Damage assessment in multilayered MEMS structures under thermal fatigue

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Abstract
This paper reports on the application of a Physics of Failure (PoF) methodology to assessing the reliability of a micro electro mechanical system (MEMS). Numerical simulations, based on the finite element method (FEM) using a sub-domain approach was used to examine the damage onset due to temperature variations (e.g. yielding of metals which may lead to thermal fatigue). In this work remeshing techniques were employed in order to develop a damage tolerance approach based on the assumption that initial flaws exist in the multi-layered.

1. Introduction
Physics of Failure (PoF) methodologies have become well established tools for evaluating the risks of failure in electronics [1]. The Polynoe Programme is committed at improving the understanding, the modelling and the prediction of the reliability of DC MEMS switches through a PoF approach [1]. Typical failure modes observed in MEMS devices and their packages include fatigue, interface delamination, and die cracking. In particular, delamination can cause shorting or mechanical impedance [2]. This research aims, firstly, to understand the effects of temperature variations as a possible cause of damage, such as yielding in the metal layers, and subsequent failure (e.g. interfacial delamination, fracture) in multilayered MEMS packages. The particular MEMS considered in this work are DC MEMS switches, but the methodology is applicable to a range of devices manufactured using similar technology. However, the construction of full-scale finite element models of MEMS devices such as DC switches which are detailed enough to accurately resolve the stresses within each region of the model is difficult due to their complex geometry. Hence, an accurate determination of local stresses can be achieved by the use of a sub-domain or representative volume element (RVE) in which the effect of temperature variations on the global stress/strain field at the local micro-structural scale of the device can be computed more accurately [3]. The sub-domain adopted in this study is three-dimensional (3D) which allows the determination of accurate and realistic tri-axial stress/strain fields within the FE model. This methodology consents to a detailed understanding of the effects of thermal loading conditions on the stress/strain distribution at micro-structural level and in particular near the materials interfaces [4, 5]. The second part of this study aims to simulate the delamination in metal layers caused by high stress gradients. In fact, the high stress gradients, due to the material mismatch, might lead to inter-layer damage with the presence of cracks. In this paper a conceptual model is presented for a software framework, based on the remeshing tool Zencrack combined with FE code ABAQUS [6], which allows efficient and automatic simulation of non-planar 3D crack propagation.

2. 3D Finite Element Modelling
2.1. Micromechanical model
The full-scale numerical model of the multilayered DC MEMS switch used in this research is shown in figure 1 and figure 2. The switch in figure 1 consists of suspended metal beams (e.g. nickel) that can be activated using electrostatic forces to make contact with the opposite gold contact electrodes. The sub-domain of MEMS used in this study, which allows the application of a vast combination of boundary conditions to simulate realistic situation, is depicted in figure 3 and figure 4.
The numerical model has been developed by assuming an ideal Si(100) layer of 20µm [7] with uniform material properties. The non-metal layers are forced to undergo the same average displacement \( \langle u \rangle \) along the x-axis (face B1 in figure 3) and y-axis (face B2 in figure 3). The average displacement \( \langle u \rangle \) can be expressed by the following equation:

\[
\langle u \rangle = \frac{1}{V} \int_{\Psi} u(x) \, dV
\]

where \( \Psi \) is the non-metal region of the representative volume element of the DC MEMS (grey area in Figure 2). Therefore, the kinematic constraint in \( \Psi \) are:

\[
\begin{align*}
  u_x (W,y,z) &= \langle u \rangle \\
  u_y (x,W,z) &= \langle u \rangle
\end{align*}
\]

where \( u_x \) and \( u_y \) are the displacement along the x- and y- axes respectively and W is the width of the representative volume element (RVE) along the x- and y-axes. The bottom face at \( z = 0 \) is constrained along the z-axis. Symmetric boundary conditions are applied in the planes at \( x = 0 \) and \( y = 0 \), therefore the displacements are:

\[
\begin{align*}
  u_x (0,y,z) &= 0 \\
  u_y (x,0,z) &= 0
\end{align*}
\]

