11.1 Damage and fracture processes of metallic materials

A. Context and state of the art

A.1. Failure mechanisms

When a metallic material is submitted to excessive loading, damage processes occur at the microscale, leading to final macroscopic failure. Depending on materials, environmental and loading conditions, failure can be brittle (cleavage and intergranular fracture) or ductile.
Cleavage fracture preferentially occurs according to metals dense atomic planes with cleavage cracks crossing grain boundaries. **Intergranular fracture** is usually observed for polycrystalline metals exhibiting segregation of impurities at grain boundaries. The transition between cleavage and intergranular fracture is a function of the ratio between the free energy per unit area of the boundary and the free energy of a surface exposed by cleavage. At a macroscopic scale, this transition can also be analyzed through the ratio between macroscopic shear modulus and bulk modulus respectively. Definition of cleavage stress, mechanisms of stress intensification, multiple barriers models and crossing of grain boundaries are reviewed in (Pineau et al. 2016). **Ductile fracture** is observed after significant plastic deformation and occurs after microvoids or shear bands develop in the metal matrix, around inclusions or other discontinuities such as grain boundaries. At the microscale, ductile damage is associated with voids nucleation, growth and coalescence under high and moderate stress triaxiality ratio[1], or shear band formation under low stress triaxiality. At the macroscale, ductile damage is represented as the progressive degradation material's behavior through stiffness and strength decrease (See Pineau et al. 2016 and Cao 2013 for a detailed review).

A.2. Modeling ductile damage

Ductile damage is usually described using three main approaches:

- **Uncoupled failure criteria**: a damage variable is defined as the integral of a function of stress state over the plastic strain path. Failure occurs when this function reaches a critical value. In this approach, the damage variable is not coupled with the material behavior law, which makes it impossible to predict material softening due to damage growth. It is however a robust approach with limited number of parameters that needs to be identified. The Johnson-Cook or Bao-Wierzbicki failure criteria were able to predict failure patterns with fairly good accuracy for impact problems on metallic structures (Kolopp 2012).

- **Phenomenological damage models**: damage is associated with one of the internal constitutive variables that accounts for the influence of the irreversible process which occurs in materials microstructure. Ranging from 0 (undamaged material) and 1 (failure), this damage variable is coupled with the material behavior and enables to predict progressive softening of the material. Just like any other coupled damage model, numerical localization issues may occur and may require the use of non-local damage theories (El khaoulani & Bouchard 2013). The Lemaitre damage model is the most used model in this approach. The damage driving variable depends on stress triaxiality ratio and recent extensions were proposed to account for the Lode angle as well (Cao et al. 2014).

- **Micromechanical approaches**: based on the initial porous solid plasticity theory proposed by Gurson, damage is accounted for through the use of void volume fraction in the plastic yield

[1] Stress triaxiality ratio is defined as the ratio between hydrostatic pressure and equivalent von Mises stress. High positive values correspond to a tensile state whereas negative values correspond to compression.

surface. This void volume fraction follows nucleation, growth and coalescence laws and ductile damage is then taken into account by this porosity term that progressively shrinks the yield surface. See (Benzerga and Besson 2010) for a review of this class of models and (Cao et al. 2013) for details of implementation.

Each approach has advantages and drawbacks, and no universal theory prevails. Whatever the models used, it is important to stress out the **importance of models calibration**. The identification of material parameters must be done for loading conditions as close as possible as to the one undergone by the material in the final application studied. Robust and efficient inverse analysis procedures coupled with global and local relevant observables should be used.

It is important to stress out that these failure mechanisms are sensitive to many parameters, among which:

- **Stress state**: stress state is defined in a unique way using stress triaxiality ratio and Lode angle. Strain to fracture clearly depends on these two parameters, but it has also been shown recently that, like in geomaterials (See Theme 11.2 Properties, damage, and rupture of manufactured and geo materials), pressure sensitivity was shown to be important for accurate prediction of metallic materials under multi-axial loading conditions (Bai & Wierzbicki 2008, Cao 2013).
- **Temperature effect**: depending on temperature, metallic materials can switch from brittle fracture (low temperature) to ductile fracture (higher temperature) and ductility tends to increase with temperature.
- **Strain rate**: strain rate strongly influences both material behavior and failure mechanisms. By increasing strain rate, two competing mechanisms occur simultaneously: increase of hardening (partly due to higher uniform dislocation distribution for the same amount of strain) and softening due to local self-heating generated by strain localization. Separating both effects is often difficult and requires the use of local observables.
- **Loading path**: damage models calibration is usually achieved using monotonic laboratory experimental tests. The application of these calibrated models to complex loading path (multi-axial & non proportional loading) is subject to caution (Gachet et al. 2014).

