Coupled Analysis of Fracture Mechanics and Piezoelectricity in Active Layers in the Abaqus Code Operated through the Isight Tool

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Abstract: *This paper describes a new computational approach aimed at investigating the crack propagation inside smart structures equipped with surface bonded piezoelectric layers, when the electromechanical coupling due to piezoelectric phenomenon is exploited. The Abaqus code is used to perform a prediction of both the fracture mechanics and the coupled response of the structure, through a suitable connection between the two solution environments, being provided by the Isight tool. A preliminary analysis is shown and some significant results are proposed.*

Keywords: *Composites, Coupled Analysis, Crack Propagation, Dynamics, Fracture, Piezoelectric Structures, Smart Materials.*

1. Introduction

Piezoelectric materials are exploited in several smart structures for actuation, sensing, energy harvesting and health monitoring purposes [1]. An increasing demand of industry concerns a reliable prediction of failure mechanism of piezoceramic layers in case of fracture, fatigue and creep. In some application like actuation, vibration energy harvesting and health monitoring this task looks extremely relevant for the design activity, because of loading conditions applied and of functions provided by the smart material. A key issue is currently the analysis of crack propagation through the piezoelectric layer while its active behavior is exploited [2]. Analytical methods already proposed in the literature may be ineffective when geometry of structure is rather complicate, or structural behavior is nonlinear, like in case of a large vibration amplitude [3]. Therefore a reliable computational approach to cope with those cases is a goal of the current research activity performed in this field.

Basically crack propagation has to be investigated in association with the piezoelectric phenomenon either in condition of direct or indirect effect, i.e. when mechanical strain induces an electric charge distribution within the material or electric field applies a mechanical strain through the electromechanical coupling. The Finite Element Method (in the following simply FEM) is highly recommended as a recognized approach also by some technical standards where 'design by rules' is substituted by a 'design by analysis', during an advanced step of design operation. Commercial codes provide nowadays the numerical tools for a straight analysis of the electromechanical coupling between strain and voltage in piezoelectric continuous media, as well as crack behavior is described by calculating the so–called 'Stress Intensity Factor' (SIF) within the region around the tip and the 'J–integral' is used to calculate the energy release rate of crack [4]. Those calculations allow predicting even the crack path. In case of a coupled system the fracture mechanics has to be associated to local effects induced by the piezoelectric phenomenon. The Abaqus code is daily used to investigate both the fracture mechanics [5] and the piezoelectric effect, but these analyses are performed separately. In present case numerical solutions of the two above mentioned problems were connected and coupled by means of the ISIGHT tool. This approach allowed investigating in details the reaction applied by the electromechanical coupling to the crack propagation at the tip. A complete procedure was defined and a numerical tool was built up as they are herein described together with some preliminary numerical results.

2. Coupled behavior of smart piezoelectric structures

To clarify the goal of the proposed analysis it can be briefly summarized herein the context of applications and the cases to be investigated. In active vibration control some piezoelectric layers are surface bonded on a main structure or embedded inside. They are either used as an actuator to apply a control action, by exploiting the imposed electric field, or as a sensor, by resorting to direct piezoelectric effect, which allows monitoring the mechanical strain of the structure. In both roles very often actions are not so large to induce a severe failure of piezoelectric layers, in regular operation. In fact, in case of structural health monitoring (SHM) goal is detecting a damage occurring inside the structure and piezoelectric layers might be exposed to a failure, if crack reaches the interface between smart material and main structure. Moreover, vibration energy harvesting (VEH) is aimed at recovering some amount of energy being usually dissipated by resorting to a suitable conversion into electric charge. It can be then used as an autonomous power supply to operate some sensor. In this case very often vibration amplitude is sufficiently large to increase the risk of crack nucleation either on the structure or directly on the piezoelectric, thus making prediction of its propagation critical for the reliability of the whole system. These applications of piezoelectric transducers were fairly recently proposed and they made the issue of describing the crack behavior in presence of electromechanical coupling a relevant topic of mechanics of smart materials. This goal is even more strategic at microscale, as in micro–electro–mechanical systems (MEMS).

