , and angular rotation of the structure,  $\theta$ , about the midpoint of the remaining ligament, (W - D), due to a unit force applied at the center of mass of the plate in a direction perpendicular to the long axis of the beam, were used to determine the relationship between angular rotation and maximum principal stress.

Modal and quasi-static structural analyses of cracked, notched, cantilever-beam structures were performed using the same material properties and

finite element package. Akin to the uncracked structures, small deformations and elastic isotropy were assumed, displacements of nodes at the base of the cantilever structure were set to zero, and the material properties of an ideal polycrystalline silicon aggregate were used. The model of the fatigue characterization structure, with a single crack located on the centerline of the notch, was constructed with six-node, triangular, plane-strain elements. The singularity at the crack-tip was modeled with twelve circumferential, unskewed elements, 1/20 of the crack length in size. The remaining element size was refined until model convergence was achieved. As with the uncracked structure, a subspace extraction method was used to determine the eigenvalues and eigenvectors for the system, establishing the first in-plane natural frequency and mode shape of the structure. Structural analyses of the cracked structure were performed using six-node triangular plane-stress elements with thickness equal to that of the structure in a configuration that was otherwise identical to the models used for the modal analyses. A unit force was applied at the center of mass of the plate in a direction perpendicular to the long axis of the beam and the resulting angular rotation used to establish the specimen rotational compliance  $(s_{\theta} = 1/k_{\theta})$ . The stress-intensity was then calculated from the displacement field immediately behind the crack-tip (Anderson, 1995; Broek, 1986). The size of the crack was gradually increased to establish the nondimensional compliance, sEt, and stress-intensity geometry function, f(a/(W-D)), for the cracked characterization structure using standard fracture-mechanics procedures (Anderson, 1995; Broek, 1986).

To evaluate the stability of cracks in structures under the resonant loading conditions, a lumped parameter modeling approach was used. The dynamic behavior of the system was modeled as a damped, forced, mass-spring oscillator that was driven at or near its natural frequency,  $f_0$ . The stiffness of the spring, k, and crack-driving force, K, were determined from fracture-mechanics solutions (e.g., Tada et al., 2000) and the mass of the model system established by the geometry of the structure. The amplitude of motion and the associated driving force for crack advance were determined from the relationship between the amplitude and frequency of the excitation waveform and the damping characteristics and natural frequency of the system (e.g., French, 1971), as detailed in the Appendix A. The damping of the system was assumed to be proportional to the velocity of the mass in the system, as is typical of many simple systems.

Crack stability under resonant loading was evaluated by calculating the maximum stressintensity,  $K_{\text{max}} = \Delta K / (1 - R)$ , where  $\Delta K$  is the stress-intensity range and R is the load ratio, for an applied force or moment amplitude. From the system compliance, the natural frequency of the resonator could then be determined. The crack was extended, lowering the natural frequency of the structure, but the excitation frequency remained unchanged. The new stress amplitude was determined using the revised structure compliance, thus permitting the associated crack-driving force to be calculated. The process of extending the crack and calculating the new stress amplitude was repeated to generate a plot of the driving force as a function of crack length. The effect of damping on the system was investigated by modifying the quality factor of the initial configuration,  $Q_0$ , as defined in the Appendix A.

This general procedure was applied first using compliance and stress-intensity solutions in the literature for three common geometries summarized in Table 1 (after Tada et al., 2000): a micronscale, edge-cracked beam in bending  $(t = 2 \mu m)$ ,  $W = 19.5 \ \mu m$ ), a single-edge-cracked plate in tension  $(t = 2 \ \mu m, W = 10 \ \mu m, L = 20 \ \mu m)$ , and a center-cracked plate in tension ( $t = 2 \mu m$ , W = 5 $\mu m$ ,  $L = 20 \mu m$ ), where t is the thickness, W is the width, and L is the length of the specimen. The edge-cracked beam in bending was attached to a mass with a mass-polar moment of inertia the same as the mass in the structure shown in Fig. 1  $(J_{\theta} = 1.024 \times 10^{-17} \text{ kg m}^2)$ , giving an initial natural frequency of 96.2 kHz. The edge-cracked and center-cracked plates in tension were modeled with a  $4.1288 \times 10^{-5}$  kg mass that gave an initial natural frequency of 14.1 and 10 kHz, respectively. In a gravitational field, this corresponded to a tensile preload of  $\sim 20$  MPa, a small fraction of the strength of silicon structural films (3-5 GPa

C.L. Muhlstein et al. | Mechanics of Materials xxx (2003) xxx-xxx

Table 1

Fracture-mechanics solutions for the mode I stress-intensity factor,  $K_{I}$ , and compliance, s, of the edge-cracked beam in bending, edge-cracked plate in tension, and the center-cracked plate in tension geometries (Tada et al., 2000)

*		
Description	$K_{\rm I} = \sigma \sqrt{\pi a} \cdot f\left(\frac{a}{W}\right)$	$s = \frac{1}{k}$
Center-cracked plate in tension	$f\left(\frac{a}{W}\right) = \left\{1 - 0.025\left(\frac{a}{W}\right)^2 + 0.06\left(\frac{a}{W}\right)^4\right\}\sqrt{\sec\left(\frac{\pi a}{2W}\right)}$	$s(\frac{a}{W}) = \frac{2a}{EW} \left( -1.071 + 0.25 \left(\frac{a}{W}\right) - 0.357 \left(\frac{a}{W}\right)^2 + 0.121 \left(\frac{a}{W}\right)^3 - 0.047 \left(\frac{a}{W}\right)^4 \right)^4$
		$+0.008\left(rac{a}{W} ight)^5-1.071\cdotrac{\log\left(1-rac{a}{W} ight)}{rac{a}{W}} ight)+rac{L}{2EWt}$
Edge-cracked plate in bending	$f\left(\frac{a}{W}\right) = \frac{6\sqrt{2\tan\left(\frac{aa}{2W}\right)}}{\cos\left(\frac{\pi m}{2W}\right)} \left[0.923 + 0.199\left\{1 - \sin\left(\frac{\pi a}{2W}\right)\right\}^4\right]$	$s_{\theta}\left(\frac{a}{W}\right) = \frac{24}{EW^2} \left(\frac{a/W}{1-a/W}\right)^2 \left\{5.93 - 19.69\left(\frac{a}{W}\right) + 37.14\left(\frac{a}{W}\right)^2$
		$-35.84 \left(\frac{a}{W}\right)^3 + 13.12 \left(\frac{a}{W}\right)^4 + \frac{12L}{EW^3 t}$
Single-edge notched plate in tension	$e \ f(\frac{a}{W}) = \sqrt{\frac{2W}{\pi a} \tan\left(\frac{\pi a}{2W}\right)} \cdot \frac{0.752 + 2.02(\frac{a}{W}) + 0.37(1 - \sin\left(\frac{\pi a}{2W}\right))^3}{\cos\left(\frac{\pi a}{2W}\right)}$	$s\left(\frac{a}{W}\right) = \frac{2a}{EW} \left(\frac{a/W}{\left(1-a/W\right)^2}\right) \left\{ 0.99 - \frac{a}{W} \left(1-\frac{a}{W}\right) \left(1.3 - 1.2\left(\frac{a}{W}\right) + 0.7\left(\frac{a}{W}\right)^2\right) \right\} + \frac{L}{2EW}$

