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# Modelling of damage due to particles and grain boundaries

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**Abstract:**

Two types of damage growth models are presented here, for the cases where damage nucleation sites are randomly spread in the matrix and where they are located at grain boundaries. In the former case, the cavity can be due both to fragmentation or decohesion, and the model is based on a 3D FEM description, whereas in the latter case, account must be taken of textures and grain shapes, which is done via a self-consistent scheme.

## Introduction:

Hard particles are often present in aluminum alloys for different reasons, and their high stiffness makes that they play the role of stress concentrators. This can induce fracture of those particles or debonding of those with respect to the surrounding matrix. Three stages are known to represent the whole damage mechanism: cavity nucleation, which occurs due to fracture or debonding, cavity growth, which depends on the strain path and trixiality, and coalescence, which is the linkage of those cavities, and that can lead to final fracture. Depending on average distance between those hard particles, the different stages can be of different importance. For a rather random and dilute distribution of particles, the growth mechanism is particularly important since it has to be quite significant to lead to coalescence and overall fracture. However, when those particles are present at grain boundaries, ie with a realatively small interspacing, then a local coalescence (that will be called meso-damage) can occur, which creates a cavity that needs, in turn, to grow significantly to lead to overall fracture. Those two cases will here be investigated. In the first case, a simple model based on a Finite Element representation will be proposed, whereas in the second case, an alternative model based on a micromechanics approach in elastoplasticity will be shown.

## Damage growth due to a random dilute distribution of hard particles: Modelling

The large majority of the work done on cavity growth is based on the modelling of simple cavities in a matrix, taking account or not of the cavity shape. It is usually done either by making use of the variational principle [1-4], or by micromechanical approaches [5, 6], or by FE method [7-18]. Very little has been done for the case of cavities created by fracture of debonding of hard particles. The present study is based on a 3D FE representation of an initially spherical particle which exhibits fragmentation or decohesion (fig.1a-d). On each face a master mode is connected to a spring element, so that its displacement is monitored according to a given prescribed stress ratio. In particular, this enables us to add some hydrostatic stresses in order to investigate the effect of triaxiality. Each master node controls as well the displacement of all nodes of the same corresponding sample face. The FE structure is built by means of three types of linear isoparametric elements, ie tetraedra, prisms and hexaedra. The matrix behaviour is described by means of the Prandl-Reuss equations in large

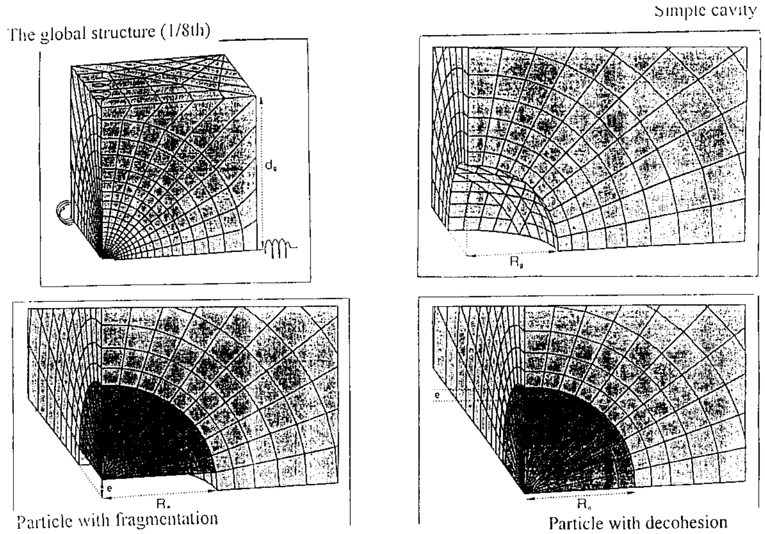


**Figure 1:** Representation of 1/8 th of the 3D global F.E. structure (a). Local view of the mesh for the case of a simple cavity (b), of a particle with a fragmented zone (c), and of a particle exhibiting an initial decohesion (d)

