Is it possible to open beverage packages virtually?

Physical tests in combination with virtual tests in Abaqus.

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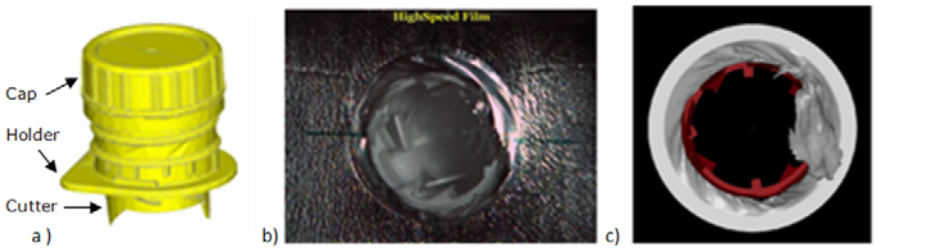
Abstract: The opening mechanism in a beverage package, where a mixed mode failure occurs, is a rather complex phenomenon. A better knowledge in respect of fracture mechanics is needed for the proactive prediction of the overall opening performance. Reliable material data used for virtual simulation of the opening mechanism is extracted by characterization and calibration of the packaging materials. Knowledge of how to choose appropriate constitutive models for the continuum material and how the damage initiates and propagates to various loading conditions is of great interest. The virtual tests, replicating the physical tests, are performed with the aid of the finite element method. Non-linear material response, anisotropic material behaviour, large deformation and fracture mechanics are identified effects that are all included in the virtual model. The results presented in this paper show possible selections of material models in conjunction with material damage models, adequately describing thin polymer films behaviour. Comparison between the physical test and the virtual test, exerted to fracture Mode I – Centre Cracked Tension, showed a good correlation for the chosen modeling technique.

Keywords: brittle, CCT, constitutive model, damage initiation, damage evolution, damage propagation, deformation, ductile, fracture mechanics, LEFM, material modeling, Mode I, NLFM, opening performance, plasticity, polymer, polymer film.

1. Introduction

To open a package virtually, as shown in Figure 1, is today possible with SIMULIA software's. Physical tests in combination with virtual tests to characterize thin polymer films have been concerned in this work. Defining a finite element modeling strategy and a physical test procedure is critical for determining the general material behaviour of polymers used in opening applications.



a) Geometry of the opening concept: Cap, Holder and Cutter
b) Physical test of the opening concept with polymer cutters
c) Virtual test of the opening concept with polymer cutters

Figure 1. Physical and virtual opening of a beverage package, inside view.

2. Materials considered in this work

2.1 General properties of polymers

The word polymer has its origin from the two Greek words; poly – meaning “many” and meros – meaning “part”. The term was introduced in 1833 by the Swedish chemist Jöns Jacob Berzelius (Wikipedia, 2012). This definition is rather good to utilize when describing the micro and macro mechanical behaviour of polymers. A polymer consists of many repeating units called “monomers”, building combinations of larger networks. The physical properties and different mechanisms involved in the mechanical behaviour of the different polymer materials originate from the monomer composition. The type of monomer, how they are arranged, chain length, how the long molecule chains fold and interact with each other, crystallinity and how the crystallites are interacting determine the material properties. The combination of the stated effects occurs both in the macroscopic continuum response and also during damage process, damage initiation and evolution. A basic understanding of the micro mechanics is very useful when understanding the macroscopic behaviour of the polymer films. The mechanical properties are highly influenced by the manufacturing process; the material/molecular orientation, production speed and operating temperatures. Other effects are temperature, humidity, viscoelastic and strain rate dependency.

2.2 Mechanical behaviour of polymers

When the polymer networks are stretched, the amorphous regions are extended, molecular folds and large subgroups are restricted and the molecules orient themselves along a preferred direction, resulting in enhanced orientation and increased order. This described phenomenon, depicted in Figure 2, have a significant effect in an opening application where a damage initiation and damage evolution occur. One very ductile polymer, Low-Density PolyEthylene (LDPE), and one much more brittle polymer film, PolyproPylene (PP), were chosen to illustrate the different polymer behaviors and physical mechanisms in this article.

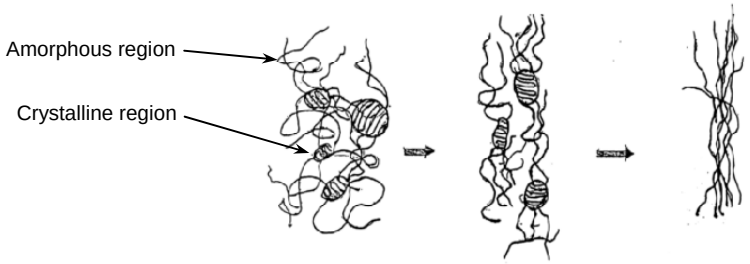


Figure 2. Molecular stretching of a polymeric material, (www.engr.utk.edu, 2011).

The initial physical response, when stretching a polymer, is given by the electrostatic bonding forces between molecules e.g. van der Waals forces and/or H-bonds and mechanical entanglement in between the molecular chains. These somewhat weaker bonds are often referred to as secondary bonds. The primary bonds, commonly covalent in polymers, are very strong compared to the secondary bonds. This can be one of the reasons for the often pronounced final strain hardening behaviour occurring in many polymers.

