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Prediction of shear crack formation of Lithium-ion batteries under rod indentation: Comparison of seven failure criteria

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Abstract:

One of the major catastrophic events in the accidents involving electric vehicles is the electric short circuit, leading to the thermal runaway, and possible fire and explosion. The short circuit is a result of the development of local or through-thickness fracture inside a cell. Fracture of the discrete layered structure of lithium-ion batteries is a complex problem involving six materials with completely different deformation and fracture properties. The homogenized model of the deformation of batteries has emerged as the best compromise between simplicity and accuracy, and therefore the well-established Deshpande–Fleck model of crushable foams is used in the present analysis to describe the deformation behavior. For the fracture description of battery cells, the authors follow the experience accumulated over the decades in predicting failure of metals and geomaterials. The constitutive description of these classes of materials gained in complexity, requiring elaborated experimental techniques for the determination of material parameters. However, the choice of possible tests for pouch or cylindrical cells is very limited, which hinders the complexity in fracture models. Those tests are typically in-plane and out-of-plane compression tests because it is almost impossible to subject an individual pouch battery to tensile or shear loading. Therefore, out of vast literature in the field of fracture, only the simplest models are considered. In this study, the seven simplest fracture models, involving only one or maximum two material constants, are coupled with the homogenized Deshpande–Fleck model to study the fracture behavior of pouch cells. Their performance is critically evaluated in terms of the capability of predicting the initiation and propagation of crack under mechanical transverse loading.

1 Introduction

An abundance of many apparently similar constitutive models in the libraries of the general purpose commercial finite element codes causes often difficulties for the average users in the industry and academia. The range of applicability of a given model is not clearly stated nor the calibration procedure is explained in the users' manuals. Two decades ago, the advanced high-strength steels (AHSS) were making its way to the automotive industry and there was an urgent need of having reliable and accurate necking and fracture models for these new grades of steel. The paper on "Calibration and Evaluation of Seven Fracture Models" that appeared in 2005 was welcomed by the community and appreciated by many follow-up studies for revealing the insights of different models [1]. This was followed in 2006 by another paper on "Evaluation of Six Fracture Models for High-Velocity Perforation" [2]. Since then several fundamental phenomenological and physics-based papers appeared and prediction of ductile fracture in a broad class of practical problems has been resolved [3-13].

Today, mechanic's community is facing a new challenge of prediction safety limits of lithium-ion batteries subjected to mechanical loading. There are two types of computational models of batteries [14]. The first is based on the homogenized material model such as the crushable foam model in LS-Dyna [15, 16], or the Deshpande-Fleck model in Abaqus [17, 18], which treats the layered battery structure as a homogenized medium (Figure 1). Such or similar model can predict the global plastic resistance of various cells, as measured by the load-displacement curve with good accuracy. These results are important to calculate the crash energy absorption of cells, battery modules and battery packs for electric vehicles but cannot predict the peak force and the amount of intrusion into battery causing the electric short circuit. A separate criterion is needed to make this prediction. Sahraei et al. [19] proposed the

criterion based on the critical value of the maximum principal strain. The homogenized models are easy to calibrate with a small number of tests but the question to transferability of material data from one type of tests to the other has not been fully resolved.

Figure 1 The discrete layered structure of the battery cell treated as a continuum.

In the alternative approach, all components of the layered structure of a cell are tested and calibrated with the most suitable constitutive flow and fracture models. Theoretically, the detailed battery model should be applicable to all type of batteries (cylindrical, pouch and prismatic) and all loading conditions. In reality, difficulties arise in testing and calibrating of individual components, for example, predicting plastic and fracture behavior of this aluminum and copper foils, which serve as current collectors for the anode and cathode. The reason is a small thickness of the foils (10-20 microns) which make tests under various stress stated a real challenge. A separate difficulty is to model and calibrate the granular coating of the electrodes. This difficulty was overcome by the investigating team of the present authors using a series of geomechanical tests including axial compression, Brazilian, and confined compression tests [20, 21]. With the existing experimental data of the other battery components [18, 22], a detailed computational model was subsequently established, which can successfully predict the load–displacement curve, the peak load, the displacement to the

electrical short circuit, and the shear failure of the cell [21].

In summary, each of the above two approaches has its own advantages and limitations. The family of homogenized models is easy to implement and calibrate, but each type of battery and especially loading conditions may require a separate calibration. The detailed model, on the other hand, is very general but the extraction of material and fracture data of each of the six different materials within a cell is time-consuming, difficult, and often subjected to large uncertainties or errors.

