Polysilicon MEMS fatigue and fracture characterization via on chip testing

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SUMMARY. In order to characterize the fatigue behaviour and determine the fracture energy of polysilicon used in micro-systems, an on-chip testing device has been designed and fabricated. The experimental set-up is able to continuously measure the elastic stiffness decrease and therefore to evidence fatigue of polysilicon 15-μm thick films and to allow for the introduction of a sharp crack at the notch of the tested specimen. A fracture test can be carried out, and, by combining experimental data and numerical simulations in the context of linear elastic fracture mechanics, an estimate of fracture energy can be obtained. In the paper it is also shown that numerical, cohesive approaches taking into account for the polycrystalline morphology can adopt the obtained fracture energy data in order to reproduce the experimental crack path.

1 INTRODUCTION

Polysilicon thin film fatigue [1] mechanisms are neither fully qualitatively understood, nor quantitatively characterized: in fact, in the literature a wide spreading exists between experimental fatigue data for polysilicon [2, 3, 4] because of material polycrystalline structure, whose grain size is comparable with specimen overall dimensions (mainly thickness) and because of the influence of micro-defects.

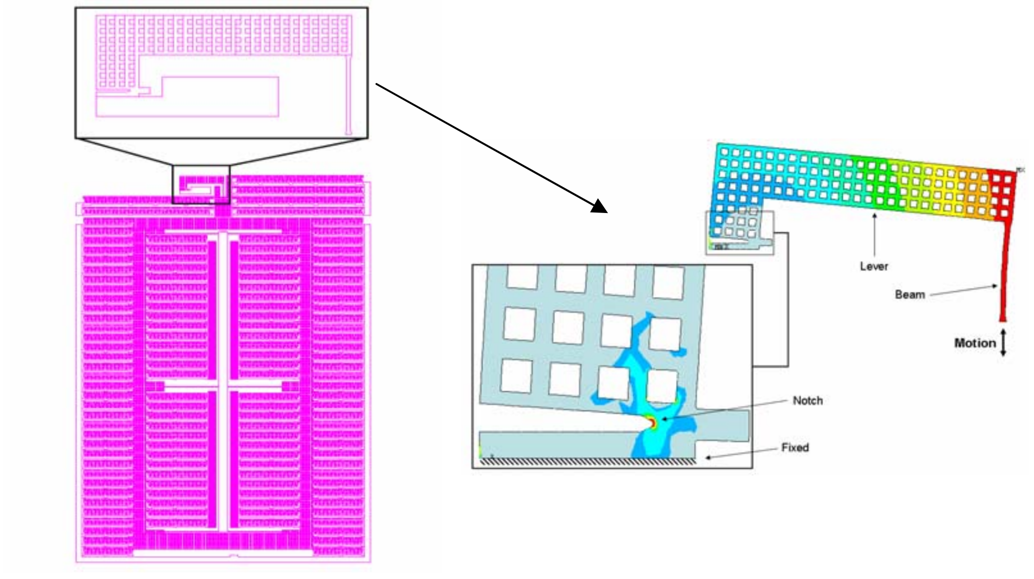
Polysilicon fracture characterization remains also difficult, because of dependence of fracture parameters on specimen size, measurement technique, and, again, the presence of defects. Moreover, mainly indirect experimental approaches must be followed for Micro Electro Mechanical Systems (MEMS) differently from the standardized techniques adopted at the macro-scale. Taking into account polysilicon MEMS, a classification for these approaches distinguishes between *off-chip* and *on-chip* testing, being the former related to some actuating and sensing apparatus external to the MEMS (e.g. load cells, micro-regulation screws, or micro-indentation [5]) and the latter related to mechanical parts for actuating and sensing built with the same micromachining process used for the MEMS.

In this work an on-chip test structure (see [6], [7]) is adopted to obtain fatigue and quasi-static fracture tests for epitaxial polysilicon obtained via the THELMA^{TM} process by STMicroelectronics. By means of a combined experimental-numerical procedure, values of critical fracture energy G_{IC} for polysilicon are obtained. The experimental results are also compared with a numerical finite element simulation of the fracture process based on the use of cohesive interface elements.