Once damage reaches its critical value, fracture occurs and needs to be modeled.

A.3. Modeling fracture

Modeling fracture has always been a « hot » scientific research topic with applications initially in civil engineering and fatigue mechanics. For brittle fracture and within the context of finite element analyses, the prediction of crack paths was based on linear elastic fracture mechanics (LEFM) theory and different numerical techniques were developed to propagate a crack in a mesh automatically: **discrete crack propagation** with automatic remeshing (Carter et al. 2000, Bouchard et al. 2003) (Figure 1.a and 1.b), **extended finite element method** (XFEM) based on level set functions and enrichment of elements containing the crack (Moes et al. 1999) or **cohesive zone models** (CZM) which defines progressive failure at interfaces using a traction-separation law (Chen et al. 2013). In this context, the accuracy of stress fields at cracks tip is essential since crack propagation is driven by stress intensity factors (or strain energy release rate for energetic approaches). For ductile fracture, more basic approaches, such as the **kill-element technique** (Figure 1.c), can be used. This technique consists in deleting elements once a critical damage value is reached. This implies volume loss when elements are deleted, and anisotropic mesh adaptation based both on damage fields and gradient of damage was proposed to improve ductile failure prediction in (El Khaoulani and Bouchard 2012).

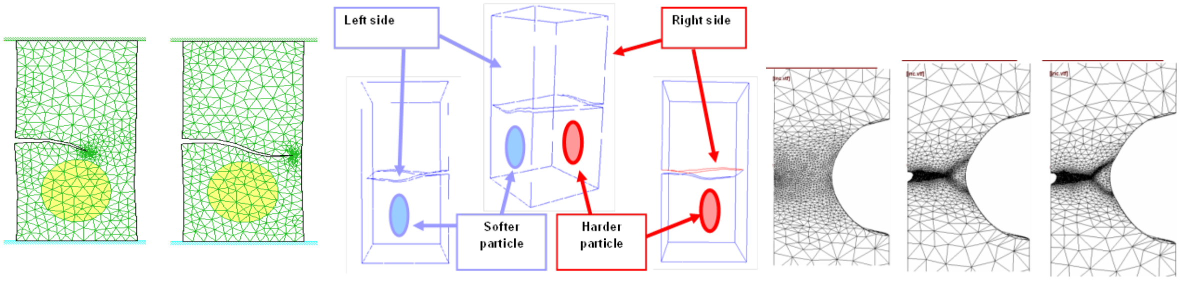
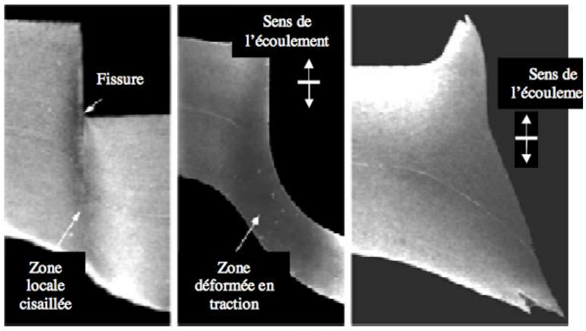


Figure 1. a) 2D and b) 3D discrete crack propagation in a composite structure using automatic remeshing; c) kill-element technique coupled with anisotropic mesh adaptation for the modeling of cup-cone ductile fracture of a tensile specimen.