The present paper is concerned with the analysis of the homogenized models of materials and fracture. With the objective of introducing some order in this evolving field, seven well-established fracture criteria are critically evaluated and compared for the most accurate prediction of battery failure. Various models are rated not only for their capability of predicting the peak load and corresponding displacement to failure but also how well they describe the initiation point and orientation of the fracture plane across the thickness of the cell. The analysis consists of four steps. The jelly roll, or more precisely the stack of electrodes inside the pouch cover is modeled by the Deshpande–Fleck constitutive formulation. Two parameters define the yield surface, as well as the hardening law, are determined from uniaxial compression and hydrostatic compression tests, previously reported by the present investigating team [23]. The same plasticity model is used for all subsequent fracture study.

In the next step, the fracture parameters are calibrated from one type of indentation tests to match the measured and predicted displacement to failure. Then the failure criterion is introduced as a user subroutine and the element deletion technique is used to visualize the

initiation and propagation of the crack under the punch. Different tests are used for calibration and validation. The magnitude of peak force and displacement to failure is predicted for all seven failure criteria with various degrees of accuracy. The Johnson–Cook (JC) and the Cockcroft–Latham (CL) fracture models emerge here as winners. The ultimate test for the capabilities of various models is the ability to predict correctly the sequence of initiation and propagation of cracks. Again, the JC and CL provide a correct path of the through-thickness shear crack of all seven models.

The present paper not only reports on a new study on fracture but offers to the battery community a powerful tool for constructing the failure envelope of the lithium-ion batteries subjected to mechanical loading.

2 Constitutive model – modified Deshpande–Fleck model

In this study, the Deshpande–Fleck model [24] is further extended by coupling it with a failure criterion in order to model crack initiation, propagation, and final fracture. A failure indicator is formulated to account for the accumulation of damage and once it reaches unity the crack is initiated by setting the stress and the stiffness to zero. To visualize the crack initiation and propagation, the element deletion technique is used in Abaqus/Explicit code.

The model is formulated in the range of small strains, where the additive strain decomposition is used. The total strain rate of the solid materials is decomposed into elastic and plastic parts:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p \quad \text{Eq. 1}$$

Therefore, the volumetric strain rate, $\dot{\varepsilon}_v \equiv \text{tr}[\dot{\boldsymbol{\varepsilon}}]$, is also decomposed into two parts:

$$\dot{\varepsilon}_v = \dot{\varepsilon}_v^e + \dot{\varepsilon}_v^p \quad \text{Eq. 2}$$

For the stress–strain correlation, Hook’s law applies:

$$\boldsymbol{\sigma} = \mathbb{C}:\boldsymbol{\varepsilon}^e \quad \text{Eq. 3}$$

where $\mathbb{C}$ is the stiffness matrix. Consequently, stress deviator, $\mathbf{s}$, and the hydrostatic stress, p , are defined as below:

$$\mathbf{s} = 2G\boldsymbol{\varepsilon}_d^e; p = K\varepsilon_v^e \quad \text{Eq. 4}$$

where $\boldsymbol{\varepsilon}_d^e$ is the elastic strain deviator; G and K are, respectively, the shear modulus and bulk modulus, defined by:

$$G = \frac{E}{2(1 + \nu)}; K = \frac{E}{3(1 - 2\nu)} \quad \text{Eq. 5}$$

where E is the Young’s modulus and ν is the Poisson’s ratio. Therefore, the Deshpande–Fleck yield function is expressed as:

$$\Phi = \sqrt{q^2 + \alpha^2 \left[p - \frac{p_c - p_t}{2} \right]^2} - \alpha \frac{p_c + p_t}{2} \leq 0 \quad \text{Eq. 6}$$

where p_c and p_t are the cut-off pressure under hydrostatic compression and tension, respectively; q is defined the same as the von Mises equivalent stress $\bar{\sigma}$:

$$q = \bar{\sigma} = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}} = \sqrt{\frac{3}{2}} \|\mathbf{s}\| \quad \text{Eq. 7}$$

α is defined by:

$$\alpha = \frac{3k}{\sqrt{(3k_t + k)(3 - k)}} \quad \text{Eq. 8}$$

where k and k_t are given as:

$$k = \frac{\sigma_c^0}{p_c^0} \text{ and } k_t = \frac{p_t}{p_c^0} \quad \text{Eq. 9}$$

where σ_c^0 and p_c^0 are the initial yield stress under the uniaxial compression and the initial pressure under hydrostatic pressure. A geometric illustration of these variables are shown in Figure 2.