(Greek et al., 1999, 1997; Kapels et al., 1999; Sharpe et al., 1998, 1999; Tsuchiya et al., 1997, 1998)). The lumped model was then applied to the notched cantilever-beam fatigue structure (Fig. 1) using results from the finite element models to establish the appropriate compliance and stress–intensity factors. The mass polar moment of inertia,  $J_{\theta}$ , of the micromechanical fatigue characterization structure was calculated from the geometry of the plate and found to be  $1.024 \times 10^{-17}$  kgm<sup>2</sup>. This mass-spring system model corresponds to an initial natural frequency of ~43.5 kHz.

The finite element and lumped-parameter dynamic models were applied to experimental results from previously reported stress-life fatigue data (Muhlstein et al., 2001a). The linear relationship between the maximum principal stress,  $\sigma_1$ , and the angular rotation of the structure provided the basis for determining the nominal stress from the experimentally measured angular rotation. The dynamic model of the structure was then utilized to evaluate the crack-growth rates in the structure using the following procedure. The measured natural frequency of the structure,  $f_{crack}$ , was normalized with respect to the initial natural frequency of the structure,  $f_0$ . A linear interpolation of the normalized natural frequency as a function of normalized crack length, a/(W-D), developed from the dynamic model was used to determine the crack length as a function of time. The maximum stress-intensity immediately prior to failure was taken as an estimate of the fracture toughness of the material.

#### 3. Results

#### 3.1. Resonant-loaded beams with holes

Polycrystalline silicon–germanium fatigue characterization structures similar in geometry to Fig. 1 were excited with a continuously increasing stress amplitude at a fixed frequency in laboratory air until motion ceased. The single notched specimen with a centrally located hole had a first inplane bending mode natural frequency of 16.88 kHz and failed at an excitation torque of  $\sim 4.7 \times 10^{-10}$  N m. The double-notched specimen with a centrally located hole had a first in-plane bending mode natural frequency of 23.17 kHz and failed at an excitation torque of  $\sim 5.7 \times 10^{-10}$  N m. In both cases the specimens were ramped manually and failure occurred in less than 5 s, corresponding to excitation ramp rates in excess of  $1 \times 10^{-10}$  N m/s. Observation of the single and double-notched beams with centrally located holes using the scanning electron microscope revealed cracks emanating from the root of the notch that terminated at the hole, as shown in Fig. 3.

#### 3.2. Dynamic and quasi-static finite element analyses

The dynamic and quasi-static behavior of the uncracked fatigue characterization structure was evaluated using the finite element methods described above. The first in-plane natural frequency of the structure,  $f_0$ , was extracted from the finite element models and the mode-shape evaluated by inspection of the exaggerated displacements. The natural frequency of the uncracked structure was found to be 43,217 kHz for both the full (t = 1.97 $\mu$ m) and unit thickness ( $t = 1 \mu$ m) plane-stress models. The torsional stiffness,  $k_{\theta}$ , of the uncracked structure due to a unit force applied at the center of mass of the toroidal plate in a direction normal to the long axis of the cantilever beam was found to be  $7.6605 \times 10^{-7}$  N m/rad. When  $k_{\theta}$  is combined with the calculated mass polar moment of inertia, the natural frequency of the mass-spring system is calculated to be 43,531 kHz. The maximum principal stress at the root of the notch due to a unit force applied at the center of mass was linearly related to the angular rotation of the mass  $(1.0107 \times 10^{11} \text{ Pa/rad})$ . The spatial distribution of the stresses along the centerline of the notch was extracted from the finite element solution and are shown in Fig. 4(a) where the principal stress,  $\sigma_1$ , is normalized by the outer fiber principal stress in the beam remote from the notch,  $\sigma_{1,\infty}$ , and the distance from the notch root, r, is normalized by the remaining ligament size, (W - D). The calculated stress concentration factor, SCF, was found to be 2.04. The maximum principal stress along the centerline of the notch decreases as  $1/r^2$  for r/(W-D > 0.1, as shown by the curve fit in Fig. 4(b).



Fig. 4. Stress-concentration effects of the notch in the cantilever beam in the fatigue characterization structure. (a) The normalized stress  $(\sigma_1/\sigma_{1,\infty})$  at location, r, along the centerline of the notch is shown as a function of the remaining ligament (W - D) of the cantilever-beam structure. The stress concentration factor, SCF, from the finite element model is similar to general results from (Noda and Takase, 1999). (b) The  $1/r^2$ decay of the maximum principal stress near the root of the notch.

Similar to the previous case, the dynamic behavior of the cracked fatigue characterization structure was also evaluated using finite element methods. The first in-plane natural frequency of the cracked structure,  $f_{\rm crack}$ , was extracted from the model and the mode-shape was evaluated by inspection of the exaggerated displacements. The relationship between normalized crack length (a/(W-D)) and normalized natural frequency  $(f_{\rm crack}/f_0)$  for the plane-stress model is shown in

Fig. 5 and fit to the ninth-order polynomial shown in Table 2. Although the relationship is nonlinear, in the early stages of crack growth a  $\sim 1$  Hz change in natural frequency corresponds to  $\sim 1$  nm of crack extension. Interpolation methods should be used when calculating small normalized crack lengths, i.e., a/(W - D) < 0.01, since the quality of the curve fit in this range is poor.

Standard fracture-mechanics analyses were used to determine the compliance, s, and stress-intensity factor, K, for the cracked fatigue characterization structure from the plane-strain finite



Fig. 5. (a) The relationship between normalized crack length (a/(W - D)) and normalized natural frequency  $(f_{crack}/f_0)$  for the plane-stress (full-thickness) finite element model of the notched cantilever beam in the fatigue characterization structure. (b) The behavior for small (a/(W - D)) and the associated ninth-order polynomial fit from Table 2 are shown.