A.4. Impact failure modes

Impact failure analyses are usually split in 4 categories depending on impact velocities: low (v< 10m/s) and moderate (10 m/s < v < 200 m/s) impact velocities, high ballistic velocities for military applications (200 m/s < v < 800 m/s), ultra-high velocities for aerospace applications (800 m/s < v < 5 000 m/s) and even more for planetary and asteroid impact problems. In addition to the complexity of failure mechanisms at such high velocities, the identification of material and damage parameters requires very sophisticated instrumented test benches.

For ballistic applications it has been shown that the shape of the projectile influences the failure mode (Børvik et al. 2001, *Figure 2*). Flat projectiles are the most critical because they induce shear bands (in front of the projectile) that initiate fracture. Smooth conical projectiles are less critical, they induce a stretched plastically deformed area before leading to fracture. Finally, hemispherical projectiles are the least critical. The impacted material exhibits more plastic strain and thinning before leading to final failure in petal shape. Each of these failure modes is related to a certain amount of absorbed energy before failure (Gupta et al. 2007).



Flat – smooth conical – hemispherical

Figure 2. Influence of projectile shape on failure modes (Børvik et al. 2001).

B. Current activity

At CEMEF, modeling damage and fracture is usually dedicated to the prediction of defects during material forming processes. Different metallic materials are studied (steel grades, aluminum alloys, zinc, zirconium, copper …) under different metallurgical states (strain hardened, recovery state, carbonitrided …) which may generate gradient of microstructure and mechanical properties. The range of temperature is usually from room temperature to ~1200°C and strain rates range from very low (10^{-3} s^{-1}) to moderate strain rates (~200 s^{-1}). In some very particular cases, strain rates can increase up to $10^4 s^{-1}$ (magneto-forming) and even 10^6 s^{-1} which is obtained very locally under blast impacts for shot-peening surface treatment processes for example. Predicting failure for such manufacturing processes require:

- the development of adapted elastic-viscoplastic material behavior laws and appropriate damage models;
- the identification of material and damage parameters based on representative experiments and robust inverse analysis procedures;
- the development of numerical techniques to model coupled damage and fracture at macroscale;

- the development of micromechanical analyses dedicated to voids nucleation, growth and coalescence mechanism at the microscale to feed macroscopic damage models with more physical data.

B.1: Modeling damage for complex loading path

During manufacturing processes, materials are submitted to large plastic strain, multiaxial loading as well as non-proportional loading. Accounting for such complex loading paths requires:

- the development and use of enhanced damage models handling various stress states (stress triaxiality ratio and Lode angle) and their coupling with the material behavior law (Bouchard et al. 2011, Cao et al. 2014);
- the design of adapted specimen geometries for reaching various stress states: smooth/notched and round/plane strain tensile specimens, shear induced specimens, hat-shape axisymmetric and butterfly specimens …
- the analysis of non-monotonic loading path (Gachet et al. 2014);
- the validation of numerical prediction with fully instrumented semi-industrial tests as close as possible to industrial tests.

B.2: Identification of material behavior and damage parameters

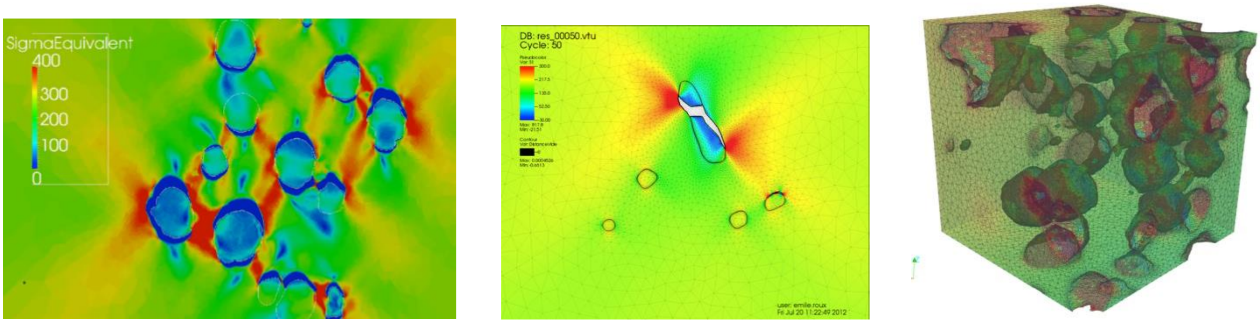
Calibration of damage models require the use of inverse analysis with adequate global and local observables. Due to the large number of parameters that need to be identified (both for material behavior law and damage models) and to the complexity of the competing mechanisms (hardening, self-heating, damage …), the use of digital image correlation is essential to get local observables (surface displacements, local strains in localized necking area …). These observables can be used in an inverse analysis framework where material parameters are identified iteratively by minimizing a cost function. This cost function is built upon the difference (least squares) between experimental and numerical observables. The use of enriched local observables is obviously improving the identification procedure and in particular the decoupling between competing mechanisms. The software MOOPI (Modular sOftware dedicated to Optimization and Parameters Identification) was developed to handle sensitivity analyses, optimization problems and inverse analysis (Roux and Bouchard 2013, Roux and Bouchard 2015). MOOPI is general enough to be coupled with any other numerical software and could be useful within the C4PO project.