2 ON-CHIP TESTING AND EXPERIMENTAL RESULTS

A micro-system was designed and built for the on-chip execution of fracture and fatigue tests on the epitaxial polysilicon, *epipoly*, produced with the THELMA^{TM} process by STMicroelectronics (Figure 1a). The thickness of the material is 15 μm, this value is large enough to require a complex actuation mechanism in a plane parallel to the one of the wafer and able to bring the specimen up to rupture; the actuation mechanism is based on a set of comb finger capacitors, a very common choice for MEMS structures. The multi-comb finger capacitive actuator is used in order to apply a force directed in the plane of the MEMS structure to a lever system which concentrates the imposed stress to a very localized zone where a notch is machined (see boxed zoom in Figure 1a and Figure 1b). This layout aims to replicate the macro-scale configurations (like e.g. a compact tension specimen) typical of fracture and fatigue tests. Sensing, instead, is obtained with interdigitated comb fingers similarly disposed as for actuation. The whole device takes up a 1600 x 2250 μm^2 rectangular area. A more detailed description of the device can be found in [6], [7].

When a voltage difference is applied to the device, the comb-finger actuators move and load the device as shown in Figure 1b. The capacitance change of the sensing part is measured and related to the displacement imposed on the extremity of the load beam through an electrostatic relation. This causes the rotation of the lever arm and the creation of the desired state of stress in the notch. The force produced by the actuator for every imposed voltage is computed again using an electrostatic relation. From this information it is then possible to obtain the force versus displacement responses of the device.



(*a*) (*b*)

Figure 1: The experimental device. (a) Overview, in the boxed zoom: detail of the fracture specimen. (b) Deformed shape of the specimen and contour plot of principal tensile stress of the notched zone.

The MEMS structures used in this work are tested in a clean room environment directly on the wafer. Basic mechanical parameters, like the elastic stiffness, the damping coefficient and the resonance frequency, have been evaluated from experimental *C*-*V* curves and downward step responses curves [7]. Fatigue tests are carried out by imposing sinusoidal load signals in the range $R = \sigma_{\max}/\sigma_{\max} = -0.3 \div +0.6$.

The fatigue experimental procedure can be also used to obtain pre-cracking during fracture tests, henceforth assuring the sharp crack condition at the crack tip, a non trivial task at the micro-scale (see, e.g., [8]). Once the sharp crack is obtained, a monotonic load is applied until the specimen is broken, i.e. the crack has propagated through the ligament.

As shown in section 3, by combining the results of numerical simulations with the experimental ones, it is possible to compute the value of the fracture energy by the measurement of the crack length, the estimate of the stress intensity factor at the current crack size through linear elastic fracture mechanics and the determination of the value for which the crack restarts propagation.

In order to start the fracture test having more sharply separated surfaces, fatigue cycles are applied to the MEMS test device with the aim to create small micro-cracks, beginning at the notch root, from which the fracture will start propagation. The complete experimental procedure is resumed below.

- The peak displacement of the MEMS movable mass during fatigue cycles is continuously monitored by means of the electronic readout setup; an increase in the peak displacement is ascribed to an elastic stiffness decrease, caused by the nucleation of a micro-crack.
- Taking into account the statistical data obtained during a previous fatigue campaign [7], [9], it is known the range of elastic stiffness decrease that a device can survive before catastrophically reaching the rupture.
- Taking into account previously obtained final fracture paths [9], simulations are performed in order to evaluate the relationship between the elastic stiffness decrease in the said range and the crack propagation length into polysilicon. These simulations will be described in section 3.
- Each device is stressed up to a certain, monitored, elastic stiffness decrease. The fatigue cycles are then interrupted and the estimated micro-crack length is evaluated with the aid of the simulations.
- The device is then monotonically driven to the fracture by means of a slowly increasing force applied through 10 mV increasing voltage steps on the actuator capacitance.