 Table 2

 Curve fits of the modal and fracture-mechanics solutions for the notched, cantilever beam in the fatigue characterization structure shown in Fig. 1

Description	Validity	Function
Natural frequency	$0 < \frac{a}{(W-D)} \leqslant 0.85$	$\frac{f_{\rm crack}}{f_0} = 1.004 - 0.07804 \left(\frac{a}{(W-D)}\right) - 8.6569 \left(\frac{a}{(W-D)}\right)^2 + 51.736 \left(\frac{a}{(W-D)}\right)^3$
		$-201.93 \left(\frac{a}{(W-D)}\right)^{4} + 508.61 \left(\frac{a}{(W-D)}\right)^{5} - 815.53 \left(\frac{a}{(W-D)}\right)^{6} + 801.57 \left(\frac{a}{(W-D)}\right)^{7}$
		$-439.42 \left(\frac{a}{(W-D)}\right)^8 + 102.78 \left(\frac{a}{(W-D)}\right)^9$
Nondimensional compliance	$0 < rac{a}{(W-D)} \leqslant 0.2$	$sEt = 3.9856 \times 10^{11} + 2.441 \times 10^9 \left(\frac{a}{(W-D)}\right) + 1.0302 \times 10^{13} \left(\frac{a}{(W-D)}\right)^2 - 1.021 \times 10^{14} \left(\frac{a}{(W-D)}\right)^3$
		$+9.5484 \times 10^{14} {\left(\frac{a}{(W-D)}\right)}^4 - 6.5976 \times 10^{15} {\left(\frac{a}{(W-D)}\right)}^5 + 3.1801 \times 10^{16} {\left(\frac{a}{(W-D)}\right)}^6$
		$-9.8133  imes 10^{16} {\left(rac{a}{(W-D)} ight)}^7 + 1.7071  imes 10^{17} {\left(rac{a}{(W-D)} ight)}^8 - 1.2397  imes 10^{17} {\left(rac{a}{(W-D)} ight)}^9$
Nondimensional compliance	$0.2 < rac{a}{(W-D)} \leqslant 0.85$	$sEt = 3.5995 \times 10^{11} + 4.421 \times 10^{12} \left(\frac{a}{(W-D)}\right) - 1.2201 \times 10^{14} \left(\frac{a}{(W-D)}\right)^2 + 1.5956 \times 10^{15} \left(\frac{a}{(W-D)}\right)^3$
		$-1.0488  imes 10^{16} {\left(rac{a}{(W-D)} ight)}^4 + 3.9005  imes 10^{16} {\left(rac{a}{(W-D)} ight)}^5 - 8.5419  imes 10^{16} {\left(rac{a}{(W-D)} ight)}^6$
		$+1.0923  imes 10^{17} {a \over (W-D)}^7 - 7.5486  imes 10^{16} {a \over (W-D)}^8 + 2.182  imes 10^{16} {a \over (W-D)}^9$
Stress-intensity factor geometric	$0 < rac{a}{(W-D)} \leqslant 0.85$	$f\left(\frac{a}{(W-D)}\right) = 1.7672 - 12.179\left(\frac{a}{(W-D)}\right) + 86.447\left(\frac{a}{(W-D)}\right)^2 - 310.86\left(\frac{a}{(W-D)}\right)^3$
Tunction		$+291.74 \left(\frac{a}{(W-D)} ight)^4 + 1890.8 \left(\frac{a}{(W-D)} ight)^5 - 7699.9 \left(\frac{a}{(W-D)} ight)^6 + 12676 \left(\frac{a}{(W-D)} ight)^7$
		$-10091 \left(rac{a}{(W-D)} ight)^8 + 3203 \left(rac{a}{(W-D)} ight)^9$

element model detailed in the previous section. The compliance of the cracked structure for a given crack length was determined from the displacement of the center of mass of the toroidal plate due to a unit force applied at the center of mass in a direction perpendicular to the long axis of the beam. The equivalent angular rotation of the plate about the midpoint of the remaining ligament of the beam was determined from the geometry of the structure. From general analytical solutions, it is known that the crack-tip stresses



Fig. 6. (a) The nondimensional rotational compliance, S(a/(W - D)) = sEt, of the cracked fatigue characterization structure due to a unit point load applied at the center of mass as a function of normalized crack length, a/(W - D), determined from finite element methods. (b) The behavior for small (a/(W - D)) and the associated ninth-order polynomial fit from Table 2 are shown.

and strains are proportional to the linear-elastic crack parameter, K, and have a general functional form dependent on the mode of loading (Anderson, 1995; Broek, 1986). Thus, the location of, and stresses (or displacements) at, nodes near the crack-tip can be used to calculate K for a given applied force. This strategy was used to calculate K as a function of crack length for a unit force applied at the center of mass of the toroidal plate in a direction perpendicular to the long axis of the beam. The results of the compliance and stressintensity factor analyses were then recast in the standard functional forms used in fracture mechanics. The compliance results are shown in the standard, nondimensional compliance form (sEt =S(a/W) (Anderson, 1995; Broek, 1986) in Fig. 6 and fit with the ninth-order polynomial shown in Table 2. Similarly, the geometric function, f(a/(W-D)) (Anderson, 1995; Broek, 1986), for the stress-intensity factor  $(K = \sigma \sqrt{\pi \cdot a})$ f(a/(W-D))) of the cracked, notched, cantileverbeam structure was determined (Fig. 7) and fit to a ninth-order polynomial shown in Table 2.



Fig. 7. The geometric function, f(a/(W - D)), for the stressintensity factor,  $K = \sigma \sqrt{\pi \cdot a} \cdot f(a/(W - D))$ , of the cracked, notched, cantilever beam specimen within the fatigue characterization structure, determined from the displacement of nodes immediately behind the crack-tip.

12

#### 3.3. Lumped dynamic model

The lumped dynamic model described in Section 2.2 was applied to the three, micron-scale, resonant fatigue characterization structures, namely the edge-cracked plate in bending, single edge-cracked plate in tension, and center-cracked plate in tension; the calculated normalized cracktip parameters, as a function of normalized crack length and quality factor, are shown in Fig. 8. The model was also applied to the cracked, notched cantilever-beam fatigue characterization structure (Fig. 1) using the fracture-mechanics solutions derived above. Results are shown in Fig. 9, where the driving force for crack advance is presented as a function of crack length and quality factor. The results shown in Fig. 9(b) focus on the range of normalized crack size relevant to polycrystalline silicon structural films.

#### 3.4. Stress-life (S/N) fatigue data analysis

Previously, 28 polycrystalline silicon specimens were tested to failure in laboratory air (Muhlstein



Fig. 8. Stability of a fatigue crack in resonant-loaded fatigue characterization structures predicted by the lumped dynamic model. The normalized driving force for crack advance,  $K_{max}/K_{max,0}$ , as a function of normalized crack length, a/W, is shown for the (a) edge-cracked plate in bending, (b) edge-cracked plate in tension and (c) center-cracked plate in tension. In heavily damped systems (i.e., low  $Q_0$ ), the fatigue-crack growth rate will accelerate (dK/d(a/W) > 0). As the damping in the system is decreased (i.e., increasing  $Q_0$ ), the crack growth rate will decelerate and possibly arrest (dK/d(a/W) < 0).