For battery cells, different from the original isotropic hardening of the Deshpande–Fleck model, volumetric hardening law is applied [25]. It implies that during the hardening, the yield stress under hydrostatic tension p_t keeps as a constant, while the yield stress under hydrostatic compression evolves:

$$p_t = \text{const.}; p_c = p_c(\varepsilon_v) \quad \text{Eq. 10}$$

where ε_v is the volumetric compacting plastic strain, which controls the evolution of the yield surface in the p - q space, defined as the “equivalent” strain in the present study:

$$\varepsilon_v \equiv -\varepsilon_v^p \quad \text{Eq. 11}$$

Due to the zero plastic Poisson’s ratio, under uniaxial compression condition, $\varepsilon_{\text{axial}}^p = \varepsilon_v^p$:

therefore, the volumetric hardening can be expressed by the uniaxial compression data:

$$p_c(\varepsilon_v^p) = \frac{\sigma_c(\varepsilon_{axial}^p) \left(\frac{1}{\alpha^2} + \frac{1}{9} \right) + \frac{p_t}{3}}{p_t + \frac{\sigma_c(\varepsilon_{axial}^p)}{3}} \quad \text{Eq. 12}$$

where $\sigma_c(\varepsilon_{axial}^p)$ is the yield stress under uniaxial compression test as a function of the absolute value of axial plastic strain.

The Deshpande–Fleck model is based on the non-associated flow rule and the flow potential is defined as:

$$\Phi' = \sqrt{q^2 + \frac{9}{2}p^2} \quad \text{Eq. 13}$$

According to the flow rule, the plastic strain rate tensor is calculated by:

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\bar{\varepsilon}}^p \frac{\partial \Phi'}{\partial \boldsymbol{\sigma}} \quad \text{Eq. 14}$$

where $\dot{\bar{\varepsilon}}^p$ is the equivalent plastic strain rate, which is defined by applying the work equivalence principle:

$$\dot{\bar{\varepsilon}}^p = \frac{\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p}{\Phi'} \quad \text{Eq. 15}$$

The fracture initiation criterion is formulated as a failure indicator based on the following general equation:

$$I_f = \int_0^{\varepsilon} \frac{d(\varepsilon)}{(\varepsilon)^f} = 1 \text{ or } \int_0^{\sigma} \frac{d(\sigma)}{(\sigma)^f} = 1 \quad \text{Eq. 16}$$

where (σ) and (ε) are representing a general form of the component or equivalent value of the stress and strain tensor, respectively; $(\sigma)^f$ and $(\varepsilon)^f$ represent the general stress and strain based failure criteria, which will be specified in detail in section 3. After Eq. 16 is satisfied, the element loses its load-carrying capability and is further deleted from the model to reveal

the crack initiation and propagation pattern. It is noted that for the stress-based failure criterion, the integral representation is only valid for monotonic loading condition. In the present plane-strain indentation problem, this condition is satisfied.

Figure 2: The schematic drawing of the yield criterion and the flow potential of the Deshpande–Fleck model in the p - q space.

3 Seven failure criteria

In this study, seven well established and often used failure criteria are considered and they are i) the maximum principal stress criterion; ii) the maximum shear stress criterion; iii) Mohr–Coulomb criterion; iv) the maximum principal strain criterion; v) the critical volumetric strain criterion; vi) Cockcroft–Latham criterion and vii) Johnson–Cook criterion. They are individually explained in detail in what follows.

Criterion I: Maximum principal stress (Smax)

The Smax criterion is a very often used failure criterion for the brittle fracture prediction of body-centered cubic (bcc) structures [26, 27]. In this context, it is also often referred to as the Orowan criterion. The criterion assumes that the fracture will occur once the maximum principal stress σ_1 of the critical location of the materials subjected to loading reaches a critical value. A schematic drawing of the criterion is shown in Figure 3 (a).

$$\sigma_1 = C \quad \text{Eq. 17}$$

Criterion II: Maximum shear stress (SSmax)

As one of the oldest and still often used failure criterion, especially in geomaterials such as soils and rocks [1], the SSmax criterion assumes that fracture happens at one of the shear planes when the maximum shear stress reaches a critical value. As it is shown in Figure 3 (a), it is exactly perpendicular to the Smax criterion in the Mohr's circle representation. The formulation is defined as:

$$\tau_{\max} = C \quad \text{Eq. 18}$$

where $\tau_{\max}$ represents the maximum shear stress.