Two physical quantities are of great interest when dealing with fracture mechanics in polymers, the fracture toughness and the energy release rate. The first of these material parameters describe the amount of energy that is needed to initiate the damage and the latter the energy to create new crack surfaces, hence propagating the crack. The stress intensity factor, K_I, with the unit $MPa\sqrt{m}$ is a quantity that describes the local phenomena close to the crack tip. Stresses, strains and displacements near the vicinity of the crack are determined by this factor. This quantity is most often used in Linear Elastic Fracture Mechanics, LEFM. Energy release rate, G, with the unit J/m^2 is on the contrary describing the global material behaviour. In small scale yielding all crack tip deformation and failure is driven solely by K_I. In ductile polymer, where large deformation is common and hence a lot of energy is dissipated into plastic work this is not the case. The energy approach states that crack extension i.e. fracture, occur when the energy available for crack growth is sufficient to overcome the resistance of the material. The material resistance may include surface energy, plastic work, or other type of energy dissipated with propagating crack (Andersson, 1995). Excerting a ductile or brittle polymer to in plane tensile loading, CCT - Mode I loading conditions, leads to rather different behaviours as shown in Figure 3, (Jemal, 2011). The crack tip of the ductile polymer to the left is significantly deformed and blunted prior to crack initiation and crack propagation. In this case a lot of energy is dissipated to plastic work and visual inspection with polarized light indicate a large area affected around the newly created crack surfaces. On the contrary a lot of strain energy is stored in the strong and tough polymer film to the right and thus only a small deformation and blunting is noticeable prior to the crack initiation and propagation. A ductile polymer with extensive plastic deformation, as described earlier, has a rather slow crack growth, the damage evolution is often referred to as stable crack growth. In a brittle material, where almost no plastic deformation is noticeable, a substantially faster crack growth occurs and it is hence termed unstable crack growth. Buckling and wrinkles in the out of plane direction due to compressional stresses is also present due to the very thin polymer films.

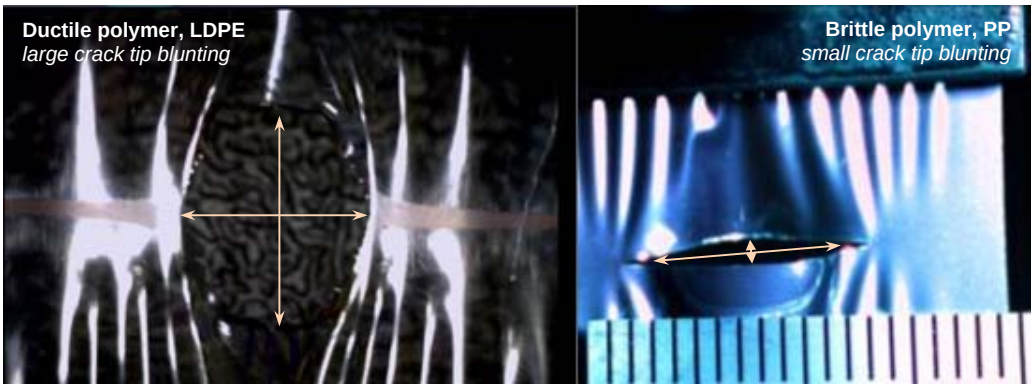


Figure 3 Crack tip blunting in two different polymer films, LDPE and PP.

One of the fundamental assumptions of fracture mechanics is that fracture toughness is indepenedent of size and geometry of the cracked body (Andersson, 1995). This is often the case, but the fracture toughness and in which manner the crack grows is heavily dependent upon the material thickness, and in our case with thin polymer film it is hard to get the “stable”/true plane-strain fracture toughness value (Mfoumou, 2004).

3. Governing theory

3.1 Constitutive models for the continuum

In linear elastic isotropic materials, the material behaviour is governed solely by Young's elastic modulus, E, and the Poisson's ratio, ν. The focus in this section will be the far more complicated anisotropic material parameters and the governing equations for thin polymer films. Studying very thin polymer films with a thickness in the μm-scale, plane stress conditions can be assumed. In these polymer films the in-plane dimensions, mm-scale, is several magnitudes larger than the thickness direction, μm. The plane stress orthotropic linear elastic relation, described for paper materials (Mäkelä, 2003), is given by Hooke's law and is defined by the equation

$$\boldsymbol{\sigma} = \boldsymbol{C}\boldsymbol{\varepsilon}^e = \begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{12}\end{bmatrix} = \frac{1}{(1-\upsilon_{12}\upsilon_{21})}\begin{bmatrix}E_1 & \upsilon_{21}E_1 & 0\\ \upsilon_{12}E_2 & E_2 & 0\\ 0 & 0 & G_{12}(1-\upsilon_{12}\upsilon_{21})\end{bmatrix}\begin{bmatrix}\varepsilon_{11}^e\\ \varepsilon_{22}^e\\ \gamma_{12}^e\end{bmatrix} \tag{1}$$

where index 1 and 2 refers to the two principal material directions orthogonal to each other, often denoted MD and CD for paper materials. The engineering shear strain above is denoted γ_{12}^e. Some of the material parameters are rather straight forward to measure with appropriate physical tests. Other parameters are rather difficult to measure experimentally and are not routinely determined. Among the difficult parameters are for instance the in-plane shear modulus, G_{12}, and the Poisson's ratios υ_{12} and υ_{21}. An approximate value of G_{12} can be calculated by the formula (Gibson, 1994)

$$G_{12} = G_{MDCD} = \frac{1}{\frac{4}{E_{45^\circ}} - \frac{1}{E_{MD}} - \frac{1}{E_{CD}} + \frac{2\nu_{MDCD}}{E_{MD}}} \tag{2}$$