According to the above mentioned issues, crack propagation is currently analyzed in:

- piezoelectric structures, without any other structural support, in case of both the roles of actuator and sensor, even in self–sensing configuration;
- damaged structures with surface bonded sensors for SHM, to detect an early transition of crack from the structure to the piezoelectric layer;
- in VEH, to analyze the crack propagation rate and its path through the composite structure.

A suitable computational process was therefore assessed to cover all the above mentioned cases.

3. Phenomenology of crack propagation in piezoelectric layers

It is known that crack propagation is effect of mechanical load applied to material surrounding the crack tip, being the rate of propagation depending on the energy balance and on the opening mode in fracture (I,II,III). Path strictly depends on load, constraints, material and mode. State of stress and crack length are both relevant for propagation, therefore in the literature the 'Stress Intensity Factor' (SIF), namely K, was defined to consider both those contributions to predict the propagation and in particular its stability, in comparison to the material toughness, for a given fracture mode, being referred to as K_c. Rate of propagation is finite until that SIF is lower than toughness, but as soon as it overcomes this value, crack proceeds very fast, in practice unstably [4].

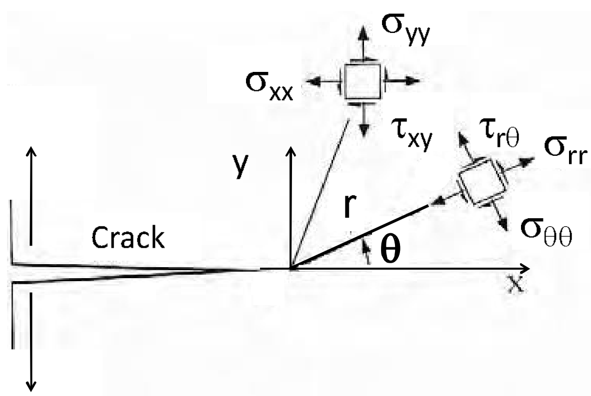

Figure 1. Description of stress components around the crack tip.

Basically, for simple geometries, SIF is defined by some analytical approach in a local reference by using polar coordinates as the distance from the crack tip, r, and its angular location, θ, with respect to the crack line and to the opening mode, e.g. SIF (K) and stress components (σ_{ij}) are related as follows :

$$\sigma_{ij} = \frac{K_I}{\sqrt{2\pi r}} f(\theta) \quad (1)$$

From the computational point of view crack tip is corresponding to a singularity, i.e. to a very sharp notch, which needs to be analyzed by a suitable numerical approach, being able to follow the opening mode and to recognize the non–holonomic (variable with both the configuration and time) compatibility of boundary conditions associated to the displacements inside the material. Energy released rate of crack is usually computed by resorting to the J–integral (JI). It describes the energy of a region around the crack tip limited by a selected contour as C_1 and C_2 in Fig.2. This integral is applied to the total length of contour C, it is defined by a local coordinate s and by a orthogonal versor n, and includes the density of elastic energy associated to strain, W_e, the stress applied to the contour, σ_{ij}, and the corresponding mechanical displacement, u.

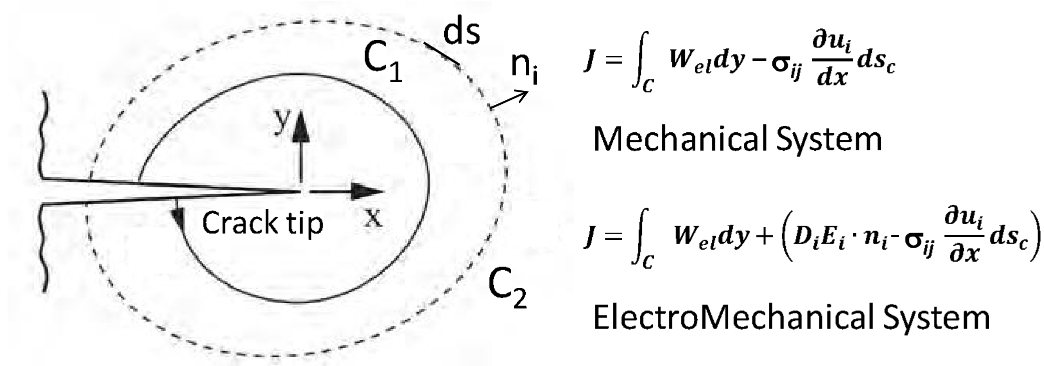

Figure 2. Definition of J-integral applied to fracture mechanics of a mechanical system and to piezoceramic material.