The top face at \( z = H \), is free to move on the z-direction. The faces A1 and A2 in the metal regions, ideally, undergo an average displacement \( \langle U \rangle \) (i=number of metal layers). The average displacements \( \langle U \rangle \) can be expressed by the following equation:

\[
\langle U \rangle = \frac{1}{V} \int_{\Omega} U_i(x) \, dV
\]

where \( \Omega \) are the metal layer regions of the representative volume element. However, the layers of different materials are assumed to be perfectly bonded together at their interfaces and because of their different coefficient of thermal expansion (CTE) under thermal loading the final distorted shape is different from the ideal configuration (figure 5a). A more realistic deformed shape is shown in figure 5b.
In FE results presented in Maligno et al. [7] have highlighted that these boundary conditions represent a critical configurations especially in the plating base where damage is to be expected due to the effect of a highly localised stress/strain field.

2.2. Materials

Metal multi-user MEMS processes (MetalMUMPs) provide a procedure for constructing micro devices [8]. The metal part of the RVE is composed of three layers, i.e., plating copper base (0.55 µm), electroplated nickel (20 µm) and a top layer of gold (0.5 µm), as shown in figure 1(b). The MetalMUMPs process flow [8] also describes the naming convention for the various layers. The non metal layers are composed by:

1. N-type (100) silicon (Si).
2. Silicon Oxide (SiO2).
3. Silicon Nitride (Si3N4).
4. Polysilicon.
5. Polysilicon.

All of the materials properties used in this research are temperature-dependant. The variation of $E$ (GPa) and the coefficient of thermal expansion $\alpha$ (°C$^{-1}$) with the temperature for the nickel are [9-13]:

\[
\begin{align*}
E(T) & \approx 230 \cdot (1-0.000286T) \\
\alpha(T) & = 13 \cdot 10^{-6} \cdot (1+0.000343T)
\end{align*}
\]

The nickel layer undergoes a linear kinematic hardening material behaviour and the kinematic strain hardening rate $H$ (i.e. the slope of the uniaxial stress–strain curve beyond yielding) has been experimentally evaluated to be 4GPa (+2%). For the plating copper (Cu) base, the material properties of the passivated copper films and the kinematic hardening model been considered. The linear dependence of initial yield strength with temperature can be described by the following relationship [13]:

\[
\sigma_y = \sigma_0 \cdot \left(1 - \frac{T}{T_0}\right)
\]

where $\sigma_y$ is the initial yield strength, $T$ is temperature, and $\sigma_0$ and $T_0$ are reference constants. For passivated copper films, reliable results have been obtained with $\sigma_0=305$MPa, $T_0=1090K$ and $H=77$GPa [17]. For the thin gold layer an elastic-perfectly plastic constitutive model has been adopted to simulate the material behaviour. The materials properties obtained by several sources, e.g. [14-18], are summarised in Table-1.

2.3 Loading conditions for thermal fatigue analysis

In the present analysis, the temperature variation applied to estimate the life of the multilayered RVE under the described boundary condition is a cyclic thermal loading: from 0°C to 150°C. Moreover, effects of residual stresses arising during manufacturing processes were considered. In fact, electroplated metal thin films comprising nickel, copper and gold are commonly used for micro-electromechanical systems (MEMS) as they provide a simple technology with superior material properties and device performances. It is known that the microstructure and mechanical properties of a plated thin film depend upon the plating conditions such as temperature, concentration and current density [20]. Thus, in this study, an attempt to understand the effect of temperature on residual stress build-up has been investigated. Electroplating processes in general take place at relatively low temperatures (≤140°C) [7]. In Maligno et al [7] was also shown that, in general, starting from temperatures of circa 80°C, yielding processes are likely to occur in the plating base (Cu layer). Therefore, to take into account the effect of the fabrication process, the loading conditions include a thermal cooling from 80°C to 0°C followed by a cyclic thermal loading from 0°C to 150°C. Thermal cooling from the initial temperature has been applied to all the layers. Moreover, the metal layers have been assumed to undergo the same time-independent cooling rate. The materials are assumed to be stress free. The total induced strain of the layers due to thermal cooling can be expressed as:

\[
\begin{align*}
\sigma_y = \sigma_0 \cdot \left(1 - \frac{T}{T_0}\right)
\end{align*}
\]
\[ \text{de}_{ij} = \delta_{ij} \alpha(T) dT \]

where \( \text{de}_{ij} \) is the total strain increment, \( \alpha(T) \) the thermal expansion coefficient which is dependent on the temperature, \( dT \) the temperature change and \( \delta_{ij} \) is the Kronecker delta.