Criterion III: Mohr-Coulomb failure model (MC)

Continuing the previous two criteria, Smax and SSmax, a natural extension is to combine both the shear stress and the principal stress in a linear form, which is the MC criterion. It has been

used mainly for the description of the plasticity and failure behavior for geomaterials and more recently was shown to describe ductile fracture of metals [32]. It basically assumes that fracture is triggered once the maximum value of the combination of shear stress and normal stress reaches a critical value. The formulation is expressed:

$$\max\{\tau + C_1\sigma_n\} = C_2 \quad \text{Eq. 19}$$

where τ and σ_n are the shear and normal stresses on the fracture plane; C_1 and C_2 are the fitting parameters, which are often referred to as the “friction” parameter related to the friction angle φ and the “cohesion” parameter, respectively. A schematic drawing of the MC criterion is also given in Figure 3 (b).

Figure 3: Schematic illustration of (a) Smax and SSmax failure criteria and (b) MC criterion.

Criterion IV: Maximum principal strain ($E_{\max}$)

The maximum principal strain criterion has not been a popular failure criterion in the conventional metal society. However, for battery's failure prediction, it has been applied to several types of batteries especially coupled with the crushable foam plasticity model in the LS-DYNA code [19, 23]. The model formulation is simply expressed in the following equation and the failure is assumed to occur once the maximum principal strain ε_1 of a local material point reaches a critical value C .

$$\varepsilon_1 = C \quad \text{Eq. 20}$$

Criterion V: Constant volumetric strain (Evol)

The Evol criterion is equivalent to the constant equivalent Mises plastic strain criterion in the metal failure applications. The Mises strain loses its relevance for the concerned materials due to the compressible properties of the battery cells as well as the volumetric hardening law in the plasticity model formulation. Fracture is triggered immediately once a critical volumetric strain is first reached in any element of the material during deformation and the equation of the criterion is shown below.

$$\varepsilon_v = C \quad \text{Eq. 21}$$

Criterion VI: Cockcroft–Latham failure model (CL)

CL failure criterion proposed by Cockcroft and Latham [28] is an extension of the Smax criterion, from purely stress based formulation to a stress–strain one. The model has been recently used in the fracture prediction of metals during material forming [29] as well as under the high-speed impact loading [30]. The model assumes that failure happens once the accumulated work of the positive maximum principal stress over the equivalent strain reaches a critical value, as shown in the following equation.

$$\int_0^{\bar{\varepsilon}_f} \langle \sigma_1 \rangle d\bar{\varepsilon} = C; \langle \sigma_1 \rangle = \begin{cases} \sigma_1, & \sigma_1 > 0 \\ 0, & \sigma_1 \leq 0 \end{cases} \quad \text{Eq. 22}$$

where symbol $\langle \cdot \rangle$ is the Macaulay bracket, which takes the value of σ_1 only when $\sigma_1 > 0$ and sets the value as zero when $\sigma_1 \leq 0$, and $\bar{\varepsilon}_f$ is the failure strain. For an implicit formulation of the model, the CL model is more often applied in the following form modified by Oh, Chen et al. [31].

$$\int_0^{\bar{\varepsilon}_f} \frac{\langle \sigma_1 \rangle}{\bar{\sigma}} d\bar{\varepsilon} = C' \quad \text{Eq. 23}$$

Although there is only one parameter involved in the model, it is offering an automatic

dependency of the failure strain on stress triaxiality and Lode angle parameter. Assuming proportional loading the failure criterion can be transformed into the strain–stress triaxiality–Lode angle parameter space, as shown in the Eq. 24. The formulation also indicates a changeable cut-off value of the failure strain once the denominator of Eq. 24 is zero. A more detailed discussion of the criterion compared to others is referred to Bai and Wierzbicki [32].

$$\bar{\varepsilon}_f = \frac{3C'}{3\eta + 2\cos\left(\frac{\pi}{6}(1 - \bar{\theta})\right)} \quad \text{Eq. 24}$$

where η is the stress triaxiality and $\bar{\theta}$ represents the Lode angle parameter as defined in Bai and Wierzbicki [3]. It is noted that in the present study the equivalent strain that is being evaluated is not the Mises equivalent plastic strain as for metals. Instead, the volumetric compacting plastic strain is used as the equivalent strain, as defined in Table 1.