Crack propagation can be investigated by resorting to the well known relation between J–I, referred to as J, and the energy release rate, G [4]:

$$J = \mathrm{G} = -\frac{\partial \mathrm{W}}{\partial \mathrm{a}} \tag{2}$$

where W describes the total energy associated to the crack system, while a is the crack length. Some authors ([2],[3]) investigated the role of piezoelectric effect upon the crack propagation through analytical approaches, by including into the J–I the electromechanical energy associated to the electric field (Fig.2). Electromechanical coupling in piezoelectric material is described by the coupled constitutive laws of material as follows:

$$T_{ij} = C_{ijkl}(S_{kl} - S'_{kl}) - e_{kij}E_k$$
$$D_i = e_{ijk}\left(S_{jk} - S'_{jk}\right) + \epsilon_{ij}E_j + P_i \tag{3}$$

According to the Standards of Piezoelectricity [1], symbols are defined. Mechanical stress components are T_{ij} (instead of σ to avoid any misunderstanding with surface electric charge) and strains are S_{kl}, being S'_{kl} the residual strain induced by polarization P_i. C_{ijkl} are the elastic coefficients, being e_{kij} the piezoelectric coefficients. E_k is the electric field and D_i is the electric displacement along a given direction i, while $\in_{ij}$ is the dielectric permittivity of material. The main problem in case of industrial applications is that geometry sometimes does not allow an easy prediction of coupled behavior in presence of crack. Moreover, in many commercial Finite Element codes the two analyses, dealing with fracture mechanics and piezoelectric effect, are usually run separately in different tasks of numerical solution.

Behavior of material around the tip is strictly important to define the propagation rate, the path and the stress distribution. It is known that in ductile material plastic behavior at tip may decrease the propagation rate and affects the stress distribution, since a local yielding effect occurs. A sort of stop–and–go transition occurs in propagation, being due to material hardening around the tip, if opening effect is sufficiently large. In case of active piezoelectric layer electric charge distribution changes with opening, because it is coupled with the mechanical strains and new free surfaces are generated. This effect may introduce an electromechanical attraction between the two crack lips, being depending on the electric nature of crack. It can be permeable, impermeable or semi-permeable to the electric charge. Around the tip stress concentration may even affect the electric field and can induce some local electromechanical actions, which superpose to the mechanical behavior. All those phenomena may have a large influence upon the crack propagation, although they depend on the direction of piezoelectric polarization and of crack, respectively.

4. Numerical method

A first activity was herein performed to investigate the case of Linear Elastic Fracture Mechanics (LEFM) of coupled metallic and piezoceramic specimens. According to the literature this is a main task to be considered, although under certain operating conditions metallic structure might undergo yielding, being herein neglected. The literature proposed some numerical approaches to investigate the fracture behavior as Finite Elements, Boundary Elements, Meshless methods and the so–called Extended Finite Element Method (XFEM), being available in the Abaqus code. The XFEM extends the classical Finite Element Method (FEM) approach, because it allows analyzing discontinuities in the displacement field, like those due to the crack opening. Therefore the main goal of numerical simulation was coupling the analysis of crack propagation, being based on the XFEM, which is associated to the computation of SIF, JI and crack path, to the prediction of the electric charge distribution, voltage and related stress occurring within the piezoelectric material. A sequential approach was implemented, i.e. electromechanical coupling was investigated by applying the mechanical load and predicting a preliminary crack propagation, then computing the displacements around the tip, thus starting an analysis of piezoelectric phenomenon to calculate the stress induced around the tip. Mechanical loading conditions were then updated and procedure was iterated up to the occurring of an unstable propagation, when it could be reached.