Thus an additional experimental test is needed in the material direction 45 degrees to the principal direction MD. This method, commonly used in paperboard material, can definitely be applicable for thin polymer film where shear testing is a rather complicated physical test due to the very ductile and flexible material. In addition to these equations the compliance matrix, the inverse of the stiffness matrix C defined earlier, is symmetric and described in the equations below

$$\frac{\upsilon_{12}}{E_1} = \frac{\upsilon_{21}}{E_2} \Rightarrow \upsilon_{21} = \frac{E_2\upsilon_{12}}{E_1} \tag{3}$$

The plastic properties of the material has also to be considered, Hill's potential function, with an elliptical shape in the deviatoric plane compared to the von Mises circular shape can be utilized (Ristinmaa, 2005). Anisotropic yield criterion can be described as an extension of the von Mises function which can be expressed in terms of rectangular Cartesian stress components as

$$f(\sigma) = \sqrt{F(\sigma_{22}-\sigma_{11})^2 + G(\sigma_{33}-\sigma_{11})^2 + H(\sigma_{11}-\sigma_{22})^2 + 2L{\sigma_{23}}^2 + 2M{\sigma_{31}}^2 + 2N{\sigma_{12}}^2} \tag{4}$$

where $F, G, H, L, M,$ and N are constants obtained by physical tests of the material in different orientations. The different constants are defined according to the Abaqus Analysis User's Manual (Abaqus, 2012) or other comprehensive theoretical books within this field. When defining plasticity in Abaqus, it is important to use true stress and true strain quantities instead of nominal stress and nominal strain, especially for ductile polymers where large deformations are present.

The selection of true stress/strain components is done to account for the rather large reduction of the initial cross sectional area A_0, often referred as necking, when the material is exerted to tensile loading. The nominal stress and strain is expressed by

$$\sigma_{nominal/engineering} = \frac{F}{A_0} \qquad \varepsilon_{nominal/engineering} = \frac{\Delta l}{L_0} \tag{5}$$

True stress and strain quantities is defined by the two equations

$$\sigma_{true} = \sigma_{nominal}(1 + \varepsilon_{nominal}) \qquad \varepsilon_{true} = ln(1 + \varepsilon_{nominal}) \tag{6}$$

The above two relations, true stress and strain, are valid only prior to necking. True plastic strain is thus expressed as

$$\varepsilon^p_{true} = \varepsilon_{true} - \left(\frac{\sigma_{true}}{E}\right) \tag{7}$$

3.2 Introduction to the basic concepts in fracture mechanics theory

General literature introducing the field of fracture mechanics for instance (Andersson, 1995), (Broberg, 1999) and (Nilsson, 2001) is easily found. However it is very hard to find books that in detail describe the non linear response of polymer materials exerted to different loading conditions accompanied with fracture mechanics. It is challenging to find appropriate damage models and a general introduction to the numerical tools for simulating continuum damage in polymer materials. A lot of inspiration to this work has hence been collected from several sources; articles, polymer books, user manuals and also the above mentioned literature. In this section, an introduction to the different notations, variables and quantities used for fracture mechanics is presented. Adopting LEFM and utilizing an infinite plate with a centre cracked panel exerted to in-plane tensile loading the stress intensity factor, K_I, is described by

$$K_I = \sigma\sqrt{\pi a}, \qquad [MPa\sqrt{m}] \tag{8}$$

where σ is the stress and a is half the crack length for a centre crack. The fracture Mode I stress intensity factor K_I for a crack through a finite plate is given as (Andersson, 1995)

$$K_I = \sigma\sqrt{\pi a} \cdot F\left(\frac{a}{W}\right) = \sigma\sqrt{\pi a} \cdot \left[\frac{2W}{\pi a} tan\left(\frac{\pi a}{2W}\right)\right]^{1/2} \tag{9}$$

A more accurate solution for a crack through in a finite plate obtained from finite element analysis, (Andersson, 1995) is given by

$$K_I = \sigma\sqrt{\pi a \cdot} F\left(\frac{a}{W}\right) = \sigma\sqrt{\pi a} \cdot \left[sec\left(\frac{\pi a}{2W}\right)^{1/2}\right]\left[1 - 0.025\left(\frac{a}{W}\right)^2 + 0.06\left(\frac{a}{W}\right)^4\right] \tag{10}$$

where the trigonometric function is defined by $\sec(x) = 1/\cos(x)$ and W denotes half of the total sample width, $2W$. The critical value of the stress intensity factor, K_{Ic}, for a linear elastic material is refeered to as fracture toughness.

The energy release rate, G, defined as the rate of change in potential energy with crack surface area for a linear elastic material, link the stress intensity factor with the elastic material parameter.