Fig. 9. Stability of a fatigue crack in the resonant-loaded fatigue characterization structure (Fig. 1) predicted by the lumped dynamic model. (a) The normalized driving force for crack advance,  $K_{\text{max}}/K_{\text{max},0}$ , is shown as a function of normalized crack length, a/(W-D), for the notched cantilever-beam specimen within this structure. Similar to the geometries shown in Fig. 8, the fatigue-crack growth rate will accelerate (dK/d(a/(W - D) > 0 in heavily damped systems (i.e., low  $Q_0$ ) and will decelerate and possibly arrest (dK/d(a/W) < 0) if the damping in the system is decreased (i.e., high  $Q_0$ ). (b) Results from the lumped dynamic model for normalized crack lengths relevant to fatigue characterization of polycrystalline silicon (a/(W - D) <0.015). Fatigue cracks tested in air ( $Q_0 \sim 100$ ) are always subjected to increasing driving force gradients. However, when the damping is reduced (e.g.,  $Q_0 \sim 10,000$  in vacuum) the cracks may arrest due to purely mechanical effects.

et al., 2001a). The fatigue lives,  $N_{\rm f}$ , varied from ~10 s to 34 days (3 × 10<sup>5</sup> to 1.2 × 10<sup>11</sup> cycles) over an angular rotation amplitude,  $\theta$ , of ~0.02 to 0.04

radians at R = -1. The silicon films displayed "metal-like" S/N behavior, with an endurance strength at 10<sup>9</sup>-10<sup>10</sup> cycles of roughly half the (single-cycle) fracture strength. The relationship between angular rotation and maximum principal stress determined using the finite element model was used to calculate the applied stress amplitude which ranged from  $\sim 2.2$  to 4.4 GPa (Fig. 10). For each specimen, the crack length as a function of accumulated cycles was determined from a linear interpolation of the finite element model-derived relationships between natural frequency and crack length shown in Fig. 5. A representative result of the calculated crack length as a function of time is shown in Fig. 11. The final crack lengths measured immediately prior to failure,  $a_{\rm f}$ , from the normalized natural frequency for the specimens in Fig. 10 are shown as a function of specimen life,  $N_{\rm f}$ , in Fig. 12. The applied stress amplitude for a given test and the crack size just prior to failure were used to estimate the fracture toughness of the material,  $K_c$ (Fig. 13). For the thin-film polysilicon fatigue tests, calculated critical crack sizes ranged from  $\sim$ 5.5 to 66 nm, depending on the applied stress amplitude. The average fracture toughness measured by this technique for failure of the polycrystalline silicon films was 0.85 MPa  $\sqrt{m}$ . These crack sizes are consistent with those observed ex-



Fig. 10. Typical stress-life (S/N) fatigue behavior of  $\sim 2 \mu m$ -thick, polycrystalline silicon obtained using the micron-scale fatigue characterization structure under fully reversed, tension-compression loading at 40 kHz in moist room air (Muhlstein et al., 2000, 2001a).

C.L. Muhlstein et al. | Mechanics of Materials xxx (2003) xxx-xxx



Fig. 11. Damage accumulation in polycrystalline silicon, shown by experimentally measured decrease in resonant frequency,  $f_{\rm crack}$ , with time during the fatigue test ( $N_{\rm f} = 2.19 \times 10^{10}$  cycles at  $\sigma_a = 2.71$  GPa), with the corresponding computed increase in crack length *a*.



Fig. 12. Decrease in normalized natural frequency,  $1 - (f_{\text{crack}}/f_0)$ , and the associated final crack size,  $a_f$ , as a function of specimen life.

perimentally in the high voltage transmission electron microscope, as detailed in Muhlstein et al., 2002a,b.

#### 4. Discussion

The finite element and numerical models provide important insight into the dynamic behavior of crack-free structures and the stresses in the vi-



Fig. 13. Computed fracture toughness,  $K_c$ , values determined from the estimated crack length immediately prior to failure, i.e., the critical crack size,  $a_c$ , for the given applied stress amplitude. The average fracture toughness (dashed line) was calculated to be 0.85 MPa  $\sqrt{m}$ .

cinity of the notched beam fatigue characterization specimens. Similarly, the models of the cracked structure can be used to determine the size and stability of cracks, as well as the fracture toughness of the material. The purpose of this section is to discuss the implications of the models for the behavior of the structure and the fatigue resistance of polycrystalline silicon.

Comparison of the various models of the dynamic behavior of the crack-free fatigue characterization structure provides useful insight into the behavior of the structure. The agreement between the first in-plane natural frequency predicted by the unit and full-thickness finite element models of the fatigue characterization structure and the 0.7% difference between the plane-stress finite element and the mass-spring description establish that the use of a mass-spring idealization is reasonable. However, there is a marked difference between the predicted natural frequency of the plane-stress model (43,217 Hz) and what is typically observed experimentally (41,693 Hz) (Muhlstein et al., 2001a). Since the stiffness of the structure is proportional to the elastic modulus, the experimentally observed Young's modulus appears to be about 152 GPa, i.e., some 7% below the ideal polycrystalline value (Simmons and Wang, 1971).

It is believed that this is not an anomalously low elastic modulus, but rather arises from the compliance of the "anchor" at the base of the cantilever structure (Van Arsdell, 1997). Consequently, the use of idealized, polycrystalline aggregate elastic properties and perfectly clamped boundary conditions provide a conservative estimate of the applied stress amplitudes during S/N fatigue testing. While the built-in assumption for the base of the fatigue characterization structure may introduce up to a 7% error in the calculated stress amplitude, the general trends observed in S/N and dynamic behavior should be faithfully represented.

Maximum principal stresses at the root of the notch, determined from the plane-stress finite element model of the crack-free fatigue characterization structure, gave values proportional to the angular rotation of the resonant mass  $(1.0107 \times$  $10^{11}$  Pa/rad). The stress field falls off at a rate proportional to  $1/r^2$  and the effects of the notch are most important for r/(W - D) < 0.1 (within  $0.65 \,\mu\text{m}$  of the root) as shown in Fig. 4(b). General solutions for V-shaped notches in flat plates loaded in bending, developed by Noda et al. (1995), give an SCF of 2.03 for the present notched cantilever beam, which compares favorably with the finite element solutions in the present study and the simplified (beam-only) models used previously (Muhlstein et al., 2001a). While understanding the notch stress distribution and dynamic behavior of the structure are important, the behavior of cracked fatigue specimens is particularly useful.