4.1 Use of the Abaqus code

The Abaqus code is used to perform the prediction of crack propagation and to investigate the piezoelectric effect. It is applied first to model the geometry of the structure and to define and locate the initial crack. Properties of materials are inputted, but features are different for metals and piezoceramics. Elastic properties and mechanical strength are provided to the code in both cases, but piezoelectric material needs that orientation is assigned, together with piezoelectric coefficients. Volumes of crack and structure, respectively, are merged as separated parts inside the model, then meshed, as soon as element type, shape and mesh technique are selected. A dynamic implicit solution is used to predict the crack opening, as a nonlinear geometric solution whose time steps time are kept sufficiently small to assure the numerical convergence, within a given maximum number of increments. Crack is created by Abaqus code through the XFEM approach, to predict the propagation for a given loading condition and known constraints. Contour integral option is used to calculate JI and SIF. Results consist for the fracture mechanics module of crack growth maps, crack angles and crack propagation rate. A dedicated module of the code deals with the electromechanical behavior of piezoelectric layers. Finite elements with piezoelectric properties are associated to numerical solutions which include both the stress and strain analysis and the distribution of voltage and electric charge, respectively, for given boundary conditions. In particular, constraints in this case include mechanical inhibition of some degree of freedom (displacement and rotation) and similar boundary conditions applied to voltage and charge.

Loading conditions consist of static and more often dynamic mechanical actions and of applied electric fields. A complete electromechanical coupling is therefore created. This allows converting the mechanical energy into an electric storage and electric energy into a mechanical work.

4.2 Use of the Isight tool

As it was previously stated the Abaqus software is unable to perform a prediction of the fracture mechanics and of an active piezoelectric material by taking into account its electromechanical coupling. A suitable procedure to create a link between the fracture mechanics and the piezoelectric analysis could be tested by resorting to an integrated model, being developed into the Isight environment. This tool is currently used to combine cross–domain models to provide a unique simulation process flow. Execution is automated, since the Isight tool can manipulate and transfer numerical data between two process steps and run multiple simulations. In this case it allowed introducing all the required piezoelectric properties inside the process flow performed to predict the calculation of JI and SIF and the crack propagation when piezoelectric layers react to the mechanical loading because of the electromechanical coupling.

5. Development of the simulation flow

Structure is first modeled inside the Abaqus code, by providing all the mechanical properties of material and relevant information about crack (load, boundary conditions, geometry, initial length), then it is meshed. To input the electrical properties of the piezoelectric layer the same geometry is modeled as a separated case, through some piezoelectric elements. Prediction of fracture in presence of piezoelectric phenomenon is performed by running the two analyses as a sequence, thus making the two above mentioned models interacting each other, inside the Isight tool. As Fig.2 shows the tool developed computes the SIF and the JI by resorting to a concatenation of computational loops.

5.1 Use case 1: piezoelectric operated as a sensor or as a vibration energy harvester

When piezoelectric layer just behaves like a sensor, i.e. no external voltage is applied, model of the cracked structure described into the Abaqus code is transferred into the Isight tool in subroutine 'Crack' which computes SIF and JI, as it does in case of a metallic structure. Results are then collected by 'Post–Crack' module and used in 'Piezo' section, together with the second model including the piezoelectric elements. Displacements induced by the mechanical actions applied to the piezoelectric layer and the voltage distribution is computed by through the typical solution performed in case of dynamic behavior of a piezoelectric material. It is appreciated that the new configuration of voltage actually induces a local piezoelectric effect upon material, which affects the boundary conditions of load around the crack tip. Therefore displacements just computed are written ('Write') and used ('SubMod') to refine both the SIF and JI previously calculated, which now include the electromechanical coupling. Subroutine 'SIF_F' is run to show the main numerical results. This procedure is applied for each load step, by following an iterative solution. Convergence is assured step by step.

5.2 Use case 2: piezoelectric operated as an actuator

When strain inside the piezoelectric layer is induced by the electric field applied by a control system, i.e. piezoelectric layer behaves as an actuator; option 'voltage driven' is followed. Task 'Model' computes the loads applied to the structure as a consequence of the electric field excitation, and both the preliminary SIF and JI are found as in option 'Force driven'. Then correction due to the capability of sensing still present in the layer is calculated by 'SubModV' and corrected SIF and JI are shown through the 'SIF_V' subroutine.