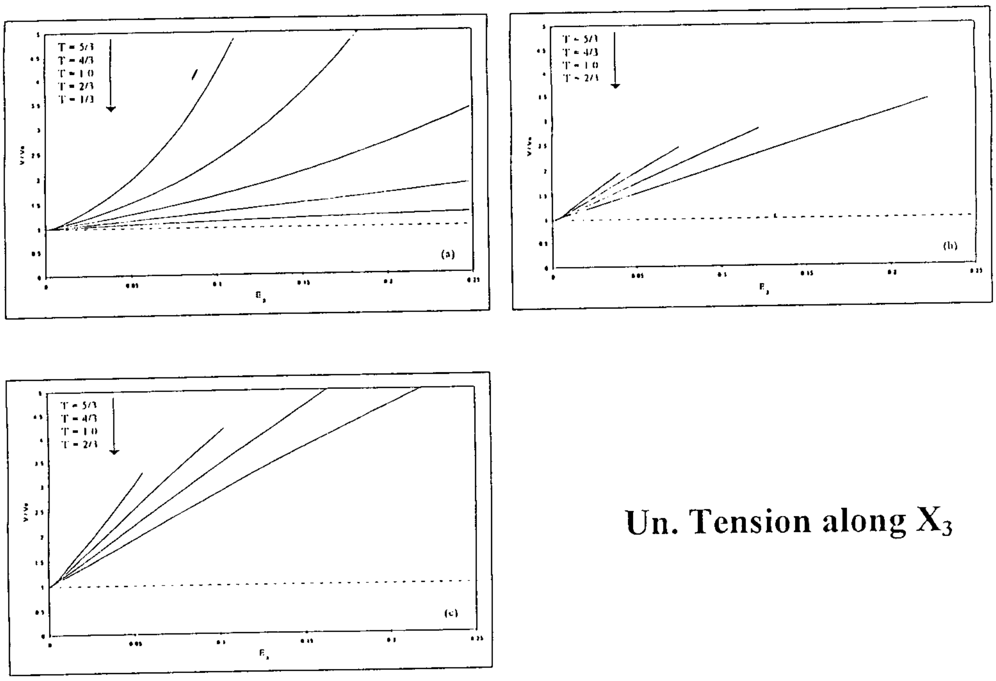


**Figure 2:** Evolution of the relative cavity volume change versus axial strain in uniaxial tension along the fragmentation plane normal, for the case of the simple cavity (a), the broken particle (b) and the decohesion (c). Note the linear increase in the latter cases as opposed to the exponential increase in the first case. Curves are obtained for different amounts of triaxiality T.

strain isotropic elastoplasticity fitting the appropriate elastic and hardening parameters to the real behaviour of the material. Different tests were done to this FE sample, for different stress ratios, and the cavity volume was recorded as a function of axial strain and triaxiality. The triaxiality factor is simply the ratio of the hydrostatic stress to the flow stress. A typical result shown on fig.2 seems to demonstrate that, although the cavity growth for simple cavities (fig.2a) is exponential with strain, as has often been found, it is linear with axial strain (figs2b,c), for the cases of fragmentation and decohesion. In all cases the rate of cavity growth is increased with an increasing triaxiality. This case corresponds to a strain path that tends to open the cavity, in collaboration with the positive triaxiality. Another interesting case, shown on figs3a-c, is the case where the tension is done orthogonal to the fracture plane normal, so that the strain path tends to close the cavity. Of course, the simple cavity case is same as found previously, ie an exponential ,dependence of the cavity volume with respect to the axial strain (which is negative in this case), whereas a linear dependence is found for the cases of fragmentation and decohesion. However, an interesting point is that the triaxiality, if it is large enough, can somewhat prevent the cavity closing, bringing therefore a competitive effect. It is possible to represent the rate of cavity growth as a function of the triaxiality factor, figs 4a-c. Fig.4a shows the case of the simple cavity, compared with the results of Rice-Tracey [1] and those more recent of Huang [2]. It can be roughly observed that the FEM results lie between the ones of these authors. This is explained by the fact that those theoretical results do not account for the shape changes in the cavity growth, which is done in our FEM estimation, and it is known that elongated cavities tend to have a smaller volume increase than spherical voids, which explains why FEM results lie below the more exact results of Huang. Another interesting point is for zero triaxiality, which was simulated as equibiaxial tension-compression. In this case an initially spherical void will become flat, with a decreasing volume, which can be explained on a morphological argument. It means that the rate of growth, tends to be negative, and not zero as would be obtained for spherical voids. Most interesting are the curves of figs4b and c, where a difference is observed depending on whether the triaxiality competes or not with the strain-path to open the cavities, in the fragmentation and decohesion cases. Both upper and lower curves can be well fitted by an exponential, and a rather general formulation has been found that covers all those cases:

