# **Fracture Mechanics Prevention: Comprehensive Approach-based Modelling?**

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Abstract: The paper presented focuses on fatigue crack growth observation in the microstructure of magnesium alloy AZ 91D using finite element software ADINA. ADINA offers a wide range of capabilities based on reliable and efficient finite element procedures. For this reason, ADINA is often chosen for applications where reliability and safety is of critical importance in different industries such as biomedical, automotive, nuclear, forming, civil engineering, hi-tech and others, e.g., in the dynamic analysis of bridge structures – earthquake analysis, in biomedical applications, in the design of nuclear reactors or in studies on safety. This work shows efficiency and good correlation between experimental and numerical results and verifies this program for its utilization in the field of fatigue endurance determination and evaluation.

*Keywords: microstructure; modelling and simulation; material fatigue; experiments; cracks and defects; reliability and personnel security* 

# 1 Introduction

The fatigue of metallic structural components is a widespread failure in different industrial branches. The fatigue process is very sensitive to a great amount of both external and internal factors that, with each of them on its own but especially when acting simultaneously, can affect the fatigue resistance of materials, parts and constructions. Fatigue tests can be performed in various experimental conditions at different loading frequencies. We have all come across examples of materials fatigue failure, whether it is the broken rail which caused trains to be delayed or the broken shaft which caused the car crash. The importance of fatigue is tied foremost to the safety of persons, whose lives depend on the reliability of a given device's operation. Cracks initiate and propagate from pre-existing flaws, material defects, or design features (fatter holes or sharp corners). In fact, most fatigue is widespread, as hundreds or even thousands of cracks are manifested in cyclic loading. The net effect of numerous fatigue cracks located in the same general area is that they synergistically interact reducing the structure's residual strength. However, the single-crack concept is still important, because ultimately, catastrophic failure can occur when a single crack goes critical and in the process envelops other adjacent cracks in a zippering effect [1].

Two basic methods are employed to predict and determine potential fatigue locations. The first is a full-scale fatigue testing, which is performed during the development process. These tests are employed to ascertain what the expected durability is. Fatigue tests, in particular, are very expensive, since they are labourintensive and require a lot of computer analysis. Decreasing expenses as well as increasing efficiency of mechanical design processes and providing operational lifetime durability of parts and machineries allow us to make progress in the field of the utilization of the computational technologies and the application of numerical methods when solving a huge amount of mechanical engineering praxes' problems. Nowadays we have several commercial programs at our disposal which allow us to solve the crack propagation. Many authors have dealt with influence of the crack growth on the functionality of the particular parts from global point of view. Available simulation programs for the simulation of fatigue crack growth can be generally divided into numerical and analytical ones. The numerical programs (FRANC/FAM, FRANC3D, ADAPCRACK3D, CRACK-TRACER, ZENCRACK) are able to predict the crack path in arbitrary 2-D or 3-D structures by using the finite element or boundary element method, the mesh-less method or the material point method. The lifetime is calculated mostly by using linear damage accumulation. However, they are often very time consuming. On the other hand, analytical programs (NASGRO, ESACRACK, AFGROW) are very fast because no model has to be built, no meshing has to be done and the analysis is very rapid. But in many cases the analytical solutions for a number of selected problems do not match the actual geometry and boundary conditions very well [1, 2, 3, 4]. ADINA is finite element software suitable for solving a large variety of problems. According to the available papers, this software has been used for static as well as dynamic analysis for instance, a composite material structure [5] and sealing ring [6] were analyzed. The composite structure was subjected to static pull conditions and stresses in the vicinity of quasi rigid inclusions, which were bonded into the base material, were investigated. The sealing ring was analyzed for undesired vibrations which occurred after it was subjected to pressure impulse load. ADINA is thus fully capable of solving fracture mechanics problems in general with large amount of options in stack under various loading conditions or thermal conditions utilizing a wide variety of material models. There is also the ability to model rupture criteria and thus it is possible to model material damage caused by cavities or impurities and its progression under cyclical load or under creep conditions. Our task was to verify the FEM ADINA for fatigue crack growth observation and its correlation with experimental results.