### 2.4 Loading conditions for crack propagation analysis

The crack propagation studies are based on the linear elastic fracture mechanics (LEFM) approach. The sub-domain used in the fracture mechanics studies has been slightly modified by adding a portion of a cantilever beam of DC MEMS switches (figure 1). In the present analysis, initially two temperature variations have been applied in order to investigate the effect of the boundary conditions on failure onset within the multilayered MEMS structure, namely:

- Cyclic thermal loading: from 0°C to 150°C.
- Cyclic thermal loading: from -50°C to 150°C.

Also, a cyclic displacement in the z-direction has been superimposed to the cyclic thermal load to take into account the higher strains measured in the plastic FE analyses and, to consider the displacements of the cantilever beam during the DC MEMS switches functioning life. Therefore, according to the Polynoe Programme’s mission profiles, two different displacements have been applied:

- Axial Displacement (z-direction): 0.1\( \mu \)m and 0.5\( \mu \)m (figure 6a)
- Bending Displacement (z-direction): 0.1\( \mu \)m and 0.5\( \mu \)m (figure 6b)

### Table 1: Mechanical and thermal properties of the MEMS materials

| Material   | \( E \) (GPa) 20°C | \( E \) (GPa) 400°C | \( \nu \) (20°C) | \( \nu \) (400°C) | \( \alpha(T) \) (10\(^{-6}\), °C\(^{-1}\)) 20°C | \( \alpha(T) \) (10\(^{-6}\), °C\(^{-1}\)) 400°C | \( \sigma_y \) (metal) (20°C) | \( \sigma_y \) (metal) (400°C) | \( \sigma_{ult} \) (non-metal) (MPa) 20°C | \( \sigma_{ult} \) (non-metal) (MPa) 400°C |
|------------|---------------------|---------------------|-----------------|-----------------|---------------------------------------------|---------------------------------------------|---------------------------|---------------------------|-----------------------------|-----------------------------|
| Ni         | 20                   | 110                 | 370             | 143             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |
| Cu         | 400                  | 93                  | 19.6            | 52              | Equation (2)                                | Equation (3)                                | 486                                     | 460                                      | 3790                         | 2000                        |
| Au         | 20                   | 75                  | 14.2            | 5.2             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |
| SiO\(_2\)  | 400                  | 59.7                | 15.02           | 4.7             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |
| SiN\(_4\) | 20                   | 71.4                | 0.52            | 3.1             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |
| Si         | 400                  | 71.4                | 0.25            | 4.8             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |
| Polysilicon|                     | 260                 | 0.28            | 4.7             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |
|            |                     | 130                 | 0.23            | 2.6             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |
|            |                     | 160                 | 0.23            | 4.2             | Equation (2)                                | Equation (3)                                | 155                                     | 486                                      | 3790                         | 2000                        |

### 3. Local Stress Analysis

Yielding is detected at the temperature of approximately 65°C in the copper plating base. The FE analyses have shown that the applied loading and boundary conditions are of vital importance on the yielding onset. The Cu plating base undergoes severe stress concentration at the interface with the Polysilicon. Due to the effect of the highly stiffer non-metallic substrates the Cu film shows only totally negligible displacement at the Cu/Polysilicon interface. The high interfacial stresses generate the initial yielding onset and, a probable, successive interfacial delamination. The trend of the von Mises and Tresca stresses along the edge of the sub-domain are shown figure 7 at Cu/Polysilicon interface. FE
results have proven that the Tresca failure criterion is more conservative (circa 13.5%) than the von Mises criterion. According to the two failure criteria, the corner of the sub-domain at the Cu/Polysilicon and the edges of the Cu thin film, at Cu/Polysilicon interface, are particularly at risk of failure. The Cu/Ni interface displays lower levels of stress (at the same temperature) and no yielding has been detected within the gold (Au) and nickel (Ni) film layers (figure 8).