Criterion VII: Johnson–Cook failure model (JC)

Since several decades ago, it has been proven by experimental work [33–37] and theoretical calculation based on long cylindrical and spherical voids [38, 39] that the failure strain of metals is dependent on the stress triaxiality. One of the most commonly used failure criteria in this context is the JC criterion, which was derived phenomenologically by Johnson and Cook [35] in a comprehensive experimental companion involving several alloys under various stress states, strain rates, and temperatures. Excluding the effects of the latter two factors, the JC criterion for quasi-static condition used is simply expressed in the following equation.

$$\int_0^{\bar{\varepsilon}_f} \frac{d\bar{\varepsilon}}{C_1 \cdot \exp(-C_2\eta)} = 1 \quad \text{Eq. 25}$$

where C_1 and C_2 are the fitting parameters. It is noted in the current form of the JC criterion, the third constant that shifts the failure curve vertically in the space of strain and stress triaxiality is omitted for the ease of the parameter calibration. The fracture is considered to

occur when the accumulated damage, expressed as the fraction of the strain increment to its failure strain under the current stress state, reaches one. Under proportional loading, it is reduced to a simple criterion only based on the fracture strain, as shown in Eq. 26. Therefore, the chosen form in Eq. 25 has the advantage to overcome a certain level of the non-proportional loading effect.

$$\bar{\varepsilon}_f = C_1 \cdot \exp(-C_2 \eta) \quad \text{Eq. 26}$$

It is also noted that the same definition of the equivalent strain is used as for the Cockcroft-Latham fracture model. By comparing Eq. 24 and Eq. 26, it is seen that the Cockcroft-Latham fracture model is more general because it includes the dependence on the Lode angle parameter while the JC criterion does not. The employed seven failure criteria are summarized in Table 1. In total, there are three criteria in the pure stress space, two in the strain space and two in the mixed stress-strain space.

Table 1: The seven failure criteria and their formulations investigated in the study.

Criteria	Equations	Parameters	Formulation space
Max. principal stress (Smax)	$\sigma_1 = C$	C	Stress
Max. shear stress (SSmax)	$\tau_{\max} = C$	C	Stress
Mohr-Coulomb (MC)	$\max\{\tau + C_1 \sigma_n\} = C_2$	C_1, C_2	Stress
Max. principal strain (Emax)	$\varepsilon_1 = C$	C	Strain
Const. volumetric strain (Evol)	$\varepsilon_v = C$	C	Strain
Cockcroft-Latham (CL)	$\int_0^{\varepsilon_v^f} \langle \sigma_1 \rangle d\varepsilon_v = C$	C	Mixed stress-strain
Johnson-Cook (JC)	$\int_0^{\varepsilon_v^f} \frac{d\varepsilon_v}{C_1 \cdot \exp(-C_2 \eta)} = 1$	C_1, C_2	Mixed stress-strain

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4 Modeling of deformation behavior

4.1 Experiments and FE model

In this study, the pouch cells with 26.3 Ah are used. The cell dimensions are 232 mm (L) x 153 mm (W) x 7.5 mm (T) with alternating layers of 20 anodes, 19 cathodes, and separators in between them. For detailed information about the cells, the readers are referred to Chuang et al. (1). The indentation tests that are investigated in this study are the ones under a cylindrical punch with two different punch diameters 15 mm and 28.6 mm. Both of these two loadings are creating, in general, a plane-strain compression on the batteries. The tests were conducted under quasi-static condition at zero percent state of charge with open circuit voltage about 3V. For the detailed testing procedures, the readers are referred to Chuang et al. (1) and Sahraei et al. (3).

The numerical models of the indentation tests are constructed in the commercial FE code Abaqus/Explicit. Due to the plane-strain compression loading condition, a 2D model is constructed with the solid plane strain elements with reduced integration point (CPE4R). In principle, symmetry can also be assumed with respect to the middle plane of the cells, but a full model is used for the latter fracture pattern investigation. As mesh is a key factor influencing the FE simulation, especially for damage and fracture investigation, consistent element type and size at the critical plastic deformation zone are used. The element size of the fine mesh at the critical zone is $0.1 \text{ mm} \times 0.1 \text{ mm}$. For the deformation behavior, such a small element is not necessary to reach a convergence of the numerical solution. However, as the element deletion method is used for the visualization of crack initiation and propagation, this size is suitable as it corresponds to a length scale that a crack is usually detected in experiments. The support surface and the punch are modeled as analytical rigid bodies, and a Coulomb friction value of 0.2 was assumed to model the contact phenomena between cells,

supporting surface, and the punch. According to the experiment, the support is fixed in all degree of freedoms, while the punch is moving down with a constant velocity to indent the cells until a displacement over the fracture limit observed in the experiments.