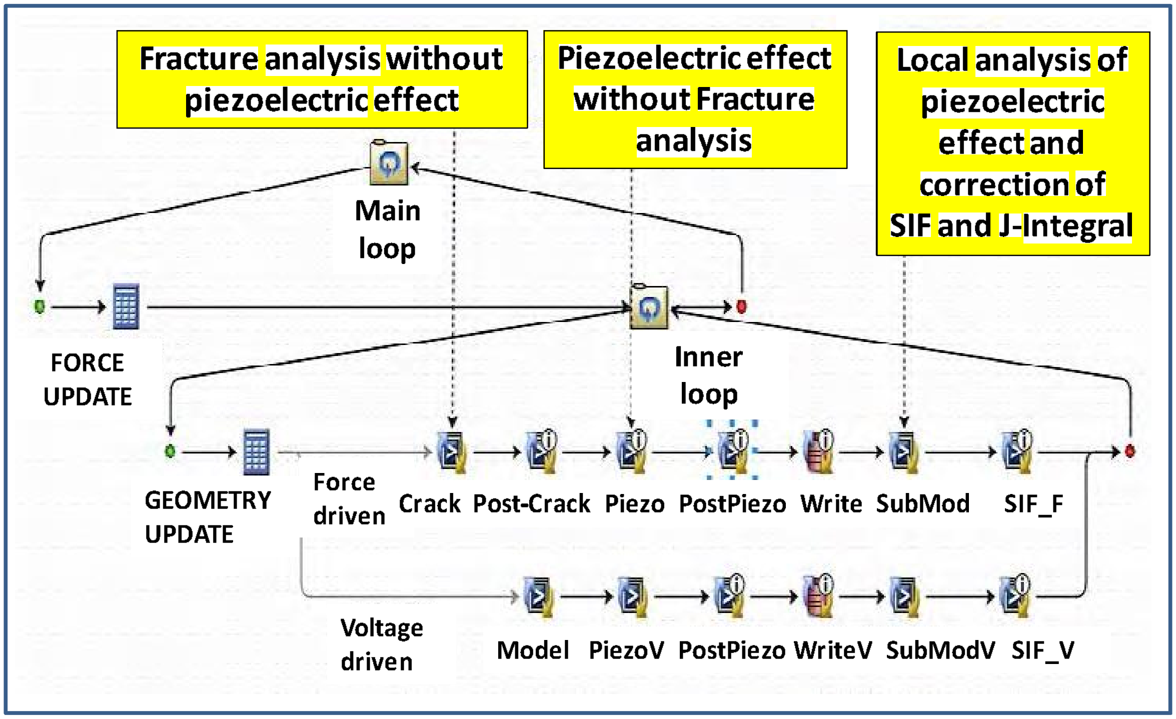

Figure 3. Toolbox developed to perform the prediction of fracture mechanics with piezoelectric effect.

5.3 Prediction of crack propagation in case of piezoelectric material

In the composite structure it was basically assumed that crack first occurs on the main metallic layer, then through the piezoelectric one, if conditions are compatible with propagation. Prediction of crack propagation requires a different implementation of the Isight tool above described. In this case propagation is investigated in terms of direction and speed. To provide those results the piezoelectric phenomenon is considered both in terms of applied strain when crack opening is driven by voltage and in terms of change of shape of piezoelectric layers. As Fig.4 describes the crack propagation model developed inside the Isight code includes some components. Properties of piezoelectric material are introduced by the module "Create Piezo Model", voltage is consequently applied and resulting displacements are recorded by running module "Run Piezo". Geometry of structure is changed by the actuation voltage. A shrinking effect occurs in the layer, which affects the geometry of the cracked structure. This change is predicted in "Grab Ux" and inputted into the XFEM module. As in case of metal the XFEM provides the computation of crack path and propagation, once that actual geometry, shape and loading conditions are known. Crack propagation and geometry of structure are step by step recorded by "Status" module. The numerical loop is closed so as for increasing voltage the crack propagation is computed by an iterative solution at each step of voltage gradually imposed, until that final rupture occurs.