Magnesium and its alloys are fascinating materials for practice. Magnesium's main advantage is its lowest specific weight out of every metal used for structural purposes, the declining availability and rising prices of raw materials, as well as the subsiding supply of metals in the world scale. The mechanical properties of pure magnesium are not favourable. It has low strength and ductility due to its crystalline structure. However, through alloying we can obtain important structural materials. Suitable alloying partially eliminates the occurrence of casting defects and considerably increases strength, toughness, resistance to corrosion and castability [7].

The outstanding features of commercially used magnesium alloys are their low specific weight, good castability, machinability and weldability in protective atmosphere. The drawbacks, which restrict their wider employment, are low modulus of elasticity, limited resistance to creeping at higher temperatures, high shrinkage during hardening and mainly by the low resistance to corrosion arising from their high chemical reactivity [8, 9].

### 2 Methodology of Simulation

Finite element software ADINA, which was used, offers two different numerical methods for the observation of the fatigue crack propagation: the line contour method and the virtual crack extension method. The model and simulation was in 2-D which is why we used the virtual crack extension method which is more suitable, efficient and easier because it uses only one analysis.

#### 2.1 Virtual Crack Extension Method

The virtual crack extension method evaluates the J-integral for a given body using the difference of the total potential energy between two configurations with slightly different cracks. The basic idea is shown in Fig. 1. This method requires only one finite element analysis. The total potential energy variation is calculated using a "virtual material shift" (zone I in Fig. 1) obtained by shifting the nodes of a domain that includes at least one of the crack front nodes.

The equivalence between the J-integral and the ratio of the total potential energy variance to the crack area increases, but this only holds for linear elastic analysis and elasto-plastic analysis when the deformation theory of plasticity is applicable. In the following, the "energy release rate" refers to the ratio of the total potential energy variation to the crack area increase. The virtual crack extension method is used in ADINA to calculate the generalized expression of the energy release rate including the effects of thermal loads, pressure loads on the faces of the crack and inertia forces.



Figure 1

The virtual crack extension method in 2D analysis

According to Figure 1, the expression of the energy release rate is:

$$G = \frac{1}{A_c} \int_V \left( \left( \sigma_{ij} \frac{\delta u_j}{\delta x_k} - W \delta_{ik} \right) \frac{\delta \Delta X_k}{\delta x_j} - f_i \frac{\delta u_j}{x_j} \Delta X_j \right) dV - \frac{1}{A_c} \int_S t_i \frac{\delta u_i}{\delta x_j} \Delta X_j dS \text{ wit}$$

h: *V*- volume of the cracked body, *S*- surface of the cracked body,  $\Delta X_k$ -components of virtual crack extension vector,  $A_c$ -increase in crack area,  $\delta_{ij}$ -Kronecker delta,  $f_i$ -components of the body force vector,  $t_i$ -components of the surface traction vector, W- $\int_{0}^{\varepsilon_{ij}} \sigma_{ij} d\varepsilon_{ij}$ .

Initial strains are included in the computation of the energy release rate.

#### 2.1.1 Virtual Material Shift



a) Description by node numbers



b) Description by element numbers



Figure 2 Description of the virtual material shift in ADINA

In order to describe a virtual material shift, a specified domain simply connected to the crack tip node must be selected (Fig. 2). The nodes inside this domain are subjected to a virtual shift in order to obtain the virtual configuration of the finite element mesh. In ADINA, each virtual shift domain can be described using node numbers, element numbers, or ring numbers (Fig. 2). It is important to verify that the virtual shift domains are simply connected. If a virtual shift domain does not contain at least one crack tip node, the fracture mechanics calculations are not performed. Several virtual shift domains can be defined simultaneously in one analysis. Only the distorted elements (zone II in Fig. 2), between the undeformed zone I and the rigid body motion zone III, contribute to the energy release rate. Therefore, the choice of the location of zone II in the finite element model will determine the accuracy of the result. It is recommended that several virtual material shifts of increasing size be used to evaluate the value of the energy release rate. Each virtual shift should enclose the next smaller virtual shift. The virtual shift size should increase equally in all directions from the plane perpendicular to the crack front.

A virtual vector is defined by its components in the global Cartesian system. An automatic calculation of the virtual vector can be requested for a given virtual material shift: in this case, the crack propagation area has been defined and the first two nodes on the generation line corresponding to the crack tip node associated with the virtual material shift are used to calculate the virtual vector. The length of the virtual vector is 1/100 of the length of the vector formed by the two nodes. It is recommended that this option be used when a crack propagation analysis is performed.