$$G=\frac{1}{V}\frac{dV}{dE_3}=A.\{1+\mathrm{sgn}[T.E_3].(e^T-1)\} \qquad (1)$$

where the parameter A depends strongly on the type of cavity considered, ie fragmentation or decohesion. In our cases, A=6.5 for decohesion and 12 for fragmentation. It is important to note that the exponential dependence on T occurs with a factor 1, instead of 3/2 for simple cavities. This strong sensitivity of the parameter A to the type of damage means that, for engineering purposes, a fitting parameter seems unavoidable, also when particles do not present the same geometry as the one presented here.

**Damage growth due to a random dilute distribution of hard particles: Application**

The present case is the one where the initial cavity volume fraction is known as $f_o$, as well as the statistical angular distribution of the damaged particles $f^D(\theta)$ and $f^F(\theta)$, that has been characterized experimentally. Knowing the definition of the damage factor:

$$D=1-V/Vo \qquad (2)$$

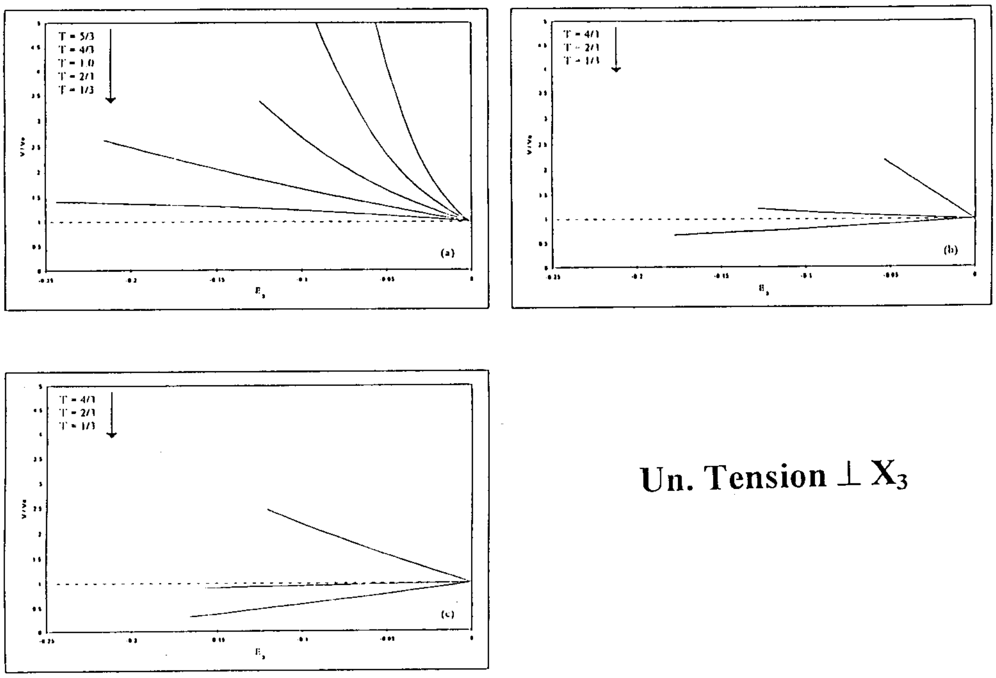


**Figure 3:** Same curves as for Fig.2 but for uniaxial tension orthogonal to the fragmentation plane normal. Note the competitive effects of the strain direction and the triaxiality.