Fatigue test results are collected in Figure 2. It is observed that while the $R > 0$ case excluded rupture for this material up to 10^9 cycles, fatigue life appears to decrease significantly when compressive stresses are applied at the lever system ($R < 0$).

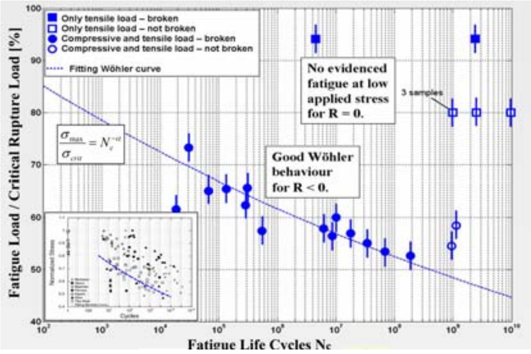


Figure 2: Fatigue test results.

As explained above, the experimental setup allows to quantify the decrease in the capacitance during the fatigue crack propagation and to link this decrease to the stiffness degradation of the structure. An example of experimental determination of elastic stiffness decrease is shown in Figure 3.

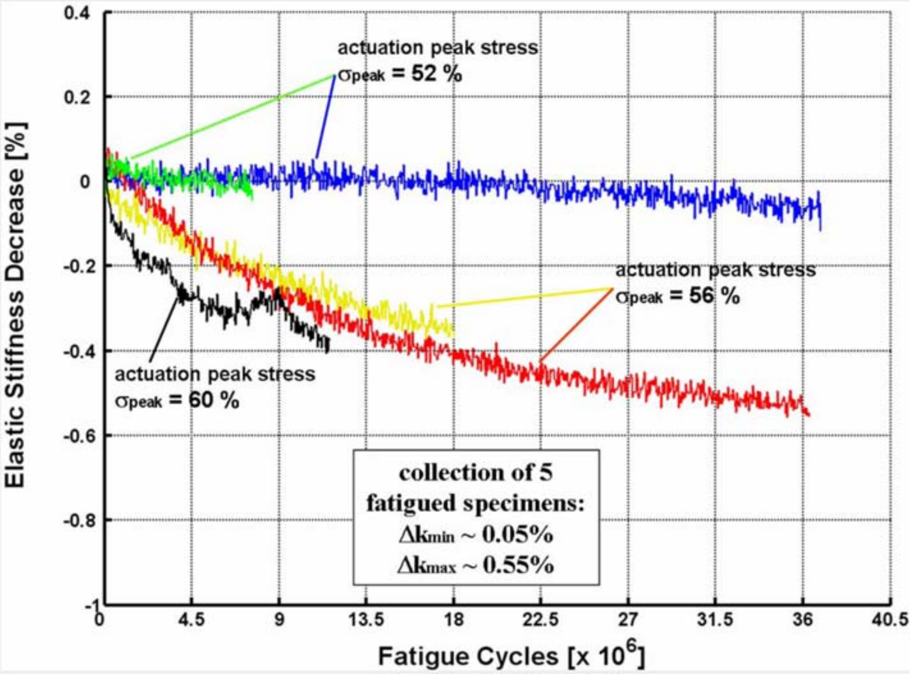


Figure 3: Elastic stiffness degradation during fatigue tests.

Typical fracture tests data are represented by load-displacement curves which remain almost straight up to complete rupture (see Figure 4).

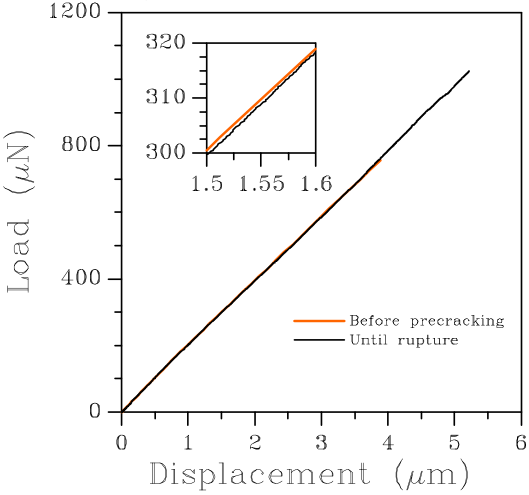


Figure 4: Typical fracture test.