B.3: Development of numerical techniques to model fracture

When damage reaches a critical value, fracture has to be modeled. Thanks to its experience in automatic remeshing, CEMEF developed and is still developing numerical techniques for fracture modeling, among which: kill-element technique with anisotropic mesh adaptation (El Khaoulani and Bouchard 2012, Cao 2014), automatic discrete crack propagation (Bouchard et al. 2013), level-set approach with anisotropic mesh adaptation (Roux et al. 2013) or with body-fitted mesh adaptation (Shakoor et al. 2015) …

B.4. Multiscale analysis of damage and fracture

Damage and fracture mechanisms analyzed at the macroscopic scale are often based on mechanisms occurring at the microscale and in particular due to geometrical and material heterogeneities. It is thus essential to model material behavior at such a scale. This requires first the ability to mesh complex 3D and heterogeneous microstructures (See Theme 5.3 Digital Material). Regarding ductile damage, it also involves the modeling of void nucleation, growth and coalescence (Figure 3). Stress-based criteria are used for particles failure and particles/matrix debonding whereas coalescence can be activated either through a local damage parameter or a minimum distance between neighboring voids. The finite element framework enables the dynamic insertion of cracks during the computation and their remeshing throughout void growth. This technique also allows accounting for complex topological events such as void coalescence. This new method is applied to study the influence of particles orientation and of loading path on micro mechanical ductile failure mechanisms. This work is in progress within the ANR project COMINSIDE, coordinated by P.-O. Bouchard, and dedicated to the understanding and modeling of ductile fracture at the microscale. In this project, in-situ laminography tensile tests are performed at ESRF. Observed experimental microstructures are meshed and exact boundary conditions are applied thanks to digital volume correlation techniques. Micromechanical nucleation and coalescence models can therefore be calibrated thanks to observations and simulations.



(a) (b) (c)

Figure 3 a) 2D particles/matrix interface debonding; b) 2D failure of a composite structure by interface debonding and particle failure; c) 3D failure of nodular cast iron in which the heterogeneous microstructure mesh comes from X-Ray tomography images.

C. Future steps

C.1. generalized non-linear material behavior laws

Metallic materials behavior laws used in metal forming are elastic-plastic or viscoplastic. Von Mises plasticity and isotropic hardening are currently used and anisotropy is dealt with using the Hill 48 anisotropic criterion in the numerical software Forge® developed at CEMEF. In order to address more complex problems, it is essential to set-up a framework in which various yield criteria (drucker-prager, pressure dependent …) and more advanced anisotropic criteria as well as anisotropic flow rules may be developed.

C.2. Impact failure processes

As shown above, even for high-speed forming processes, velocities are order of magnitudes below the ones encountered in the impact problems expected in the C4PO project. Addressing new high speed impact applications is however one of our goal within the C4PO project. From a numerical point of view, this would require the development of explicit schemes (the Forge software is based on an implicit formulation right now). In addition, the use of automatic remeshing may be useful to adapt the mesh automatically in strain localization areas. This would however require to be extremely careful with transport of mechanical fields from old meshes to new meshes and with energy conservation.