For a crack of length $2a$ in an infinite plate, i.e. the width of the plate is, $2W \gg 2a$, subjected to remote tensile stress, the energy release rate for plane stress is given as (Andersson, 1995)

$$G = \frac{{K_I}^2}{E} = \frac{\pi {\sigma_\infty}^2 a}{E} \tag{11}$$

where σ_∞ is the remotely applied stress, a is half the crack length, and E is Young's modulus. Depending on the mixture of amorphous regions and crystalline regions the fracture toughness and the energy release rate of the polymer material is quite different. The equations described in this section are valid for linear elastic materials, e.g. metals. Polymeric materials, when subjected to large deformations, are unfortunately not behaving as linear elastic materials. Therefore Elastic-Plastic Fracture Mechanics - EPFM or Non-Linear Fracture Mechanics - NLFM, is needed to adequately describe the material response more accurately. The crack surfaces with an initial sharp shape, as in our case for polymers, is moving apart prior to damage initiation. Plastic deformation blunts the sharp crack as illustrated earlier. Hence is more advanced fracture mechanical models needed to better capture this type of phenomenon. More complicated quantities and numerical tools are introduced as J-Integral, Crack Tip Opening Distance - CTOD and Essential Work of Fracture – EWF (Andersson, 1995). These quantities are often used for a more realistic description of the material behaviour in polymeric material. An enhanced model for describing material that undergoes plastic deformation is the Dugdale-Barenblatt model also referred to as the Strip Yield Model, SYM. These quantities are not further discussed in this.

4. Finite element modeling

It is beneficial to define a FE-modeling strategy as early as possible in a project. There are at least two reasons, one of them is selecting appropriate constitutive equations and hence which continuum material models and material damage models that are implemented and available in currently used software. The second reason is to understand in which analysis procedure the final application is to be solved in, Abaqus/Standard or Abaqus/Explicit. It´s preferable to calibrate the material models in the same analysis procedure and with the same specific settings as the application later will be solved in. At first it seems quite trivial to select the appropriate solver but by experience this decision can be quite tricky. Try to consider different aspects or physical mechanisms that will eventually be included in the final model, for instance contact conditions, damage initiation, damage evolution, large deformation, very small elements and time domain. Different solvers can support quite different element types, material models, stability and contact algorithms. Many of the industrial applications deal with very small elements in the thickness direction, due to the thickness of the package material laminate structure, and hence is Abaqus/Explicit not the most beneficial code due to very small time increments. Membrane or shell elements are most often used if Abaqus/Explicit is chosen as the solver. The quite recent implementation of the quasi-static procedure in the Dynamic/Implict solver is appealing to use in many applications where the total time domain in physical tests is a couple of seconds or minutes.

4.1 Material modeling in the finite element code Abaqus

In the simplest case, isotropic elastic material properties are defined for describing the continuum material behaviour. The **`*ELASTIC`** option is used to define linear elastic moduli. In an Abaqus analysis either isotropic, orthotropic or anisotropic linear elastic moduli can be defined for

describing material properties of the solid continuum elements. These options of the keyword are more thoroughly described in the different Abaqus manuals and the keyword is supported in Abaqus/Standard, Abaqus/Explicit and Abaqus/CAE. Below is an extract of the two different settings that were used in this work.

***ELASTIC, TYPE=[ANISOTROPIC | COUPLED TRACTION | ENGINEERING CONSTANTS | ISOTROPIC | LAMINA | ORTHOTROPIC | SHEAR | SHORT FIBER | TRACTION]**

Data lines to define isotropic elasticity (TYPE=ISOTROPIC):

E, ν

Data lines to define orthotropic elasticity in plane stress (TYPE=LAMINA):

$E_{MD}, E_{CD}, \nu_{MDCD}, G_{MDCD}, G_{MDZD}, G_{CDZD}$

In thin polymer film layers, implemented as shell elements, where plane stress conditions prevail only the values of $E_{MD}, E_{CD}, \upsilon_{MDCD}, G_{MDCD}, G_{MDZD}$ and G_{CDZD} are required to define an orthotropic material. The shear moduli G_{MDZD} and G_{CDZD} are included because they may be required for modeling transverse shear deformation in a shell. The Poisson's ratio υ_{CDMD} is implicitly given by the symmetry condition discussed in the previous section. In most of the engineering applications it´s not enough only to use elastic material properties describing the material, thus is yielding and hardening often needed. To specify plastic material properties, non linear behaviour, for a polymeric material is challenging, especially if the material behaves anisotropic. In this work a metal plasticity model is utilized. This model is used to specify the plastic part of the material model for elastic-plastic materials that use the von Mises or Hill yield surface. This keyword is available in Abaqus/Standard, Abaqus/Explicit and also supported in the Abaqus/CAE. Abaqus use true stress or Cauchy stresses in the ***Plastic** material card and hence has the physical test data results to be adjusted. Engineering stress or nominal stress that most often is given from the experimental test apparatus should therefore be transformed to the appropriate stress quantity used by Abaqus. This effect is significant in polymer films used in this work, exerted to high loading conditions and hence large deformations. The data needed to be put into the keyword and the specific settings is described below.

***PLASTIC, HARDENING=[ISOTROPIC | KINEMATIC | COMBINED | JOHNSSON COOK | USER]**

Data lines to define the plastic points:

$\sigma_{yield}, 0$ *Yield stress, plastic strain*

$\sigma^1, \varepsilon^1_{plastic}$

$\sigma^2, \varepsilon^2_{plastic}$

...

$\sigma^n, \varepsilon^n_{plastic}$

In an isotropic material, von Mises plasticity is most often utilized. Adopting an anisotropic continuum material with a yield function hardening gets a little more complicated. One way of introducing the asymmetric yield function is to take advantage of the Hill plasticity (Ristinmaa 2005). Define an anisotropic yield model by the keyword ***POTENTIAL**. This option is used to define stress ratios for anisotropic yield behaviour. It can be used in conjunction with material models defined by the ***PLASTIC** option. This functionality is supported in Abaqus/Standard, Abaqus/Explicit and Abaqus/CAE.