4.2 Calibration of the deformation parameters

To describe the deformation behavior of the cells, three materials properties are required, the elastic constants, the stress–strain response and the two parameters of the Deshpande–Fleck model. The elastic constants are taken from our previous study [23] and Young’s modulus is 4.2 GPa, while the Poisson’s ratio is assumed to be zero. For the stress–strain behavior, the calibrated curve from the uniaxial compression test is used as the axial strain is identical to the volumetric strain. A power-law relation of the stress and the volumetric strain, $\bar{\sigma} = A\bar{\epsilon}^n$, is employed with the constant A as 500 MPa and the exponent as 1.5. For the two parameters of the Deshpande–Fleck model, they are adapted from the previous study on a lithium-ion battery with similar architecture structure [18]. All of these materials parameter for the deformation description are summarized in Table 2.

With these calibrated parameters, the simulation of the indentation tests for both punch geometries is run in Abaqus/Explicit. The force–displacement results are shown in Figure 4 together with the experiments. A minor deviation at the beginning of the deformation is observed, which is mostly related to the fitting quality of the stress–strain behavior by a power-law equation to the experimental results. Overall, a quite good agreement between the experiments and simulation is reached, especially at the later stage of the deformation until the fracture point. This provides a good basis for the failure analysis in the following sections.

Table 2: The material constants used in the Deshpande–Fleck model.

Young’s modulus	Poisson’s ratio	A	n	k	k_t
4.2 GPa	0	500 MPa	1.5	1	10

Figure 4: The force–displacement responses of the experiment and simulation with the Deshpande–Fleck model for indentation tests with a cylindrical punch with a diameter of (a) 15 mm and (b) 28.6 mm.

4.3 Parametric study of the Deshpande–Fleck model

To further explore the influences of the two parameters of the Deshpande–Fleck model, a parametric study is designed in the following. The set the calibrated material parameters serves as the reference case. Two additional cases are derived by keeping the k_t as constant and reaching the limits of k at 0.1 and 2.9. The other two cases are setting k as a constant and k_t are set as 1 and 50. The following table summarizes the parameters for the case study.

Table 3: The five cases of the material parameters of the Deshpande–Fleck model.

Parameters	Reference case	Case I	Case II	Case III	Case IV
k	1	0.1	2.9	1	1
k_t	10	10	10	1	50

The simulation is run for the additional cases on the indentation test with the punch diameter of 15 mm. The force–displacement curves are shown in Figure 5 (a) and (b) for the study of

the influence of parameter k and k_t , respectively. It is observed that when keeping k_t as 10, both increasing and decreasing k value will result in higher forces. When considering the influence of the k_t value at a constant k value, the force response shows a monotonic pattern: increasing the k_t values will increase the force response. It is noticed that the maximum force is reached for k_t at one and a softening behavior is observed afterward. Increasing k_t value, however, shows a more homogeneous deformation, which is very similar to the previous two cases varying the k value.

To further understand the results of the parametric study, the yield locus of these five cases are plotted in the space of p and q . For each case, the initial yield locus and the evolution of it at a volumetric strain of 0.05 and 0.07 are also plotted in Figure 6. In addition, three typical loading cases of uniaxial tension, shear, and uniaxial compression are also marked in the figure. Comparing the reference case with Case I and II, it is clear that smaller k values introduce less pressure sensitivity to the yield locus. A small k value results in the yield locus closer to the Mises plasticity model. The three cases always have the same stress value for the uniaxial compression condition. However, when the k values are increased or decreased from one, the yield stress is both increased under the shear condition, which is also the reason for the increased force response under the plane-strain compression condition between the uniaxial compression and shear. For either very small or high k values, either no pressure sensitivity or very strong gradient of pressures dependence is found, which both promote a homogeneous deformation mode.

When comparing the reference case with Case III and IV, it is found that decreasing k_t value introduces pressure sensitivity or vice versa. Large k_t values also result in the yield surface toward the pressure-insensitive Mises plasticity model. At the same time, increasing the k_t value also increases the yield stress under the shear condition, which contributes to the force

increase in the plane-strain indentation test. For the very small value of k_t , a large difference of the yield stress between the uniaxial compression and the shear. This large difference creates a large gradient in any slight different stress states in-between, which contributes to the early and strong localization observed case III.