3. EVALUATION OF FRACTURE ENERGY AND NUMERICAL SIMULATION OF CRACK PROCESSES

2.1 .*Estimate of fracture energy with linear elastic fracture mechanics*

We make the (crucial) assumption that the decrease in the elastic stiffness Δk, experimentally obtained, is linked to crack growth at the notch apex. Moreover, linear elastic fracture mechanics hypotheses and isotropic elasticity in the plane transversal to silicon grain growth are assumed. A set of linear elastic finite element simulations of the specimen at varying fixed crack length are then carried out in order to numerically compute the stiffness of the system. The true crack path, i.e. as observed through optic microscope during one specific test, is adopted for the simulations. The crack path remains almost straight during the very first 100-150 nm crack propagation, while it deviates after about 1 μm; this is mainly due to the rotation of principal stress directions (see Figure 6).

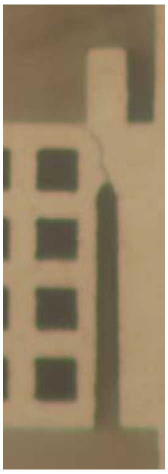


Figure 5: Experimentally determined crack path.

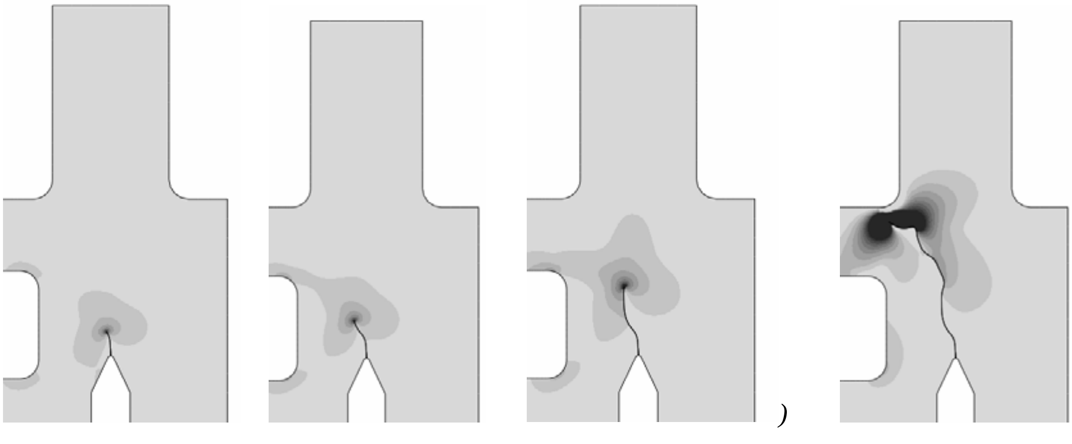
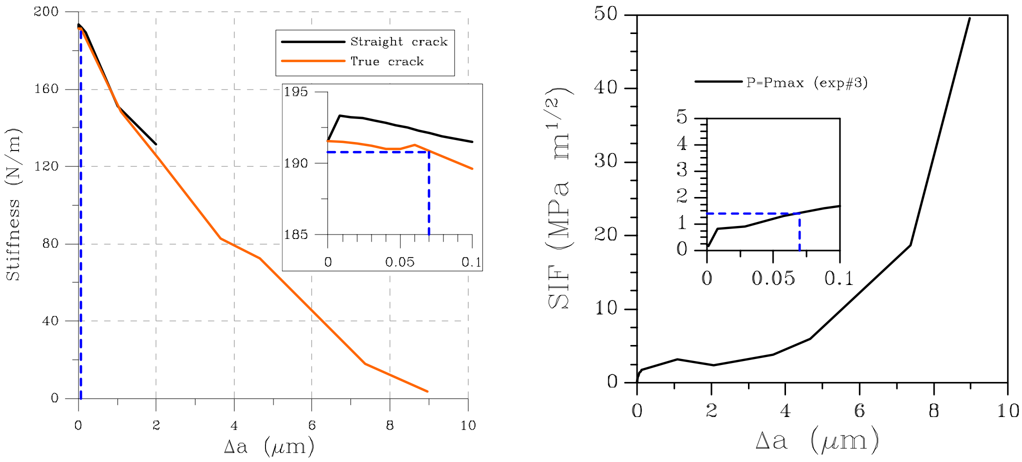


Figure 6: Maximum principal stress near the crack tip at growing crack length.