4. Thermal Cycle Analysis

Critical combinations of thermal loadings and boundary conditions might lead to damage (such interfacial delamination) in MEMS packages. The analyses have shown that the most critical area is represented by the thin copper plating base and in particular at the interface with the Polysilicon in which high stress gradients arise. Similar results have been found by research partners of the Polynoe programme, which investigated, experimentally and numerically, analogous multilayered structures under temperature cycling. High stress is localised in copper anchor of the suspended beam (figure 9).

For that reason, it is paramount that FE analyses aims to the life estimation copper layer under the thermal loading conditions prescribed by the mission profiles of the Polynoe Programme.

4.1 Coffin-Manson Rule

To estimate the fatigue failure of the copper plating base, the Coffin–Manson relationship of the form [19] has been adopted:

\[ \frac{\Delta \varepsilon^{pl}}{2} = \varepsilon_f (2N_f)^c \]

where \( \Delta \varepsilon^{pl} \) is the plastic strain amplitude, \( c \) is known as the fatigue ductility exponent, that in general varies from -0.5 to -0.7 for metals, \( (2N) \) is the number of strain reversals (cycles). The ductility \( \varepsilon_f \) of copper is smaller than the ductility of bulk copper [20-23]. Thus, in this study a ductility of 20% [19] has been assumed. Reliable strain changes in the Coffin–Manson rule can be obtained from multiple thermal cycles calculations since the metal layers undergo complex plastic deformation. These temperature cycles are illustrated in figure 10. The cycles between 0°C and 150°C are repeated until the change in the magnitude of the plastic strain reaches a steady-state value (figure 11). At the present stage of this research five cycles have been simulated. The equivalent plastic strain \( \varepsilon^{pl} \) is defined by the following relationship:

\[ \varepsilon^{pl} = \varepsilon_0 + \int_0^t \dot{\varepsilon}^{pl} \, dt \]

where \( \varepsilon_0 \) is the initial equivalent plastic strain and for classical metal (von Mises) plasticity:
\[ \dot{\epsilon}_{pl} = \sqrt{\frac{2}{3} \epsilon_{pl} : \epsilon_{pl}} \] (7)

where \( \dot{\epsilon}_{pl} \) represents the plastic strain rate tensor. The plastic strain magnitude \( p \) is defined by:

\[ p = \sqrt{\frac{2}{3} \epsilon_{pl} : \epsilon_{pl}} \] (8)

where \( \epsilon_{pl} \) is the plastic strain tensor. Both are scalar measures of the accumulated plastic strain. For proportional loadings, the measures should be equal [20]. Nevertheless, for loading with reversals, the equivalent plastic strain will continue to increase if the plastic strain rate is non-zero (regardless of sign). Therefore, plastic strain magnitude is the favourite measure and to estimate the life of the copper film, the plastic strain magnitude (PEMAG) has been considered. The plastic strain magnitude has been evaluated in critical areas of the sub-domain (e.g. at the Cu/Polysilicon interface) in which delamination or fracture initiation are expected to take place.

![Figure 10. Applied cyclic loading.](image1)

![Figure 11. Average value of the plastic strain.](image2)

### 4.2 Fatigue life estimation

Two set of analyses were performed, namely: non-residual stress analysis and residual stress analysis. In these analyses no time dependant behaviour of the materials was introduced. The results of the analyses for two extreme values of the parameter \( c \) are presented in Table-2 and table-3.

| Maximum \( \Delta \epsilon_{pl} \) (%) | Parameter \( c \) | Fatigue Life \( N_f \) |
|-----------------------------------|----------------|----------------------|
| 1.84                             | -0.5           | ≈170                 |
|                                  | -0.7           | ≈40                  |

Table 2. Life estimation of the plating base film: non residual stress analysis

| Maximum \( \Delta \epsilon_{pl} \) (%) | Parameter \( c \) | Fatigue Life \( N_f \) |
|-----------------------------------|----------------|----------------------|
| 0.16                              | -0.5           | ≈589                 |
|                                  | -0.7           | ≈78                  |

Table 3. Life estimation of the plating base film: residual stress analysis. Cooling from 80°C to 0°C.