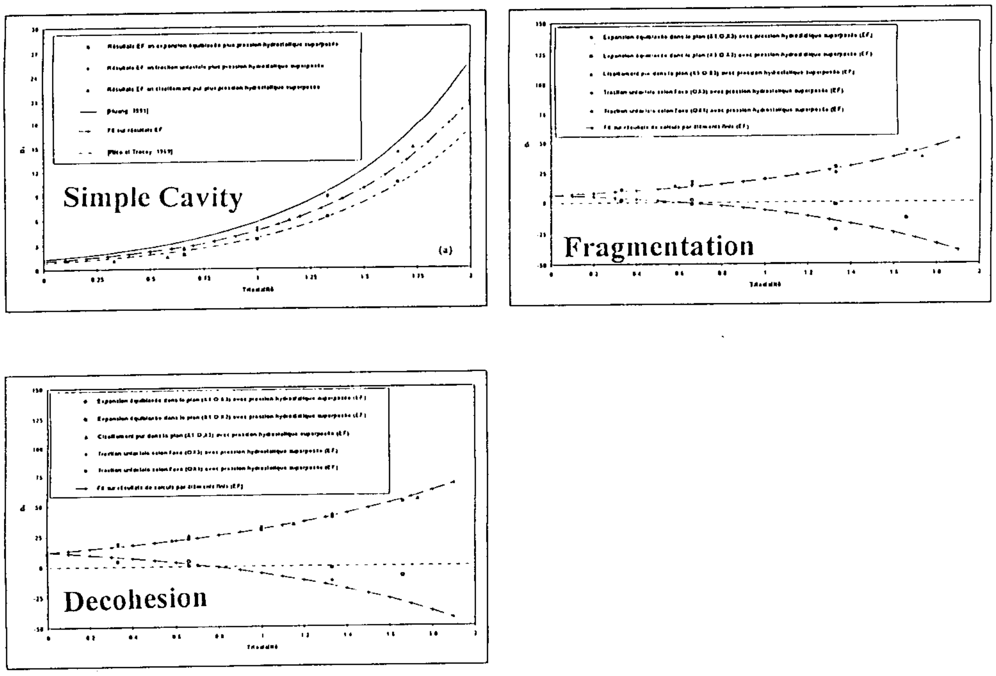


**Figure 4:** Evolution of the relative growth rate as a function of the triaxiality in the three investigated cases. Dots correspond to the FE results, and curves to analytical representations.

its evolution can be obtained by a simple relation:

$$D=(1-D).\varepsilon^{cav}.[\, f_o(1-D) + D\,] \qquad (3)$$

where $\varepsilon^{cav}$ is obtained as:

$$\varepsilon^{cav}=V^{cav}/V^{cav} \qquad (4)$$

which can be obtained by the integral over the angular statistical distribution:

$$V^{cav}= Q.\int (f^D(\theta,t).G^D(\theta,t).+ f^F(\theta,t).G^F(\theta,t))\, N_{TOT}.d\theta/\pi. \qquad (5)$$

Both quantities $G^D$ and $G^F$ are computed according to the model previously proposed, and the parameter Q is simply a fitting parameter which accounts for the fact that the particles have shapes which are not spherical. In our case, Q was adjusted to the value 2/3 and was kept constant and unique for all the laboratory tests investigated. The results of this simple model are shown and compared with the experimental results on fig.5, where a good agreement is observed.

This model, which is based on the 3D FEM results, is a kind of extension of the models of Rice and Tracey, and also of Huang, for the case of hard particles associated to fracture or decohesion. Another case will now be investigated where the hard particles are relatively clsse to each other, and located at grain boundaries.