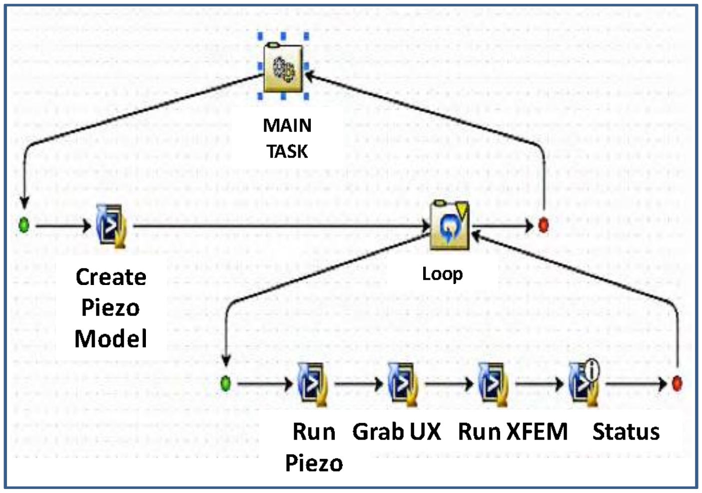

Figure 4. Isight model for the analysis of crack propagation inside the piezoelectric material

6. Numerical simulation and tests

The simulation flow above described was preliminarily validated on a case of literature to check its consistency [6]. Once that this action was performed, the numerical tool was used to investigate the main cases described in above Section 2. Two main cases of fracture modes were analyzed as are shown in Fig.5. A typical opening mode I of fracture was excited in specimen 1, since crack is perfectly located at the middle span of the composite beam and load is aligned with its length. Specimen 2 is suitable to investigate a mixed mode operation in which modes I and II are superposed. Dimensions were suggested directly by [4]. In a first set of simulations material was completely assumed to be piezoelectric PZT (d31=–150 pC/N, E=115 GPa; v=0.34; ρ=7.8 kg/m^3), while in a second one a composite with steel (E=206 GPa; v=0.3; ρ=7.89 kg/m^3) was tested.

■ **SIF and J–Integral:** Results show that in case of Mode I (1 in Fig.5) and single piezoelectric layer, crack propagates directly inside the dielectric material. The SIF grows up with both the applied mechanical load and crack length, as in steel, when electric field is weak, being induced only by crack opening and structure bending. J-integral grows nonlinearly with the SIF value. In fact, when load is generated directly by the electric field applied to the electrodes of piezoelectric layer, which are the upper and lower surfaces of the structure, the SIF increases with applied voltage, but only up to almost one half the total thickness of the structure (Fig.6). When crack length is longer than this value, it gradually decreases. This result is confirmed by the values of J-integral which slightly grows up with the SIF when crack is fairly short, then decreases. Moreover, against any intuitive interpretation J-integral is negative. Somehow energy exploited by the piezoelectric effect to apply strain to the material is dominant on the release of energy coming from the crack opening. This result can be motivated by expression of J-integral for the electromechanical coupled system described in Fig.2. Those trends were confirmed in mixed mode analysis, although sign of J-integral may depend on the dominant fracture mode in that case. In case of composite specimen with surface bonded piezoelectric layer those results were even more evident. J-integral and the SIF decrease with crack length after reaching a maximum peak, if crack is started from the steel and propagates across the metallic portion of the smart system first.

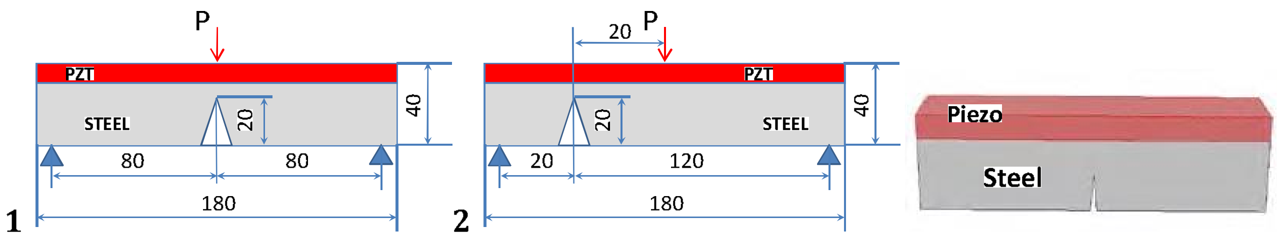

Figure 5. Test cases analyzed in numerical simulations (units are mm)

Some typical effects occurring in operation of piezoelectric structures were detected by numerical simulations. They are herein described by remarking only some peculiar behaviors.