***POTENTIAL**

Data lines to define stress ratios:

$R_{11}, R_{22}, R_{33}, R_{12}, R_{13}, R_{23}$ $\quad where\ R_{11} = \frac{\bar{\sigma}_{11}}{\sigma_{y0}}, R_{22} = \frac{\bar{\sigma}_{22}}{\sigma_{y0}}, R_{33} = \frac{\bar{\sigma}_{33}}{\sigma_{y0}}, R_{12} = \frac{\bar{\sigma}_{12}}{\tau_0}, R_{13} = \frac{\bar{\sigma}_{13}}{\tau_0}, R_{23} = \frac{\bar{\sigma}_{23}}{\tau_0}$

Two quantities, damage initiation and damage evolution, mainly define the fracture behavior of the material in fractured model analysis in Abaqus. The keyword ***DAMAGE INITIATION** Specify material properties to define the initiation of damage. This keyword is provided in the products Abaqus/Standard, Abaqus/Explicit and also supported in the Abaqus/CAE.

***DAMAGE INITIATION, CRITERION=[DUCTILE | FLD | HASHIN | HYSTERESIS ENERGY | JOHNSON COOK | MAXE | MAXS | MAXPE | MAXPS | MK | MSFLD | QUADE | QUADS | SHEAR | USER]**

ε_p^{eq} *(equivalent plastic strain at damage initiation), -p/q (stress triaxility), strain rate*

The model assumes that the equivalent plastic strain at the onset of damage is a function of stress triaxility and strain rate. The stress triaxility effect is very low for a thin polymer layer where a plane stress condition is dominating. In addition to damage initiation there is a need of describing the damage evolution. The purpose of the virtual model is to be able to predict the opening performance and thus is a complete damage model needed. The latter option ***DAMAGE EVOLUTION** specifies material properties to define the evolution of damage. This option is used to provide material properties that define the evolution of damage leading to eventual failure. It must be used in conjunction with the ***DAMAGE INITIATION** option. It can be utilized for elements with plane stress formulations; plane stress, shell, continuum shell, and membrane elements and, in Abaqus/Explicit, for elastic-plastic materials associated with any element type. This option is provided in the products Abaqus/Standard, Abaqus/Explicit and Abaqus/CAE. A lot of settings can be used in this option and the settings utilized in this work is highlighted below

***DAMAGE EVOLUTION, TYPE=[DISPLACEMENT | ENERGY | HYSTERESIS ENERGY], DEGRADATION=[MAXIMUM | MULTIPLICATIVE], SOFTENING = [LINEAR, EXPONENTIAL, TABULAR]**

Effective total or plastic displacement at failure, measured from the time of damage initiation.

The use of plasticity for a polymeric material can be questionable, one of the reasons to use this setting is that plasticity must be used in conjunction with the damage initiation and damage evolution keywords in order to get damage. This assumption is not too large simplification if the loading condition is monotic loading without any significant cyclic loading or unloading and subsequent loading. The two main keywords for modeling material damage were described above. A general discussion of the damage modeling and especially applied for polymer film materials including stages as damage initiation and damage evolution will follow. *Damage initiation* defines the point where the stiffness degradation is initiated, shown in Figure 4. Two main mechanisms can cause the fracture of a ductile polymer: ductile fracture due to the nucleation, growth and coalescence of voids and shear fracture due to shear band localization. Based on phenomenological observations, these two mechanisms call for different forms of the criteria for the onset of damage. It does not actually lead to damage unless damage evolution is also specified. *Damage evolution* defines the post damage material behavior (Abaqus, 2011). The characteristic stress-strain behavior of a material undergoing damage is shown in Figure 4. A damage variable, D, is introduced to represent the degradation of the material. In the context of an elastic-plastic material with isotropic hardening, the damage manifests itself in two forms: softening of the yield stress and decrease of the elasticity. The solid curve shown in Figure 4 represents the damaged

stress-strain response, while the dashed curve shows the continuum response if no damage occurs (Abaqus, 2011).

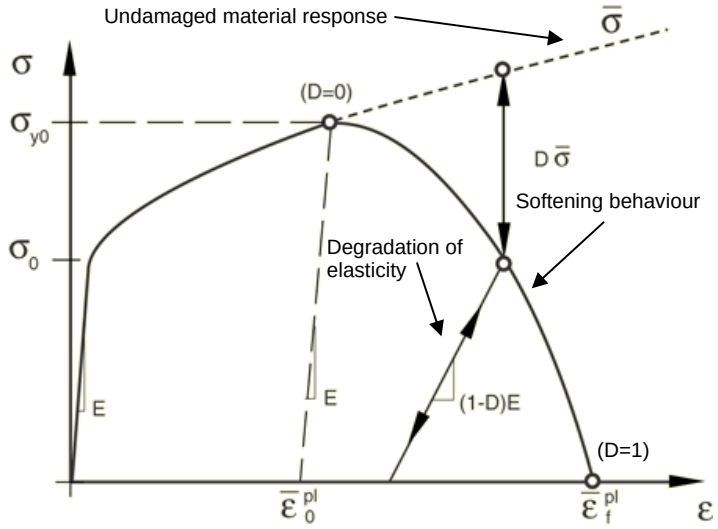


Figure 4. Stress strain response of a damaged material (Abaqus, 2011).