The comparison of the results in Table-2 and Table-3 shows a beneficial effect of the residual stress in the overall life estimation of the RVE. In fact, the manufacturing processes cause the warped shape of the copper plating base after the cooling process (figure 12a) and, in a residual stress/strain field. The application of thermal cycling loading (with an initial increasing temperature) tends to lessen this warping (figure 12b) and consequently the residual stress field.

![Figure 12. Warped shape after manufacturing processes (a) and reduced deformed shape at increasing temperatures (b).](image3)
5. Fracture Mechanics Studies

5.1 FE modelling of crack growth

The development of complex fracture planes seen in real components can in general be simulated in software by the application of appropriate modelling techniques and mixed mode fracture mechanics principles. For this work the commercial software Zencrack in combination with the FE code ABAQUS have been used to simulate fatigue crack growth in multi-layered MEMS structures. In this research the software has been adapted to describe the crack evolution in thin film in order to avoid mesh and structural distortion during the remeshing.

5.2 Crack growth criteria

In order to predict linear elastic fracture mechanics (LEFM) crack growth using FE method, three basic parameters are required: stress intensity factors (SIF), crack propagation direction (CPD) and crack growth material models, for example, the Paris equation [21]. There are several approaches to calculating SIFs such as: the crack tip opening displacement (CTOD) approach [22], the crack tip stress field approach [23] and the SIF extraction method from J-integral [24]. In the present work the SIFs are extracted from the J-integral using the method of Asaro and Shih [20], based on the following equation:

\[ J = G = \frac{1}{E} \left( K_{II}^2 + K_{III}^2 \right) + \frac{1}{2G} \left( K_{I}^2 \right) \]  

(9)

where \( E = \frac{E}{1-\nu^2} \) for three-dimensional problems. The quarter-point node technique is used by Zencrack to model the crack-tip singularity. Under mixed mode conditions it is necessary to introduce an equivalent stress intensity factor, \( K_{eq} \), considering Mode-I, II and III simultaneously. Several formulae have been proposed for \( K_{eq} \) and the most commonly used expression is [25]:

\[ K_{eq} = \sqrt{K_{I}^2 + K_{II}^2 + (1+\nu)K_{III}^2} \]  

(10)

In order to determine new crack front positions, the CPD must be computed. The maximum energy release rate criterion or the \( G \)-criterion has been adopted in these investigations. The \( G \)-criterion states that a crack will grow in the direction of maximum energy release rate. The CPD, \( \theta = \theta_0 \), is then determined by:

\[ \frac{dG}{d\theta} \bigg|_{\theta=\theta_0} = 0, \]

\[ \left( \frac{dG}{d\theta} \right)^2 \bigg|_{\theta=\theta_0} \leq 0. \]  

(11)

Numerous numerical techniques can be used to compute \( G \) such as the path independent J-integral [26, 27] and the virtual crack extension (VCE) method [27, 28]. The VCE method was applied in this research.

5.2.1 Virtual crack extension directions

At any node on a 3D crack front a “normal plane” can be defined. This is a plane that is orthogonal to the crack front tangent at the node. A series of virtual crack extensions in the normal plane will produce a distribution of energy release rates. This is shown schematically in figure 13 as energy release rate values \( G_1 \) to \( G_7 \). At some angle to the local crack plane the energy release rate will be a maximum. \( G_{\text{max}} \) denotes this maximum energy release rate. The value of \( G_{\text{max}} \) and the corresponding angle is calculated for use in crack growth prediction.