The loading conditions that develop during testing of the electrostatically actuated fatigue characterization structure are inextricably linked to its dynamic behavior. The objective is to apply large, sinusoidally varying stresses to the material to characterize the fatigue behavior. However, the electrostatic comb drive actuators have a relatively limited capacity. The typical electrostatic torque that can be applied to the structure ( $\sim 5 \times 10^{-10}$ Nm) is insufficient for fracture and fatigue characterization. However, if a time-varying force is applied to the structure at or near an appropriate resonant frequency, large, fully reversed stress amplitudes can be generated due to coupling between the excitation force and the inertial response of the system. The amplitude of motion and the corresponding stress amplitudes are then described by the equations of motion of the simple harmonic oscillator as detailed in the Appendix A. These simple relationships have two key aspects that must be understood when evaluating the behavior of the fatigue characterization structure. Firstly, when the structure is excited at its natural frequency, decreasing the damping of the system (i.e., increasing the quality factor, O) will increase the amplitude of motion for a given excitation force. However, a competing effect is at work when the structure is excited off-resonance. The amplitude of motion decreases as the excitation frequency deviates from the natural frequency of the system. The rate of decrease is much more rapid for systems with low damping (e.g., high Q). Secondly, an analogous situation arises if the excitation frequency remains fixed but the stiffness of the system changes, such as if cracking occurs. The interaction between natural frequency of a cracked structure and the excitation frequency, depicted schematically in Fig. 2, was observed experimentally as a loss of resonance in the specimens with centrally located holes. If a fatigue crack is allowed to propagate into a hole under the correct loading conditions (De Rijk, 1970; Van Leeuwen, 1970; Van Oosten Slingeland and Broek, 1973), the crack-tip tip radius is effectively "blunted", in the present case from Angstroms to micrometers, which can lead to arrest. Because the natural frequency of the structure has been radically reduced, during the next electrostatic cycle the structure is not excited at resonance since the frequency of the impulse has remained unchanged. This provides a "graceful" failure mode that prevents shorting of the electrostatic actuator when the specimen separates.

In general, under nominally linear-elastic conditions, when a constant force is applied normal to the crack plane (i.e., mode I loading), an increasing *K*-gradient results and stable crack growth is not observed in materials that do not exhibit resistance-curve behavior (Anderson, 1995; Broek, 1986; Lawn, 1993). In contrast, a mode I crack subjected to a constant displacement will usually be subjected to a decreasing *K*-gradient and stable crack propagation can occur once the applied driving force reaches the critical stress–intensity,

 $K_{\rm c}$ . Creative mechanical design can lead to exceptions to these general trends (e.g., (Fitzgerald et al., 1999; Gonzalez and Pantano, 1990)) just as rapidly varying the applied force or displacement can, in principle, be used to generate the desired crack-tip driving force and *K*-gradient. The applied stress-intensity range,  $\Delta K$ , gives the analogous driving force for fatigue-crack growth in linear-elastic solids. Fatigue cracks subjected to increasing  $\Delta K$  gradients ( $d\Delta K/da$ ) accelerate while decreasing gradients eventually lead to crack arrest. The resonant loading conditions encountered in micromechanical fatigue testing play an important role in the stability of cracks in these structures.

If a micromechanical fatigue system is modeled as a damped, forced, mass-spring oscillator that is driven at or near its natural frequency, the stiffness of and crack-driving force in the "spring" can be determined from fracture-mechanics solutions that describe the geometry of the specimen. A wide variety of solutions are summarized in handbooks, e.g., (Tada et al., 2000). The range of motion of the structure can be determined from the relationship between the amplitude and frequency of the excitation waveform and the damping characteristics and natural frequency of the system. This general approach allows the evaluation of fatigue crack stability for a wide variety of configurations and reflects the behavior of a variety of mechanical testing structures used to characterize structural films used in MEMS. If the system is driven at or near the natural frequency of the crack-free structure, the unique loading conditions depicted schematically in Fig. 2 may develop. A structure excited at  $f_0$  will begin at an amplitude of motion as defined by Eq. (A.2) in the Appendix A. As the crack advances, the natural frequency of the structure decreases. Since the excitation frequency has remained unchanged, the amplitude of motion decreases as the coupling between the structure and excitation force is reduced. If the rate of load shedding is sufficiently rapid (i.e., high enough Q), a decreasing  $\Delta K$  gradient may develop. What would seem at first glance to be a force-controlled configuration is actually limited by the change in stiffness of the structure. In the case of the micromechanical resonators for fatigue characterization, these force-controlled, displacementlimited conditions may develop when the damping in the system is altered by lowering the ambient pressure of the surrounding environment.

As noted above, the mode I compliance and stress-intensity factor solutions for edge and center-cracked plates in tension and edge-cracked beams in bending from (Tada et al., 2000) were used as test cases for the general model of crack stability under fatigue loading. In heavily damped (i.e., low *Q*) systems, the stress amplitude does not significantly change as the crack advances into the material and the loading conditions are not unlike constant force or moment conditions. The crack grows into an increasing  $\Delta K$  gradient, accelerates and eventually fails when  $K_{\text{max}}$  reaches the fracture toughness,  $K_c$ , of the material (i.e., is unstable). However, as the level of damping is reduced the driving force,  $\Delta K$ , and its gradient change significantly; the lower damping in the system leads to a rapid decrease in the applied stress amplitude as the crack advances. Once the quality factor reaches relatively high values (in excess of 1000), the gradient is such that the fatigue crack is decelerating and will eventually arrest (i.e., is stable). This phenomenon is quite general, and is observed with both edge and centrally located cracks loaded in tension or bending.

The stability of cracks in the micromechanical fatigue characterization structure is shown as a function of system damping in Fig. 9. The behavior of the structure is similar to the model systems based on edge and center-cracked plates in tension and edge-cracked beams in bending. Reducing the system damping can create decreasing driving forces and driving force gradients for fatigue crack advance. This is pertinent where fatigue testing is required for different environments. For the case of the fatigue characterization structure used by the authors, Q increases by several orders of magnitude for the audio-frequency resonator between atmospheric pressure ( $Q \sim 100$ ) and moderate vacuums of around 1 milli-Torr  $(O \sim 10,000)$ . Consequently, one would expect the mechanical loading (as well as the environmental) conditions to be significantly different for tests conducted in these two environments. This subtle, but important, interaction between the resonant

loading conditions and the driving force for crack advance can be further clarified by directing attention to the range of normalized crack length relevant to the fatigue behavior of polycrystalline silicon structural films (i.e., a/(W - D) < 0.015). The stability of these small fatigue cracks is shown as a function of the system damping in Fig. 9(b). It is well established that small-scale resonant fatigue tests conducted in air at atmospheric pressure lead to failure of the micromechanical structure (Fig. 10). This is a direct consequence of the fact that fatigue cracks in the structure during resonant loading are subjected to a monotonically increasing gradient in stress-intensity factor range when the damping in the system is relatively high (e.g.,  $Q \sim 100$ ), as shown in Fig. 9(b). However, if the damping in the system is reduced by conducting the test in vacuum, the driving force for fatiguecrack growth (after an initial increase) decreases as the crack grows (Fig. 9(b)). This crack arrest process is a direct result of the rapid unloading of the resonating specimen that occurs as the compliance increases when the damping in the system is relatively low (e.g.,  $Q \sim 10,000$ ). This phenomenon can lead to confusion when interpreting the results of micromechanical fatigue tests.