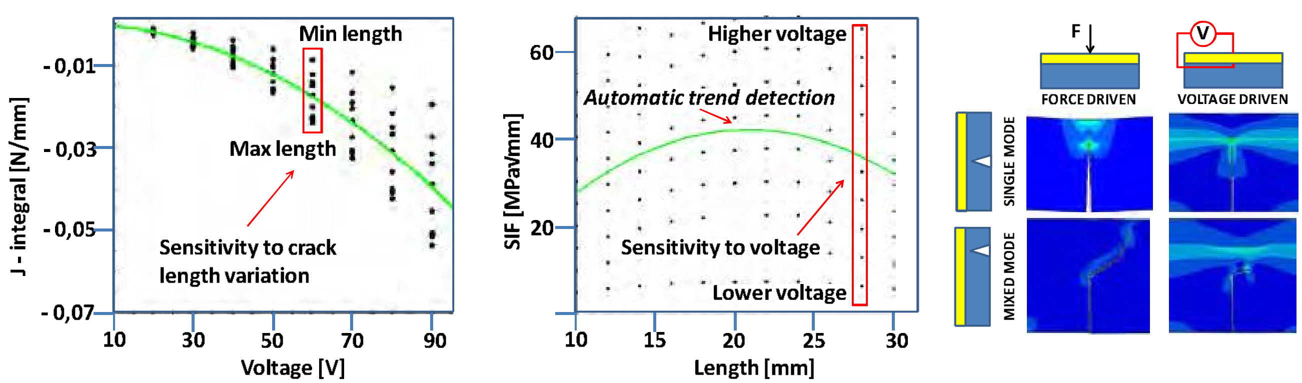

Figure 6. Relevant numerical results in voltage driven fracture of piezoelectric layer

■ **Crack propagation and rupture:** Simulations performed show that mechanical load induces a crack propagation which might grow up to the rupture of material. By converse when voltage acts as driving load, crack propagation stops when a certain critical length is reached. To start again the propagation a larger electric field is required than that it was applied as crack was stopped. A sort of 'barrier effect' is due to the boundary conditions imposed by the piezoelectric effect at crack tip. In case of a mixed mode (Fig.6), if mechanical load is applied, crack changes direction, but deviation is less evident when load is driven by voltage. In composite structures with a metallic substrate equipped with a surface bounded piezoelectric layer the crack propagates along a straight line under both mechanical force and voltage excitation in single mode, but in voltage driven condition propagation stops when crack tip reaches the interface between materials. This effect is more evident in mixed mode, because propagation changes its direction at the interface under mechanical action and breaks both materials, while in electromechanical actuation crack never breaks the piezoelectric layer, being stiffened by the applied voltage.

7. Conclusion

Crack propagation is fairly different across the steel and piezoceramic material, respectively, because of their properties. In passive configuration a crack propagation through the steel easily breaks the piezoceramic, if only a mechanical force is applied, speed of propagation increases and might make unstable the fracture. By converse when bending is driven by voltage a sort of barrier effect is opposed by the piezoelectric layer because of a superposition of phenomena. Local distribution of stress around the tip is greatly affected by the piezoelectric coupling, which can reduce the capability of material to allow cracking. In some cases stretching of piezoelectric layer increases its stiffness and apparent toughness, by reducing the crack propagation. Proximity of crack tip to free surface with concentrated electric charges seems to be favorable to reduce the crack propagation. A relevant result of this work is that both the electromechanical coupling effect and the crack direction in propagation are detected through the proposed procedure developed by resorting to the Isight program. Nevertheless, experimental validation is still to be performed. Due to high expenses related to the design and construction of the piezoelectric specimens it is worthy noticing that the numerical tool developed allows a preliminary oriented design of experiments.

8. References

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