![Figure 13. Typical energy release rate distribution at a point on a crack front](image)

5.3 Remeshing techniques

A crucial problem in 3D fracture mechanics is related to mesh generation for the FE analysis. The approach that has been adopted in this research is the use of a ‘sub modelling’ strategy which models the details of the crack region. In figure 14 is presented the use of the ‘sub modelling’ methodology in generating a cracked mesh from a user-supplied
intact component. The initial crack is placed within the copper plating base and its position is equidistant (0.25µm) from the nickel and Polysilicon layer. The initial crack dimensions are 0.1µm and 0.05µm which represent optimal values and avoid too severe mesh distortion.

Figure 14. Submodelling techniques (a), details of crack block: rectangular crack shape (b) and quarter-circle crack shape(c).

6. Crack growth results
A number of factors which may influence the crack propagation in thin film have been examined in these investigations, namely: initial crack shape, loading condition and cryogenic temperature.

6.1 Effect of initial crack shape.
Two different crack shapes have been evaluated, namely:
1) Wall-through or rectangular shape (figure 15).
2) Quarter-circle shape (figure 16).

The numerical analyses have shown that the crack direction, which has been determined with the maximum energy release rate criterion, is not influenced by the different crack shape, loading conditions and, the crack dimensions as displayed in figure 15 and figure 16. In particular, the crack evolves toward the Cu/Ni interface. The overall effect of different loading conditions is to increase/decrease the crack growth rate toward the nickel layer.

Figure 15. Rectangular crack shape: initial crack (a), final crack growth (b).

Figure 16. Quarter-circle crack shape: initial crack (a), final crack growth (b).

6.2 Effect of loading condition
The critical energy release rate ($G_c$) of the copper used in this study is 0.4 J/m² [29].

The application of thermal cycling determines a safe loading condition, in fact numerical analyses show that the $G_c$ is never reached (figure 17). In figure 17 three different loading combinations are considered for the rectangular crack shape. The coupled thermal-mechanical loadings with a displacement of 0.1µm are more likely to cause the drastic failure of the copper plating base and in particular the coupled thermal/bending displacement cycling is very likely to fail at very early stage of the crack initiation. A very drastic malfunction of the MEMS switches could be caused by the sudden failure of the copper layer if higher displacements are applied. In figure 18 it is clear that a bending displacement of 0.5µm leads to values of the critical energy release rate far beyond the $G_c$ of the copper plating base.
As far as the quarter-circle crack shape under thermal cycle loading from 0°C to 150°C, the $G_c$ is obtained for crack extension above 0.1µm as depicted in figure 19.

6.3 Effect of cryogenic temperature
A critical parameter to consider in the design of DC MEMS switches is the temperature variation and the temperature dependant material properties which has been investigated from 0°C to 150°C.

Nevertheless, in aerospace and defence applications it is worthwhile to investigate the effect of cryogenic temperatures. In this research we will study the effect of thermal cycling from -50°C to 150°C according to the mission profiles suggested by the Polynoe Programme partners. Numerical analyses on MEMS RVE under thermal cycling with a quarter-circle shape, which represents the most critical crack configuration, have been performed. The FE simulations show the detrimental effect of cryogenic temperature on the crack propagation (figure 19). In fact for initial crack dimensions equal or above 0.1µm, the critical energy release rate (and the radical failure of the copper layer) is achieved at zero-cycles.

7. Conclusion
A FEM study has been performed on multilayered MEMS structures to evaluate the reliability of these components under different loading conditions. This study is based on a sub-domain approach. The numerical simulations have shown that the most vulnerable area of multilayered MEMS switches is represented by the copper plating base. Strong stress gradients arises within the copper film due to the different material behaviour between the Cu/Polysilicon interface and Cu/Ni interface. The life estimation of copper layer is also influenced by the presence of residual stresses. Fracture mechanics studies have demonstrated that several factors could influence the drastic failure of the copper plating base and cause the malfunctions of the DC MEMS switches. In particular coupled thermal-bending displacements cyclic loadings and cryogenic temperature are very likely to lead to premature delamination of the copper layer. The effects of residual stresses on crack-growth evolution are currently being investigated. Also, the comparison of different methods and criteria for the determination of crack growth parameters (e.g. energy release rate) is also under evaluation.
Acknowledgments

This research is funded by the European Defence Agency (EDA) through the POLYNOE Programme.

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