5. Physical tests of polymer films, in-plane

The physical test procedure utilized in this work is described in the experimental work by (Mfoumou, 2004) and (Jemal, 2011). Characterizing thin material parameters with non standard dimensions of *95x230mm*, 2W x 2H, have been utilized in a number of articles (Kao-Walter, 2002). Rather large test specimens were used in order to decrease the edge effect of the centered pre-made cracks. The aim of the experimental tests is to define a test procedure for determining material properties governing damage initiation and propagation for thin polymer films. Accurate experimental data is needed for calibrating the material models used in the FE-simulations.

5.1 Physical test setup

In infinite sheet, size of crack is small compared to dimension of the sheet. In this case the crack tip conditions are not influenced by external boundaries. As the crack size increases or as the sheet size decreases, the outer boundaries start to exert an influence on the crack tip. Since a tensile stress cannot be transmitted through a crack, the lines of force are diverted around the crack, resulting in a local stress concentration. If the sheet width is restricted to $2W$, the force perpendicular to the edge must be zero on the free edge; this boundary condition cause the line of force to be compressed, which results in a higher stress intensification at the crack tip as described in (Andersson, 1995). The experimental test setup and the different material orientations of the specimens are shown in Figure 5.

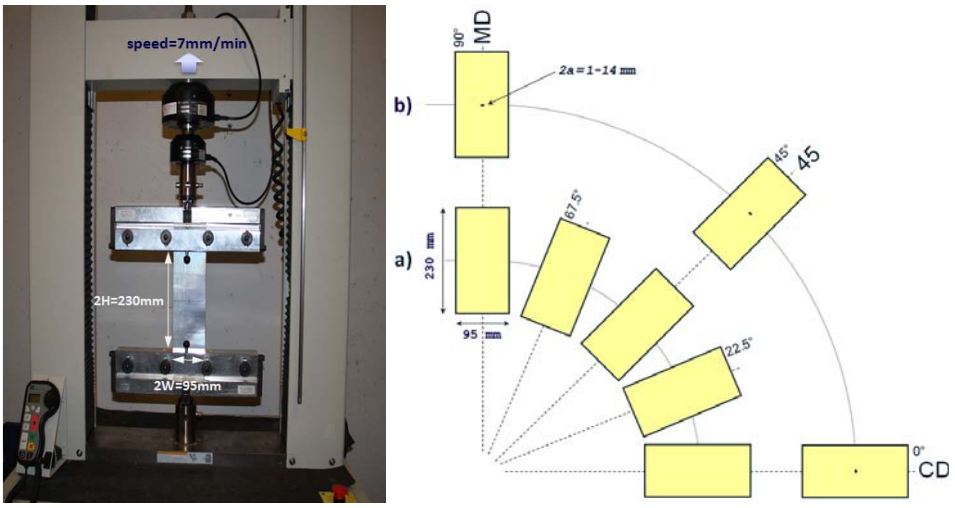


Figure 5. Physical test setup to the left, test specimens to the right.

The tensile test machine shown in Figure 5 has a pair of grippers that clamp the specimen ends. One of the grippers is stationary, the lower one, and the upper gripper moves upward. The test specimen is placed in between the grippers. The clamped specimen is loaded and extended until it breaks. The tensile test speed is constant during the test and set to $7\ mm/min$. The load and extension of the test specimen is recorded. A large reduction of the maximum loading capacity is seen if a centre crack is introduced, Figure 5 b), in the specimen compared to not introducing any crack, Figure 5 a). The response curve has the same initial slope "yielding", and "hardening" and depending on the crack size, a cut off is seen at different displacements. If a $2mm$ wide crack is introduced in the brittle polymer film a decrease of 60% of the maximum load is obtained. In a ductile polymer only a reduction of 10% of the maximum loading capacity is seen. Buckling in the out of plane direction occurs when a pre-cracked specimen, exerted to tensile loadings in the vertical directions, fracture Mode I. Formation of wrinkles, described by (Li et. al, 2005), due to compressional strains creates the out of plane "buckling" shown in Figure 6, Centre cracked tension test specimens with the dimensions $25x20\ mm, 2a = 5mm$.

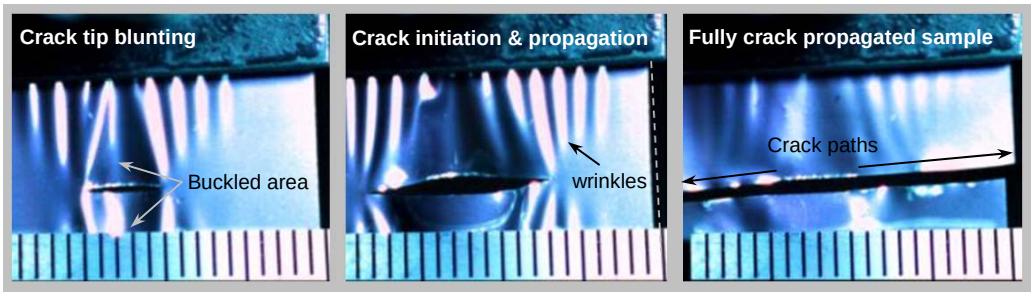


Figure 6. Crack tip blunting, initiation and propagation in thin polymer film.

This buckling effect has been shown to have a small influence on the overal result (Li et. al, 2005) and hence, this out of plane buckling, is not restricted by two polymer or glass plates in the experimental tests in this work. This is not more thoroughly investigated in this work.