C.3. Muti-objective inverse analysis

As shown above, the MOOPI software could be a very useful tool for parameters identification within the C4PO project. As an example, shot-peening modeling was studied in the DEFISURF ANR project. Shot-peening consists in impacting a metallic surface with thousands of hard shots (sub-millimeter dimensions) with velocities ranging from 10 to 100 m/s. Due to the small shot dimensions, local strain rate can rise up to 10^6 s^{-1}, which makes difficult the identification of metallic materials behavior laws at such strain rate. An innovative inverse analysis approach was developed within the ANR DEFISURF project. Single impact tests were carried out (at ENSAM Aix) with three different shot diameters and three different velocities. Inverse analysis was conducted based on two local observables: impact depth and pile-up height. The automatic inverse analysis procedure enabled the calibration of a Johnson-Cook material behavior law for such high strain rates, which was never done before. MOOPI could be really useful within the C4PO project since it can be coupled to any kind of numerical software used in impact problems. Extended MOOPI to handle more efficiently multi-objective problems is one of the tasks that could be carried out in the C4PO project.

C.4. Failure of heterogeneous structures

Planetary corpses and meteorites have heterogeneous structures. The numerical tools developed for micromechanicals analyses of metallic materials ductile fracture (See section B.4) could be extended to model failure of such heterogeneous structures. In particular, mesh adaptation (with anisotropic adaptation or body-fitted technique) are particularly well suited for describing multi-materials interfaces and their possible failure processes. Development of cohesive zone models could also be of interest for a better description of progressive failure at interfaces.

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D. International and National collaborations

- **MIT – Department of Mechanical Engineering (USA):** collaboration with Prof. D. Parks on damage and fracture of carbonitrided steel components and Prof. T. Wierzbicki on influence of stress state on ductile fracture.
- **CONICET (Argentina)**: collaboration with Prof. J. Signorelli on material behavior laws, anisotropy and ductile damage.
- **Pontificia Universidad de Chile (Chile):** collaboration with Pr. D. Celentano on ductile damage and material forming processes.
- **LMT Cachan (France)**: collaboration with Prof. F. Hild (expert in DIC and DVC analyses) within the COMINSIDE ANR project dedicated to the understanding and modeling of ductile fracture at the microscale.
- **CdM Mines ParisTech (France)**: collaboration with Dr. T. Morgeneyer (expert in X-Ray laminography at ESRF) within the COMINSIDE ANR project dedicated to the understanding and modeling of ductile fracture at the microscale.
- **ENSAM Angers (France)**: collaboration with Prof. F. Morel on the modeling of shot-peening and its impact of steel fatigue properties.

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F. Most significant publications of the team

- Bouchard, P.-O., Bay, F. and Chastel, Y. 2003, Numerical modeling of crack propagation – implementation techniques and comparison of different criteria. Computer Meth. Appl. Mech. Engng., 192, 3887-3908.
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Short CV of participants

Pierre-Olivier Bouchard, is Professor at Mines ParisTech and in charge of the Computational Machanics and Physics department at the Center for Material Processing, Sophia-Antipolis. Laureate of the ESAFORM Scientific Prize in 2005. P.-O. Bouchard is expert in damage and fracture modeling at multiple scales. He is the coordinator of the French ANR project COMINSIDE (2014-2018). He is in charge of the MECAMAT association working group dedicated to "Physics and Mechanics of Damage and Fracture". About 50 refereed publications.

Marc Bernacki, Professor in Numerical Metallurgy at CEMEF MINES-ParisTech. Expert in development of numerical methods and HPC in materials science. His main activities concern the simulation of microstructure evolution during materials forming. Head of the "Numerical Materials" committee of the SF2M. Head of the research group "MultiScale Modelling".

Daniel Pino Munoz, is Assistant Professor at CEMEF, specialized in the numerical modeling of non linear multiphysics problems. Among the other research interests, his research is mainly focused on the study of ductile and brittle fracture of materials under complex loading, plasticity modeling at different scales and mass diffusion problems. He was awarded the prize for the best PhD thesis on the field of computational mechanics in 2012 by the French Computational Structural Mechanics Association (CSMA).