Conducting tests in controlled environments is a crucial aspect of understanding the mechanisms of fatigue-crack growth. However, the results of the lumped parameter model establish that great care must be taken when interpreting micromechanical resonant fatigue data generated by testing in vacuum. Firstly, it is possible to mistake the transient increase and subsequent decrease in observed fatigue crack-growth rates as an indication of an interfacial cracking phenomenon involving a compliant layer on a stiff substrate (Beuth, 1992). Fortunately, this error can be avoided simply by evaluating the microstructure of the material. More importantly, fatigue crack-growth rates must be lower and fatigue lives must be longer for tests conducted in vacuum compared to those performed in air because of the lower stressintensity factor amplitude and the decreasing stress-intensity factor gradient. This behavior is independent of any environmentally-assisted crack-growth process. Therefore, there is a critical distinction that must be made between resonant

fatigue testing in air, "inert" atmospheres, and in vacuo. Specifically, tests in vacuum not only remove active species from the atmosphere, but also alter the driving force for fatigue-crack growth by changing the loading conditions.

One should note that analyses of resonant fatigue systems are limited by the ability to adequately model the loading conditions and by the behavior of the system as the crack becomes an appreciable fraction of the specimen. For example, the inhomogeneous distribution of stress in macroscopic resonant fatigue specimens complicates the evaluation of the stress-intensity factor (Schoeck, 1982). Fortunately, this is not a problem in the mass-spring systems used in micromechanical fatigue structures. However, in both continuous and mass-spring systems the load ratio of -1 is problematic, as the opposing faces of the crack come into contact during the compression portion of the loading cycle (and even earlier if crack-closure phenomena are active). In this study, as with most fracture-mechanics analyses, this problem is alleviated by computing the stress intensity in terms of the tensile portion of the cycle only; for this reason, the driving force results are presented in terms of  $K_{\text{max}}$ . Additionally, at long crack lengths the difference in compliance during the opening and closing portions of the loading cycle introduces significant nonlinearity in the cracked mass-spring oscillator. Furthermore, out-of-plane bending and torsional modes tend to couple with the in-plane bending mode at large normalized crack lengths (Van Arsdell, 1997). These factors can limit the range of applicability of the lumped model and finite element results. Fortunately, cracks observed experimentally in the micromechanical fatigue characterization structure modeled in this paper are usually very short (e.g., with  $a/(W-D) \ll 0.1$ ), such that these limitations are insignificant.

When the finite element and lumped parameter models are used to interpret the stress-life fatigue behavior of polysilicon, a variety of important observations can be made. If the damage accumulation (i.e., the decrease in resonant frequency) during the fatigue test is assumed to be due to the formation of a crack, the crack length can be readily determined as a function of time (Fig. 11).

While this is a simplification of the fatigue degradation process, experimental observations of cracks in structures are consistent with the observed changes in natural frequency (Muhlstein et al., 2002a,b). The crack-growth behavior determined from the change in natural frequency of the specimen (Fig. 11) suggests that the crackgrowth rates are decreasing as the crack advances. This behavior has been observed for microstructurally-small cracks, cracks growing under displacement control, cracks growing into residual stress fields, and cracks approaching interfaces. In the present case, the effect is likely related to several of these factors acting in concert, as detailed in Muhlstein et al. (2002b). If the crack-driving force at failure is taken as an estimate of the fracture toughness, the toughness of the material can be determined. The crack length estimates at failure were used with plane-strain models of the stressintensity for the notched cantilever beam structure. Results from the polysilicon fatigue tests (Fig. 13) give an average fracture toughness of  $\sim 0.85$ MPa  $\sqrt{m}$ , with critical crack sizes in the range  $\sim$ 5.5–66 nm depending on the applied stress amplitude. As prior studies (Muhlstein et al., 2002a,b) have indicated that the oxide thickness at the notch is on the order of 100 nm, it is clear that the crack initiation, growth and final (overload) processes during thin-film silicon fatigue all occur within the native oxide. The measured toughness value of  $\sim 0.85$  MPa  $\sqrt{m}$  is thus indicative of the fracture toughness of the amorphous silica reaction layer.

#### 5. Conclusions

Based on experimental and numerical analyses of resonating micromechanical fatigue structures used in micron-scale testing of structural silicon films, which incorporate experimental observations and finite element (quasi-static and dynamic) and lumped dynamic models, the following conclusions may be made:

1. The notched cantilever-beam fatigue characterization structure behaves as a lumped massspring oscillator (within 0.7%). The idealized clamped boundary conditions for the structure introduce error of  $\sim 7\%$  to the maximum principal stress at the root of the notch through the estimate of the specimen compliance.

- 2. The notch in the cantilever beam of the fatigue characterization structure influences the compliance and stress-intensity factor solutions. The influence of the notch on the maximum principal stress field falls off at a rate proportional to  $1/r^2$ , and the effects of the notch are most important within 0.65 µm of the root (i.e., a/(W D) < 0.1). This corresponds to the range of crack lengths generally of interest for stress-life fatigue characterization in micronscale structures made from brittle materials.
- 3. The dynamic response of the fatigue characterization structure is extremely sensitive to crack length. Although the relationship is nonlinear, a 1 nm extension in crack length corresponds to  $\sim$ 1 Hz change in natural frequency for short cracks.
- 4. The presence of a centrally located hole in notched micromechanical fatigue characterization structures prevents complete separation of the test specimen by blunting the crack when the resonator is driven at a fixed excitation frequency.
- 5. Fatigue crack stability in micromechanical resonators driven at a constant frequency at, or near, the natural frequency of the structure is a function of the damping characteristics of the system. Specimens in micromechanical fatigue characterization structures are subjected to force-controlled, displacement-limited loading conditions. Lowering the damping in the system, e.g., by testing in vacuo, can lead to crack arrest from purely mechanical factors. This effect must be considered in the evaluation of results from controlled environment testing using this test geometry.
- 6. Fatigue lives measured in vacuo using micromechanical fatigue resonators cannot be directly compared to atmospheric pressure data due to differences in the gradient of the applied stress-intensity range. Independent of environmental effects, fatigue crack-growth rates must be lower and fatigue lives must be longer for micromechanical resonant fatigue tests conducted

in vacuum compared to atmospheric pressure environments.