The procedure leading to the estimate of the critical stress intensity factor K_{IC} (or, equivalently, of mode-I fracture energy G_{IC}) can be resumed into the following steps.

1. *Experiment.* The original, un-cracked specimen is loaded monotonically in the elastic regime in order to evaluate the original stiffness S_0; then, fatigue pre-cracking is carried out, stopping it before a critical configuration is reached; finally, a monotonical load is again applied up to rupture, registering the maximum load P_{max}, the corresponding displacement u_{max} and the stiffness of the cracked specimen $S_{cracked}$.
2. *Numerical simulations*. The specimen stiffness $S(a)$ is numerically computed as a function of crack length (see Figure 7a); in the framework of linear elastic fracture mechanics (LEFM) the mode-I stress intensity factor (SIF) K_I (a,P) is computed as a function of the applied load at varying crack length according to the actual crack path (see Figure 7b);.
3. *Parameter identification*. The experimental stiffness $S_{cracked}$ is introduced in figure 7a in order to compute an estimate of the crack length a_{num} after fatigue pre-cracking. The obtained numerical crack length a_{num} is adopted as an input for the numerical relationship K_I (a_{num}, P_{max}) at the experimental maximum load, thus obtaining the value of SIF from Figure 7b.



(*a*)

(*b*)

Figure 7: (a) Stiffness decrease due to crack extension (LEFM). (b) Stress intensity factor for increasing crack length (experiment #3, at P_{max}=1024 N, LEFM).

The decrease in stiffness registered in step 1 is very small and collocates itself in the initial "plateau" zone (see the small box in Figure 7a) where very small stiffness variations are evidenced. This is also true for the region where K_{IC} is estimated (see Figure 7b, small box). As an example, for experiment #3, stiffness decrease is about 0.36%, the numerical crack length a_{num} turns out to be 70 nm and the SIF reads 1.42 MPa m$^{1/2}$. Other results and the values of G_{Ic} are shown in Table 1.

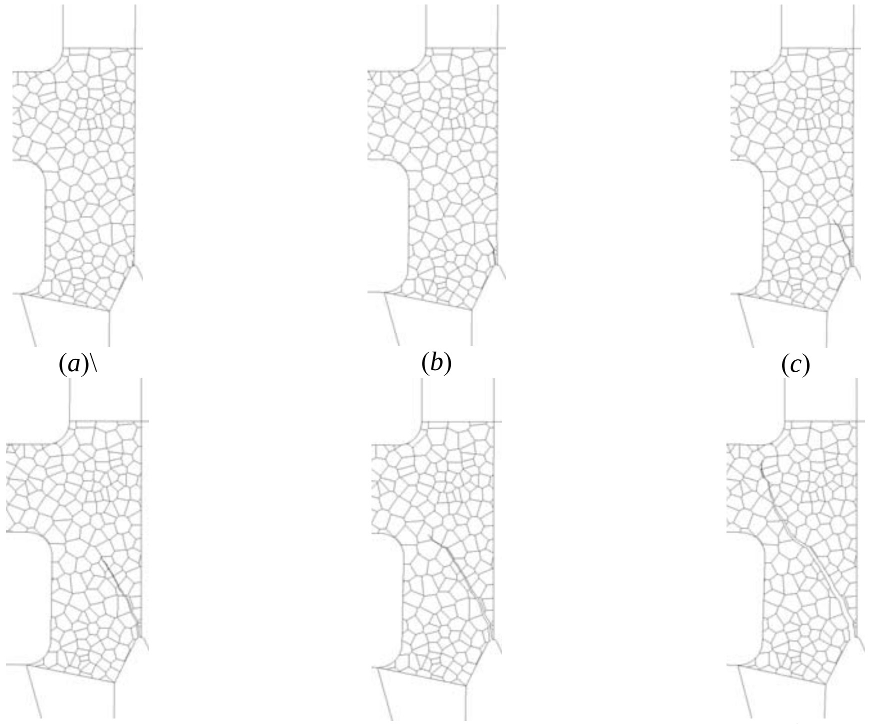
Experiment	Stiffness decrease %	a_{num} (μm)	K_{IC} (MPa m$^{1/2}$)	G_{IC} (N m^{-1})
1	0.63	0.069	1.41	13.44
2	0.20	0.058	1.31	11.60
3	0.70	0.071	1.43	13.77