For a symmetric specimen and loading, the virtual vector lies in the plane of the crack. For an asymmetric specimen and/or loading, the virtual vector direction is usually unknown in advance, because the direction of future cracking is not usually in the plane of the crack [10].

# **3** Experimental Material

Magnesium alloy AZ 91D is the most commonly used magnesium alloy. Its main advantage is its lowest specific weight out of every metal used for structural purposes, and its good castability, machinability and weldability in a protective atmosphere. Drawbacks which restrict its wider employment are its low modulus of elasticity, its limited resistance to creeping at higher temperatures, its high shrinkage during hardening and, most of all, its low resistance to corrosion arising from their high chemical reactivity [10, 11]. The low specific weight and the ability to absorb vibrations make the alloys suitable for applications in the automobile, aviation and rocket industries as well as in telecommunication and instrumentation.

The mechanical properties are shown in Table 1 the microstructure and material curve are in Figs. 3 and 4.



Table 1 Mechanical properties of Mg – alloy AZ 91D

 $Figure \; 3$  Microstructure of Mg – alloy AZ91D, mag. 100 x, etch. 5  $\% H_2 MoO_4$ 



Figure 4 Resistance curve of AZ 91D

# 4 Numerical Part

The microstructure of the material represented by tightly packed grains was modelled by using the finite-element software ADINA in accordance with the microstructure shown in Fig. 3. The geometry of each grain was modelled by Pro/Engineer software and was exported as a plain surface in IGES file to ADINA, where a 2D analysis was performed. For the sake of analysis, each surface representing individual grain of the microstructure was discretised using a finite element mesh (Fig. 5). In this case quadratic elements were used, which means that unknown quantities have been approximated by a polynomial of the second order inside of each element. Due to large gradients in the secondary fields, it is necessary to use very fine discretisation in the vicinity of the crack to achieve reasonable accuracy. Each element has prescribed its own material properties. A multi-linear plastic material model was used in the simulation. The properties of the alloy were obtained experimentally as a dependence of the displacement of the specimen on the applied force. The values were then recalculated to a relation of strain  $\varepsilon$  and effective stress  $\sigma$  (Fig. 4) according to known dimensions of the specimen. Afterwards, the stress-strain curve was imported into ADINA and applied on each element. The analysis was performed by using large deformations and large displacements incorporated into the mathematical model.





Mesh in the surrounding of the stress concentrator

Each grain was considered a standalone body and contact conditions between each pair of grains were implemented. In the microstructure model a stress concentrator was made (Fig. 6). On the boundaries, a cyclic load with amplitude 30 MPa and with frequency 25 Hz was applied, which was identical to experimental fatigue tests. These are standard loading conditions for examining the fatigue resistance of the material.



Figure 6

Model of microstructure with primary stress concentrator before applied load

A plastic zone (Fig. 7) is created in the vicinity of the crack tip in which a plastic strain is accumulated due to cyclic loading.



Figure 7 Plastic zone at the fatigue crack tip

The deformation process at the crack tip depends significantly on the mechanical properties of the material and on the environment in which the loading occurs. The limited plastic deformation, the equal values of intensity factor and the equal coefficients of asymmetry of the cycle do not guarantee the same magnitude and form of plastic zone ahead of the crack tip.



Figure 8 Fatigue crack path

The load amplitude by which the propagation of micro-failure occurs is fully dependent on the non-homogeneity of the material. The aim of the simulation was to observe the failure propagation in the microstructure (Fig. 8). A redistribution of stress was influenced by the cyclical nature of the applied load. Even though the stress is applied on the structure in a uniform manner, it does not act in the same way on each grain in the structure. Most of the stresses are cumulated in the region with certain non-homogeneity in the microstructure. In that case it was a notch and the highest stress was at the tip of crack.

### 5 Discussion of Results

Fatigue crack growth is generally divided into three regimes: near-threshold (stage I, low fatigue crack growth rate, single shear, large influence of structure, large influence of closured stress, the plastic zone at the fatigue crack tip is usually smaller than the average grain size), validity of the Paris law (stage II, medium fatigue crack growth rate, growing, little influence of structure, little influence of closured stress, the plastic zone at the fatigue crack tip is usually bigger than the average grain size) and rapid fatigue, when the crack increases its growth rate till final fracture. The first two areas are significant for the optimal selection of construction materials and for a qualified proposal of component and construction.