6. Analysis procedure in Abaqus

The purpose of the numerical model in this work is to calibrate the material parameters under Fracture Mode I tensile loading in the virtual environment, thus to predict the material continuum response and the damage process. A finite element model representing the test specimen of the polymer material was created and analyzed using a general purpose finite element program, Abaqus/Explicit. Due to convergence problems in Abaqus/Standard, because of material degradation, Abaqus/Explicit was used in this work. The number of elements varies from 20 000 to about 100 000 for the calibration and opening simulation with a simulation time in the range of one to two days on a large linux-cluster. Simulation in the realistic time scale, which is a rather slow strain rate, would require an excessive number of small time increments. To get acceptable solution time the quasi-static solution needs to be accelerated somehow. The problem is that when an event is accelerated, the state of static equilibrium evolves in to a state of dynamic equilibrium in which inertial forces become more dominant. The goal is to model the analysis in a short time period where inertial forces remain in-significant. However, size of the finite elements in an explicit analysis determines the simulation time. Common pitfalls will be discussed and presented in this section. As discussed earlier, use true stress and strain quantities. Another very general tip is not to take anything for granted; in Abaqus/Standard **NLGEOM** is not used per default, this is the case in Abaqus/Explicit. Shell elements were used throughout this work. It is very important to utilize *consistent units*, the general recommendation is always to use SI-units. Length scale, utilizing mm, and stress quantities in MPa is simple to use when pre-processing and modeling realistic applications and therefore frequently used but should be handled with great care.

To be able to visualize the element deletion in post processing, the **STATUS** filed output should be selected in the ***FIELD OUTPUT** request. Implementing a crack is very easy in Abaqus/CAE, there are several ways. One of them is for instance in the Interaction module: Tools→Partition→Face →Sketch (draw the desired crack length). When the crack is sketched this line can then be utilized in the menu Special→Crack→Assign seam (here assign the drawn crack section as a seam), this is a very effective and general technique of separating two parts by disconnecting the nodes. To be able to get a nicer visual appearance in the post processing; Mesh module: Element→Element deletion→Yes. For an analysis in Abaqus/Explicit the setting in the Job module: Double precision is important to invoke at job submission and facilitate and enhance accurate numerical results.

6.1 Calibration of constitutive model and material parameters

It´s very useful to combine physical material characterization tests with virtual tests in an effective manner to calibrate the material parameters. Thereby a standardized working procedure is created for describing the mechanical properties of a thin polymer film. With the aid of the inverse analysis technique described by (Ageno, 2008) or (Mahnken, 1996), in conjunction with an optimization software, for instance Isight, a work flow can be created. In this work it was done by experience and in a manual manner and good results was reached within a few number of

iterations, hence was it done in this primitive way and the focus was rather put on capturing the physical fracture processes. A typical response graph of the material reaction to the tensile load from the physical tensile test is presented in Figure 7. One plane of symmetry was utilized in the numerical model. In these graphs are also the virtual tensile test results from calibrated material parameters plotted. The visual appearance of both the physical tensile test and the virtual tensile test is overlaid in the picture shown in Figure 7 a and b. In the upper graph, a), was not a centre crack introduced, hence is only the continuum material depicted. Introducing a centre crack in conjunction with the appropriate damage material parameters in the virtual model reduces the loading capacity significantly and this result is depicted in Figure 7 b). The visual and the qualitative results are quite accurately describing the material behaviour for this type of polymer film according to the graph and the comparison of the virtual and physical test in the lower right hand corner. Observe that the two different graphs have not the same scales, the lower graph is significantly zoomed to be able to visualize the two graphs.

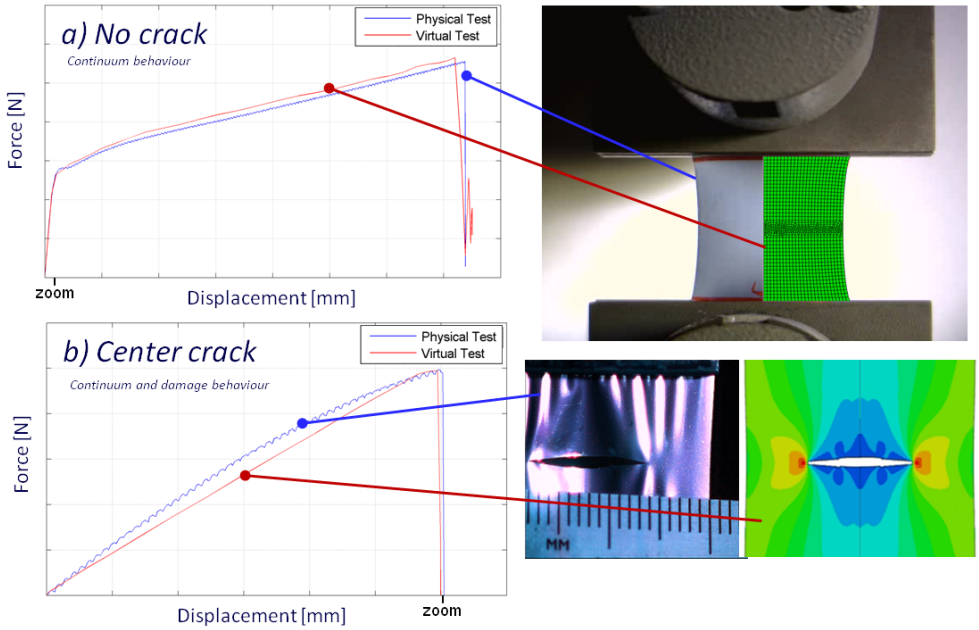


Figure 7. Physical and virtual uni-axial tensile testing of polymer film.