Table 1: LEFM evaluation of fracture energy by crossing numerical and experimental data

3.2. *Crack initiation and propagation by means of cohesive crack finite element model*

In order to further check the consistency of the experiments discussed in Section 2 and of the identification procedure for the polysilicon fracture energy discussed in sub-section 3.1, the obtained data have been used for the numerical simulation of crack initiation and propagation in the tested specimens by means of a finite element code developed and described in previous works (see e.g. [10]). The code allows for the 2D numerical simulation of a polycrystalline solid and has the following main features: grain topology is created by means of a Voronoi tessellation algorithm; the single grains can have an anisotropic elastic behaviour and random orientation; pure and mixed mode fracture is modelled through a linear softening cohesive behaviour; interface elements are automatically introduced at the boundary of adjacent quadratic triangular finite elements whenever a critical conditions is locally reached; interface elements can be inserted either between continuum elements inside grains or between grain boundaries; different inter-granular and trans-granular behaviours can be reproduced; dynamic relaxation analysis with an explicit time integration algorithm is adopted.

Figure 8 shows a sequence of crack evolution for experiment # 3, automatically computed with the above briefly described finite element model. The results can be directly compared with the crack path shown in Figure 5.



(*a*)\ (*b*) (*c*)

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Figure 8: Sequence of crack evolution during fracture
(crack propagation including grain microstructure).

An example of the numerical and experimental load-displacement curves is shown in Figure 9 again for experiment #3.

The resulting load-displacement curve, while capturing the quantitative main experimental features, shows small deviations from the linearity. In particular, the simulation evidences local rising of the stiffness, and a similar behaviour is also registered experimentally. Even if the lack of knowledge of the actual grain morphology make it impossible to quantitatively describe these local phenomena, the simulation gives qualitatively hints to the causes: these uprisings can be related to crack propagating towards grains with an elastic modulus higher than the previous ones along the crack direction. When the crack changes again its path and it encounters a lower elastic modulus grain, the stiffness decreases again.

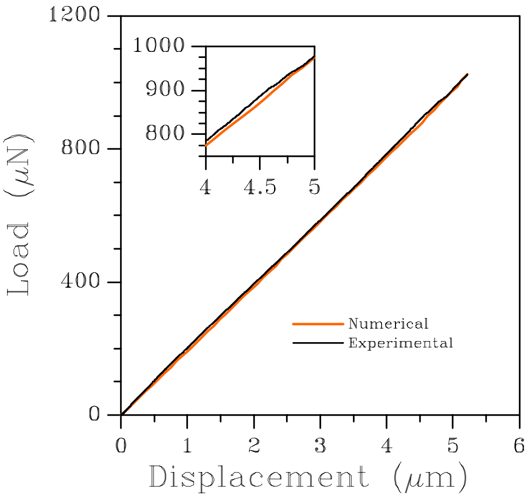

Figure 9: Comparison of numerical and experimental results by simulation with cohesive approach.

4. CONCLUSIONS

In this work fatigue and fracture tests with on-chip MEMS device have been discussed. A mixed experimental/numerical identification procedure leading to the determination of fracture energy G_{IC} of polysilicon has been proposed. Numerical simulations taking into account the morphology at the polycrystalline length-scale confirm the consistency of the numerical model and of the identification procedure.

Acknowledgements

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