After a cyclic load was applied to the microstructure model, the crack started to grow at the stress concentrator. The formation of fatigue cracks always takes place at the free surface of cyclically loaded pieces, at points of concentration of cyclic plastic deformation. At these points one can find notches of different types and origin, as well as inclusion, precipitates and imperfections of the working surface. Fatigue cracks are formed due to the not -entirely -reversible plastic deformation.

The stress concentrator (Fig. 6) was artificially made and presented the inclusion or cast defect (Fig. 3). The structure of the material (Fig. 3) was classified as a structure with patchy polyedric grains of phase  $\delta$  (grain size 1-2) and with areas of imperishable lamellar precipitate. Black points documented the occurrence of cast defects – cavities. These imperfections are considered to be stress concentrators.

The crack path in Fig. 8 is the result of a series of mechanisms associated with different stages of fatigue crack growth. The propagation started in a single grain and continued through several grains in stage I. A stage I crack growth, occurring predominantly by single slip bands (in the direction of maximum shear stress in front of the crack tip) in the direction of the primary slip system, developed because the local plastic zone (Fig. 7) became smaller than the average grain size. The crack is extraordinary effective stress and strain concentrator, together with the microstructural material parameters, the strain field at the crack tip control crack behaviour in a loaded body. The plastic zone (plastic deformed region of material at fatigue crack tip) differs markedly from the matrice structure. Its dimension is tens to hundreds of  $\mu$ m.

Under continuous cyclic loading, the primal crack became interconnected and penetrated deeply into the piece. Many micro-cracks grow only to a depth of several tens of microns and then stop. After the depth of penetration increased, the crack gradually inclined towards the direction perpendicular to the vector of the main stress, and a plastic zone appeared at the tip of the crack. The said processes could be aligned with the first stage of the propagation of the fatigue cracks, in which the crack spread in the crystallographic orientation. In the second stage, the crack spread in a non-crystallographic way. The length of the crack, corresponding to the transition from the first to the second stage of propagation, depended on the type of material and on the loading amplitude. The speed of propagation of the crack was low in the first stage, and the number of cycles necessary for its termination was small in comparison with the second stage of propagation of the crack. The first stage of the propagation of the cracks does not manifest itself for pieces with constructional, technological or metallurgical notches.

Then, the additional slip bands were activated and the crack grew in alternating glide planes perpendicular to the direction of maximum normal stress – stage II. Non-crystallographic propagation in the second stage was controlled by normal stress, while in both stages, at the usual temperatures of loading, the crack propagated in a trans-crystalline manner. The second stage of crack propagation terminates after having caused such a reduction of the carrying cross section of the piece that this would have failed by overloading.

The numerical simulation of fatigue crack growth in magnesium alloy AZ91D by ADINA was compared to experimental observation of fatigue crack trajectory (Fig. 9). Despite the elimination of the lamellar precipitate on the grain boundaries the primal fatigue crack grew transcrystalographically through the grains [12]. Both pictures (Figs. 8 and 9) show good correlation.



Figure 9 Transcrystallic growth of fatigue crack

#### Conclusions

The problems of crack propagation in the micro-scale are considerably demanding on the model accuracy. Many of the effects are manifested at the atomic scale and by using the continuum mechanics it is possible to study these effects only under the certain optimal conditions or according to the output of experimental results or other special methods.

The FEM software ADINA enables us to observe the growth of fatigue damage and crack propagation in a model as well as to observe the distribution of stress fields. It enables us to elaborate on the stress state inside of the material, based on which it is possible to predict the direction of crack propagation.

The aim of the paper was not only to simulate or model a fatigue process of a material to the final failure of the structure. Rather, the principle of the damage creation in micro-volume should be observed closely, as well as the influence of stress distribution on the fatigue crack propagation. It can be seen that even for small loads, small micro-cracks and micro-damage can be spread in the micro-structure, which causes changes inside the material. This, of course, does not necessarily mean that it will lead to a final crack which will imminently cause a failure. The direction of the crack propagation is highly dependent on the stress distribution in the structure and vice versa, which means that the crack propagation, its direction and its peed are governed by the principle of the minimum energy in the system.

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