**Case of hard particles being close and at grain boundaries:**

An Al-Zn-Mg alloy has been studied, where the damage occurs by decohesion of particles present at grain boundaries, but where the growth process leads rapidly to coalescence. This phenomenon has been studied extensively, and seems relatively well described by the Embury-Nes model [19]. However, in this case, grains are very flat as a result of the rolling process, and the material exhibits a sharp texture, both effects being important. A relevant modelling must therefore account for those. When coalescence occurs, it is first limited to the grain boundary region, and a meso-damage therefore appears, for which a significant growth process must occur before materials overall failure happens. The present model aims at describing this latter growth process, starting from the microstructural state of the material, and some critical conditions due to the Embury-Nes model, provide an estimate of the growth mechanism that will lead to overall failure.

The material is made of grains with given aspect ratios, and its plasticity is due to the cooperative effect of slip systems, which are assumed to obey the Schmid law. Since both texture and grain shapes are quite sharp, the small strain formalism is used, ie no texture nor grain shape evolution is assumed to take place here. In this model, each crystallite follows a flow law of the kind:

$$\sigma=\mathbf{L}:\varepsilon \qquad (6)$$

where **L** is the grain tangent modulus. The overall material is assumed to follow a flow law of the same kind with $\mathbf{L}^o$, its tangent modulus to be determined at each strain step, by a self-consistent procedure. For each grain, the knowledge of its orientation, of its active slip systems, of their hardening characteristics, is enough to determine uniquely the tensor **L**. Then

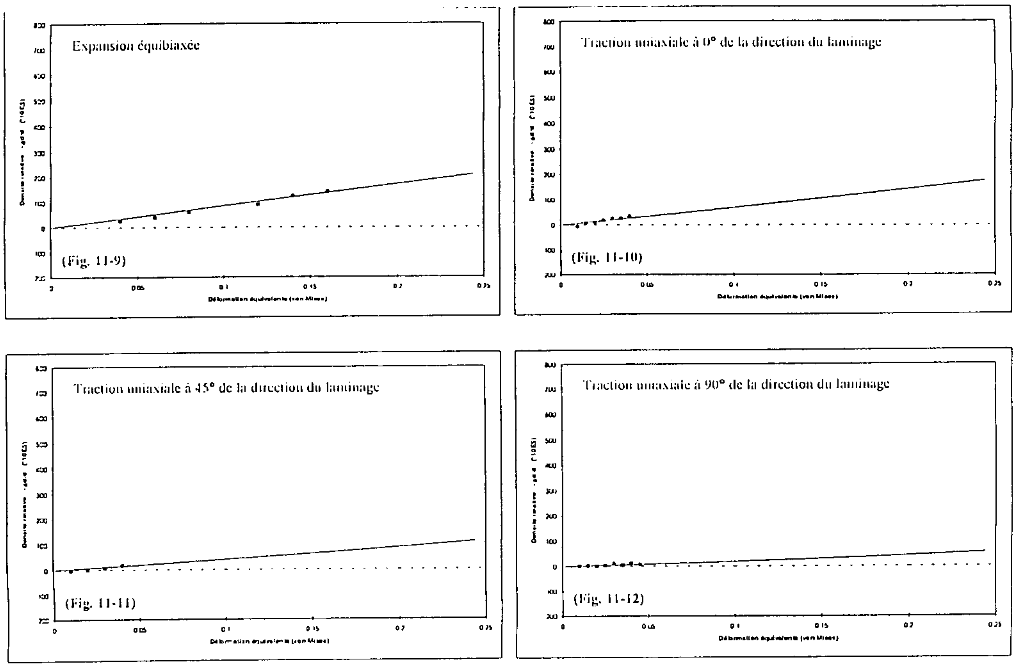


**Figure 5:** Comparison of damage results obtained by the modelling proposed with the one obtained by experimental results on a Al alloy.