7. During the fatigue of thin-film polysilicon, calculated critical crack sizes ranged from ~5.5 to 66 nm depending on the applied stress amplitude; the average toughness value was found to be 0.85 MPa  $\sqrt{m}$ . These results, together with previous studies, suggest that the processes of crack initiation, growth and final overload failure all occur within the native oxide layer.

#### Acknowledgements

This work was funded by the Director, Office of Science, Office of Basic Energy Research, Division of Materials Sciences and Engineering of the US Department of Energy under Contract no. DE-AC03-76SF00098 (for R.O.R.). The authors wish to thank Dr. S.B. Brown for his prior support, Dr. W. Van Arsdell for the original specimen design, and Dr. J.M. McNaney for helpful discussions.

# Appendix A. Forced, damped, mass-spring system equations of motion

In contrast to the systems used for macroscopic ultrasonic fatigue testing, most micromechanical fatigue characterization structures can be modeled as forced, damped, mass-spring oscillators (e.g., (Van Arsdell, 1997; Van Arsdell and Brown, 1999)). The deformation of the structure is localized to the test specimen and the attached mass, m, reduces the natural frequency,  $f_0$ , of the system. If we assume that the damping in the system is proportional to the velocity of the mass, dx/dt, and the stiffness of the specimen is given by k, the motion of the system may be described by the following second-order differential equation:

$$\frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + f_0^2 x = \frac{F_0}{m} \cos(f \cdot t),$$

$$\frac{k}{m} = f_0^2,$$

$$\frac{b}{m} = \gamma,$$
(A.1)

where x is the position of the center of mass at time, t, and f is the frequency of the applied force,  $F_0$ . The damping parameter,  $\gamma$ , is the ratio of the velocity-dependent resistive force, b, to the mass. Solutions to this equation are routinely derived in introductory texts on dynamics (e.g., French, 1971). It is convenient to introduce the quality factor,  $Q = f_0/\gamma$ , as a measure of the damping characteristics of the system. With this added notation, the solution of the amplitude of motion as a function of excitation frequency, A(f), is given by

$$A(f) = \frac{\frac{F_0}{m}}{\left[ \left( f_0^2 - f^2 \right) + \left( \frac{f \cdot f_0}{Q} \right)^2 \right]^{\frac{1}{2}}}.$$
 (A.2)

For rotational systems, e.g., where the angular rotation is a function of an applied moment, the rotational stiffness,  $k_{\theta}$ , and the mass polar moment of inertia,  $J_{\theta}$ , are used to describe the stiffness and mass of the system, respectively.

#### References

- Allameh, S.M., Gally, B., Brown, S., Soboyejo, W.O., 2000. On the evolution of surface morphology of polysilicon MEMS structures during fatigue. In: Kahn, H., de Boer, M., Judy, M., Spearing, S.M. (Eds.), Materials Science of Microelectromechanical System (MEMS) Devices III. Boston, MA. MRS, Pittsburgh, PA, pp. EE2.3.1–EE2.3.6.
- Anderson, T.L., 1995. Fracture Mechanics: Fundamentals and Applications, second ed CRC Press, Boca Raton.
- ASTM, 2001a. E 466 standard practice for conducting force controlled constant amplitude axial fatigue tests of metallic materials. Annual Book of ASTM Standards, vol. 03.01. ASTM, West Conshohocken, PA.
- ASTM, 2001b. E 647 standard test method for measurement of fatigue crack growth rates. Annual Book of ASTM Standards, vol. 03.01. ASTM, West Conshohocken, PA.
- Ballarini, R., Mullen, R.L., Yin, Y., Kahn, H., Stemmer, S., Heuer, A.H., 1997. The fracture toughness of polysilicon microdevices: a first report. Adv. Appl. Mech. 12, 915–922.
- Beuth Jr., J.L., 1992. Cracking of thin bonded films in residual tension. Int. J. Solids Struct. 29, 1657–1675.
- Broek, D., 1986. In: Martinus, N. (Ed.), Elementary Engineering Fracture Mechanics, fourth ed. Kluwer, Dordrecht; Boston: Hingham, MA.
- Brown, S.B., Van Arsdell, W., Muhlstein, C.L., 1997. Materials reliability in MEMS devices. In: Senturia, S. (Ed.), Proceedings of International Solid State Sensors and Actuators Conference (Transducers '97). IEEE, Chicago, IL, USA, pp. 591–593.

- Chati, M., Rand, R., Mukherjee, S., 1997. Modal analysis of a cracked beam. J. Sound Vib. 207, 249–270.
- Chen, C.P., Leipold, M.H., 1980. Fracture toughness of silicon. Am. Ceram. Soc. Bull. 59, 469–472.
- Chondros, T.G., Dimarogonas, A.D., Yao, J., 1998. A continuous cracked beam vibration theory. J. Sound Vib. 215, 17– 34.
- De Rijk, P., 1970. Empirical investigation on some methods for stopping the growth of fatigue cracks, TR 70021. National Aerospace Institute.
- Fitzgerald, A.M., Dauskardt, R.H., Kenny, T.W., 1999. Fracture toughness and crack growth phenomena of plasma-etched single crystal silicon. Sens. Actuators A A83, 194–199.
- Franke, A.E., Jiao, Y., Wu, M.T., King, T.J., Howe, R.T., 2000. Post-CMOS modular integration of poly-SiGe microstructures using poly-Ge sacrificial layers. Solid-State Sensor and Actuator Workshop (TRF Cat. No. 00TRF-0001) Technical Digest. Solid-State Sensor and Actuator Workshop. Hilton Head Island, SC, USA. Transducers Res. Found., pp. 18–21.
- French, A.P., 1971. Vibrations and Waves. Norton, New York.
- Gonzalez, A.C., Pantano, C.G., 1990. A compression-loaded double cantilever beam specimen. J. Am. Ceram. Soc. 73, 2534–2535.
- Greek, S., Ericson, F., Johansson, S., Schweitz, J.A., 1997. In situ tensile strength measurement and Weibull analysis of thick film and thin film micromachined polysilicon structures. Thin Solid Films 292, 247–254.
- Greek, S., Ericson, F., Johanasson, S., Furtsch, M., Rump, A., 1999. Mechanical characterization of thick polysilicon films: Young's modulus and fracture strength evaluated with microstructures. J. Micromech. Microeng. 9, 245–251.
- Kahn, H., Ballarini, R., Mullen, R.L., Heuer, A.H., 1999. Electrostatically actuated failure of microfabricated polysilicon fracture mechanics specimens. Proc. Royal Soc. A 455, 3807–3823.
- Kahn, H., Tayebi, N., Ballarini, R., Mullen, R.L., Heuer, A.H., 2000. Fracture toughness of polysilicon MEMS devices. Sens. Actuators A A82, 274–280.
- Kapels, H., Aigner, R., Binder, J., 1999. Fracture strength and fatigue of polysilicon determined by a novel thermal actuator [MEMS]. In: Proceedings of the 29th European Solid-State Device Research Conference. Leuven, Belgium. IEEE, Chicago, IL, pp. 1522–1528.
- Lawn, B.R., 1993. Fracture of Brittle Solids, second ed Cambridge University Press, Cambridge, New York.
- Mahmoud, M.A., Zaid, M.A., Harashani, S.A., 1999. Numerical frequency analysis of uniform beams with a transverse crack. Commun. Numer. Meth. Eng. 15, 709–715.
- Mayer, H., 1999. Fatigue crack growth and threshold measurements at very high frequencies. Int. Mater. Rev. 44, 1–34.
- McGuire, S.M., Fine, M.E., Achenbach, J.D., 1995. Crack detection by resonant frequency measurements. Metall. Mater. Trans. A 26A, 1123–1127.
- Muhlstein, C.L., Brown, S.B., Ritchie, R.O., 2000. High cycle fatigue of polycrystalline silicon thin films in laboratory air.