Figure 5: The force–displacement responses of the Deshpande–Fleck model for (a) various k values under a constant k_t and (b) various k_t values under a constant k .

Figure 6: The yield loci of the Deshpande–Fleck model at different volumetric strain levels for (a) reference case, (b) case I, (c) case II, (d) case III and (e) case IV.

5 Failure prediction

5.1 Failure parameter calibration of the seven criteria

Based on the parameter number of the failure model, the parameter calibration strategy is customized in two ways. For the single parameter failure model group (Smax, SSmax, Emax, Evol, and CL), the fracture parameter is simply calibrated based on the iterative fitting peak load at the force–displacement curve of the indentation test with 15 mm punch. The calibration procedure is shown in Figure 7. The single parameters for all these five criteria show a monotonic influence on the force–displacement response. The best fitting parameters are found by examining the goodness of fitting to the fracture displacement.

For the criteria with two material parameters, MC and JC, different calibration strategies are used. As the C_1 parameter in the MC model has a physical meaning, Chung et al. [23] derived the equation to correlate this parameter with the measured shear fracture angle. The correlation is shown graphically in Figure 8 (a). Therefore, this parameter is directly calculated and the parameter from the previous study is used here. The second parameter C_2 for the MC model is calibrated iteratively based on the force–displacement response of the indentation with 15 mm punch as the single parameter models. The calibration procedure is also shown in Figure 8 (b). For the JC criterion, the two parameters are actually independent on each other and no physical meaning is associated with either of them. Therefore, they are iteratively fitted based on force–displacement curves from both experiments with 15 mm and 28.6 mm indenters. A relatively large domain of these two parameters is defined in the space with rather coarse intervals of these two parameters. The optimization of these parameters with finer and finer intervals is involved until a good agreement of both experimental results is satisfied. The final fitted results are shown in Figure 9. As a summary, all the calibrated parameters are listed in Table 4.

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Figure 7: Parameter fitting procedure of the failure criteria with one parameter.

Figure 8: Parameter fitting of the MC criterion.

Figure 9: Parameter fitting of the JC criterion.

Table 4: The calibrated material parameters of the seven failure criteria.

Failure criteria	Smax C [MPa]	SSmax C [MPa]	MC C_1 [-]; C_2 [MPa]	Emax C [-]	Evol C [-]	CL C [MPa]	JC C_1 [-]; C_2 [-]
Parameters	19	36	1.1; 30	0.055	0.28	1.2	0.058; 6

5.2 Quantitative analysis of the predictive capability

After the calibration procedure of the parameters in the failure model by using the experimental data from the 15 mm punch, they are all applied to predicting the peak force in the indentation test with the 28.6 mm punch, except the JC criterion, for which both experiments are used for parameter calibration. The predicted results for the six criteria are shown in Figure 10. The three stress-based criteria show very similar performance: all of them are slightly underestimating the fracture moment of the new test. However, the extent of the underestimation is not large. The two strain-based criteria are showing controversial prediction quality: Emax criterion is overestimating the fracture displacement, while the Evol is underestimating. Both of them are showing relatively larger errors of the fracture displacement. The last criterion, CL, in the mixed stress-strain space gives a very good prediction of the fracture displacement.

For a more quantitative assessment of these criteria, the predicted fracture displacement of all seven criteria are normalized with the experimental ones for both geometries and they are presented in Figure 11. For the stress-based criteria, the Smax shows an overall minimum error in terms of the fracture displacement prediction. Both strain-based criteria are falling the bottom of the seven criteria and it is noted that the Emax gives an overestimation, which is more critical than underestimation in structural integrity analysis. The CL criterion shows very similar predictive performance to the JC criterion, almost perfect in terms of the fracture displacement prediction for both loading conditions. However, for the JC criterion, both experiments are actually involved in the parameter calibration procedure, while for the CL criterion, the indentation test with 28.6 mm is a complete prediction.

Figure 10: The force–displacement response of the six failure criteria on the indentation test with 28.6 mm punch.

Figure 11: The relative fracture displacement analysis of all sever failure criteria.

5.3 Shear fracture prediction

The fracture pattern comparison of the seven criteria with the experimental result is shown in Figure 12 for the cylindrical punch with 15 mm diameter and Figure 13 for 28.6 mm. The experimental results were revealed after the tests were completed and the punch was unloaded. As the entire cell is packed inside the metal case, it was cut in the middle to reveal the failure pattern, which also releases the internal stresses.