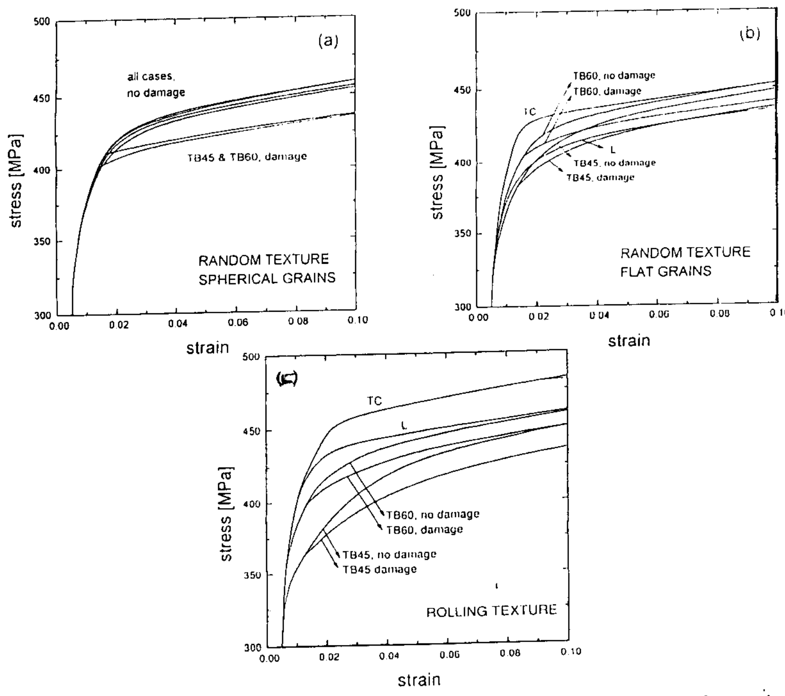


**Figure 6:** Typical stress-strain curves obtained from the elastoplastic self-consistent model including the effects of damage only (a), grain shape and damage (b), texture, grain shapes and damage (c).

an inclusion analysis provides the mechanical response of the grain in its neighbourhood, which is used, by an iterative scheme to derive the macroscopic tangent properties. This enables us to compute the state of stress in each grain and its vicinity, which, in turn helps determining the critical conditions for the occurrence of meso-damage. Once such a condition is reached, then a flat void is created which is, in turn , treated as an inclusion of zero stiffness, that is allowed to grow. However its growth will weaken the material, by decreasing the macroscopic tangent tensor, and here again, it is estimated by using the self-consistent technique.All details concerning this approach are explained by Lebensohn et al [20].

From this technique, it is possible to investigate separately the effects of texture, grain shape and damage evolution on the macroscopic behavior. As seen on fig.6a, for spherical grains and random texture, all curves, which correspond to tensile tests at different angles with respect to the RD-ND axes, lie on a unique curve, except when the damage process is set in. Fig.6b shows the case of no texture, but flat grains, where a discrepancy is expected and observed. Finally when a typical rolling texture for f.c.c. materials is used, then the tensile behavior turns out to be very different with the tensile angle, as seen on fig.6c.

Typical profiles are then obtained, and it can be observed that the texture plays a dramatic role, as compared to the one of the grain shapes.The same kind of conclusion can be drawn from the limit strains obtained from the bifurcation analysis.

This method has been applied in a companion paper by Solas et al [21], with real texture data, and is shown to provide useful results.

**Conclusions:**

The modelling of damage has been proposed for alloys having hard particles present in the matrix, in two cases, namely where those particles are rather diluted and randomly spread into the matrix, and where they are quite close to each other and distributed at the grain boundaries. In both cases decohesion or fragmentation of the particles is the source mechanism of damage, but final overal failure only occurs after significant growth. In the latter case, in turn, he damage initiation is rapidly followed by local coalescence, at the grain boundary level, and the meso-damage that is created must grow significantly again to lead to overall failure. In the former case, a reliable growth model is required, based on the local geometry, whereas in the latter case, a micromechanical model, making use of the crystallographic texture and the grain morphology is needed, since the local stresses and strains are useful. Those two types of models have been proposed, by means firstly of a 3D FE model, and secondly by means of a small strain elastoplastic self-consistent scheme. Those two approaches provide satisfactory results as compared with experiments.

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