In: Kahn, H., de Boer, M., Judy, M., Spearing, S.M. (Eds.), Materials Science of Microelectromechanical System (MEMS) Devices III. Boston, MA. MRS, Pittsburgh, PA, pp. EE5.8.1–EE5.8.6.

- Muhlstein, C.L., Brown, S.B., Ritchie, R.O., 2001a. High-cycle fatigue and durability of polycrystalline silicon films in ambient air. Sens. Actuators A 94, 177–188.
- Muhlstein, C.L., Brown, S.B., Ritchie, R.O., 2001b. High-cycle fatigue of single crystal silicon thin films. J. Microelectromech. Syst. 10, 593–600.
- Muhlstein, C.L., Stach, E.A., Ritchie, R.O., 2002a. Mechanism of fatigue in micron scale films of polycrystalline silicon for microelectromechanical systems. Appl. Phys. Lett. 80, 1532– 1534.
- Muhlstein, C.L., Stach, E.A., Ritchie, R.O., 2002b. A reactionlayer mechanism for the delayed failure of micron-scale polycrystalline silicon structural films subjected to highcycle fatigue loading. Acta Mater. 50, 3579–3595.
- Noda, N.A., Sera, M., Takase, Y., 1995. Stress concentration factors for round and flat test specimens with notches. Int. J. Fatigue 17, 163–178.
- Noda, N.A., Takase, Y., 1999. Stress concentration formulae useful for any shape of notch in a round test specimen under tension and under bending. Fatigue Fract. Eng. Mater. Struct. 22, 1071–1082.
- Ritchie, R.O., 1999. Mechanisms of fatigue-crack propagation in ductile and brittle solids. Int. J. Fract. 100, 55– 83.
- Saxena, A., Muhlstein, C.L., 1996. Fatigue crack growth testing (fracture and fatigue). In: Lampman, S.R. (Ed.), ASM Handbook, vol. 19. ASM International, Materials Park, OH, pp. 168–180.
- Schoeck, G., 1982. Calculation of the stress intensity in ultrasonic resonance. Z. Metall. 73, 576–578.
- Sharpe, W.N., Brown, S., Johnson, G.C., Knauss, W., 1998. Round-robin tests of modulus and strength of polysilicon. In: Brown, S., Gilbert, J., Guckel, H., Howe, R., Johnson, G., Krulevitch, P., Muhlstein, C. (Eds.), Microelectromechanical Structures for Materials Research. Materials Research Society, San Francisco, CA, pp. 57–65.
- Sharpe, W.N., Turner Jr., K.T., Edwards, R.L., 1999. Tensile testing of polysilicon. Exp. Mech. 39, 162–170.
- Simmons, G., Wang, H., 1971. Single Crystal Elastic Constants and Calculated Aggregate Properties: A Handbook, second ed M.I.T. Press, Cambridge, MA.
- St. John, C., 1975. The brittle-to-ductile transition in precleaved silicon single crystals. Philos. Mag., 1193–1212.
- Stanzl-Tschegg, S., Mayer, H., 2001. In: Stanzl-Tschegg, S., Mayer, H. (Eds.), Proceedings of the International Conference on Fatigue in the Very High Cycle Regime. University of Agricultural Sciences, Vienna, Austria.
- Suresh, S., 1998. Fatigue of Materials, second ed Cambridge University Press, Cambridge, England.
- Tada, H., Paris, P.C., Irwin, G.R., 2000. The Stress Analysis of Cracks Handbook, third ed ASME Press, New York.
- Tatsumi, Y., Ohsake, H., 1988. Properties of Silicon. IEE, London, UK, pp. 3– 6.

C.L. Muhlstein et al. | Mechanics of Materials xxx (2003) xxx-xxx

- Tsuchiya, T., Sakata, J., Taga, Y., 1997. Tensile strength and fracture toughness of surface micromachined polycrystalline silicon thin films prepared under various conditions. In: Cammarata, R.C., Nastasi, M., Busso, E.P., Oliver, W.C. (Eds.), Thin-Films-Stresses and Mechanical Properties VII. Boston, MA, USA. Mater. Res. Soc, Pittsburgh, PA, pp. 285–290.
- Tsuchiya, T., Tabata, O., Skakata, J., Taga, Y., 1998. Specimen size effect on tensile strength of surface-micromachined polycrystalline silicon thin films. J. Microelectromech. Syst. 7, 106–113.
- Van Arsdell, W., 1997. Ph.D. Dissertation, Massachusetts Institute of Technology.

- Van Arsdell, W.W., Brown, S.B., 1999. Subcritical crack growth in silicon MEMS. J. Microelectromech. Syst. 8, 319–327.
- Van Leeuwen, H.P., 1970. The repair of fatigue cracks in lowalloy steel sheet, TR 70029. National Aerospace Institute.
- Van Oosten Slingeland, G.L., Broek, D., 1973. Fatigue Cracks Approaching Circular Holes. Delft University.
- Wong, B., Holbrook, R.J., 1987. Microindentation for fracture and stress-corrosion cracking studies in single-crystal silicon. J. Electrochem. Soc. 134, 2254–2256.
- Yokoyama, T., Chen, M.C., 1998. Vibration analysis of edgecracked beams using a line-spring model. Eng. Fract. Mech. 59, 402–409.