6.2 Visualization of virtual simulation result

Analyzing simulation results thoroughly is most often quite cumbersome, the most difficult part is to know which response factor to evaluate. The advantage when conducting physical tests combined with virtual test is that a lot clues of how to interpret the result and what to specifically look for is generated. One of the most obvious results, shown in Figure 8, is to look into the different stress and strain components, especially when the stress state is not typically homogenous and also when anisotropic films are to be evaluated. It is evidently seen that the stress field in the vicinity of the crack and close by is quite inhomogeneous. The buckled area, discussed

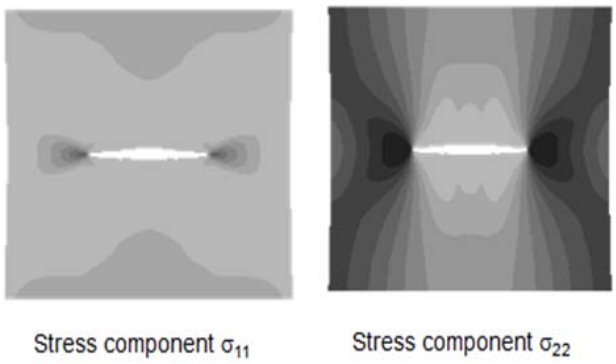


Figure 8. Stress components during Mode I tensile loading.

earlier, is also indicated in the right picture in Figure 8. The buckled area is visualized in light gray, below and over the crack surface in the centre of the specimen.

Evaluating simulation results has the advantage that depending on the number of ***FIELD OUTPUT** and ***HISTORY OUTPUT** requests a rather detailed visualization of the crack blunting, damage initiation and damage propagation can be extracted. Defining relevant response factors like force versus displacement is important to be able to quantify the accuracy of the numerical models. These variables are often used in the calibration scheme discussed earlier. Another nice feature with the simulation results is the possibility to project the damage evolution on the undeformed geometry, shown in Figure 9 for an opening simulation. Visualizing the crack path is thus possible and can be quite handy when comparing different design proposals impact on the crack propagation. This is done by post processing the undeformed state and applying the status variable on this setting. When dealing with element deletion and damage models it is important to enable the field output status variable, then the element deletion is evoked automatically in the Abaqus/Viewer by default, as described below.

```
*Output, field, time points=TimePoints-fine-output
*Element Output, directions=YES
PE, PEEQ, S, STATUS
```

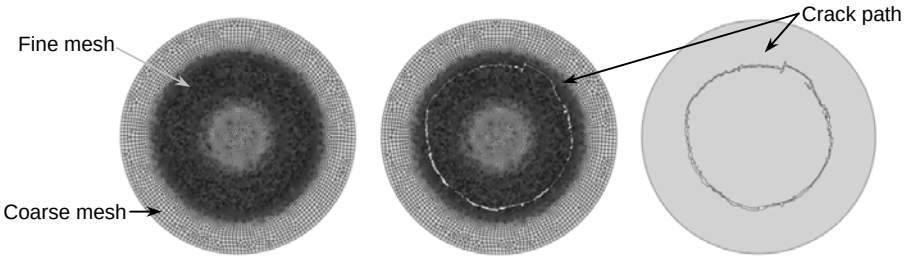


Figure 9. Visualization of the crack propagation in undeformed state

7. Results and conclusions

Many industries as aircraft, automobile and manufacturing are doing everything to avoid fracture and failure. However opening a package means on the contrary that a damage initiation is preferred and especially controlled damage propagation is wanted. Utilizing fracture mechanics knowledge in combination with good geometrical part design makes the opening process robust. The aim of this work is to simulate the initiation of the damage and afterwards controlling the crack propagation in the package material structure, in a generic opening concept. It is definitely possible both in implicit and explicit finite element codes to initiate and also propagate damage. Only a few years back it was hard to implement material damage models and the hardware was not there yet. Lately the interest has shifted from only calculating stress intensity factors and stress concentrations for LEFM to be able to do realistic simulations, for instance package openings. Doing that means that it is manageable to translate NLFM into governing constitutive equations and numerical models in Abaqus. This virtual test environment can thus be used as a tool to drive the development of new opening concepts. Geometry and shape optimization of the various polymer parts in combination with the design of laminated material structures is possible.

7.1 Future work

The continuation of this work is to define the FE modeling strategy and also to find a physical test procedure for thin polymer films exerted to fracture Mode II and Mode III. Physical characterization of the polymer films in various strain rates, humidity's and also temperatures is of high importance. A better understanding of how to experimentally measure quantities such as υ_{MDCD}, υ_{CDMD} and the shear moduli in the three different material directions is needed. A lot more exotic effects can be implemented in the virtual models, for instance the adhesion between the different materials layers in the package material structure. Simulations with the analysis procedure Implicit/Dynamic, quasi-static, can be used to compare with the current results in this work. It is advisable to start evaluating and use the eXtended Finite Element Model, XFEM, for numerical modeling in Abaqus to get rid of mesh dependency. Hopefully this technique is implemented for shell elements in Abaqus within a reasonable amount of time. New techniques such as the different meshless particle methods for instance SPH and EFG has also been shown effective in the literature capturing damage processes accurately. The material model presented in this study couldn't capture the blunting of very ductile polymer films. Therefore are material models for polymers with a significant softening behaviour of interest in further studies. In general there is a gap in Abaqus in the available constitutive models describing polymers and anisotropy in a good way.

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