For the predicted failure pattern, in general, very similar behavior is found for all these failure criteria on both geometries. The Smax criterion is giving a completely vertical fracture pattern almost through the thickness, while the SSmax is showing initially horizontal fracture pattern followed by a shear fracture after certain crack propagation. The fracture pattern from MC criterion shows a large number of element deletion and these deleted elements are either vertical or slatted to the supporting plane. The Emax criterion is showing a complicated failure pattern. In the center part of the cell, the failure pattern is slanted, while four additional crack paths are found from top and bottom on both sides of the model. In all the above four cases, the fracture pattern is not physical. A quite clean shear fracture is reached by the Evol criterion, although the crack does not propagate completely through the thickness. In the end, both of the CL and JC criteria show a clear shear fracture through the entire thickness of the battery cell, which is greatly in line with the experimental results including the slant angle. It is, however, also noted that the prediction of the exact angle of the shear fracture from experiments is not a straightforward process, due to the effect of the released internal stress by cutting off the batteries.

It is clear that all the stress-based criteria exhibit a massive element deletion, especially the Smax and MC, compared to the strain based criterion. The failure pattern of Smax and SSmax are exactly perpendicular to each other and the MC, as a combination of the shear stress and normal stress, is showing also a mixture of both of them. The distribution of the maximum

principal stress is along the vertical direction, the same as the fracture angle. Accordingly, the distribution of the maximum shear stress is inclined with 45° to the vertical axis; however, the fracture pattern is horizontal until a certain length and it follows the maximum shear stress distribution.

Grouping the prediction of all the strain-based criteria, it is concluded that shear fracture is a volumetric strain dominant process. The three criteria based on the volumetric strain all achieved very good prediction of the failure pattern for both geometries. Although a through-thickness failure is not achieved for the constant volumetric strain criterion, the overall trend and slant angle is also quite close to the experiments. However, it is also obvious that the stress state is playing a non-negligible role for the accurate prediction of the entire failure pattern and the force–displacement response for different geometries. The CL and JC criteria are taking into account this effect of the stress state and resulted in a great performance on both metrics and for both geometries. In addition, based on the illustration of these two criteria in the space of equivalent stress vs. stress triaxiality, they do show very similar pattern under the general plane-strain condition. Therefore, similar performance is reached, although the CL criterion has only one fitting parameter, which gives benefits for the experimental and fitting effort. It is also, however, noted that the performance of all these criteria shall be further investigated under different loading conditions, which is an on-going work.

Another reason for the clean shear fracture prediction from the last two criteria is that they are both based on the integral of the stress over a strain space or strain over a stress quantity space. The integration also helps to stabilize the disturbed distribution of the stress/strain calculated from the Deshpande–Fleck model as well as the loading history influence on the crack initiation.

Figure 12: The comparison of the failure pattern between the experiment and the seven failure criteria of the indentation test with 15 mm punch.

Figure 13: The comparison of the failure pattern between the experiment and the seven failure criteria of the indentation test with 28.6 mm punch.

5.4 Shear crack initiation and propagation

The fracture pattern is an important metric to assess model performance. Additionally, the fracture initiation point and its propagation direction can also reveal more details of the failure process, as the experimental result is only a post-deformation observation and without an in-situ test it cannot give details of the crack initiation spot. The initiation spot matters as it is directly related to battery positioning and possible safety control. It is very likely that the failure criterion, which gives a reasonable prediction on both force–displacement response and the fracture pattern, fails to reveal the critical point to failure for the battery.

Based on the previous comparison of force–displacement response as well as the fracture path, the following criteria (E_{max} , E_{vol} , CL , and JC) are chosen to detail the failure initiation and propagation, while the rest clearly shows fundamentally wrong failure pattern. Four consecutive intervals of the deformation are shown in Figure 14 for the E_{max} criterion. The fracture under the plane-strain condition shows a sharp fracture mode, which can be also seen from the force–displacement curve, i.e. the drop of the force is sudden and right after the maximum force is reached. Therefore, these three deformation stages are so close to each other with an infinitesimal difference in terms of the displacement of the punch. This feature additionally also raises difficulties to capture the crack initiation and propagation history from experiments. As shown in Figure 14 (a) and (b), the crack initiation location of the E_{max} criterion is actually the bottom of the batteries and then followed by a second initiation spot on the top surface right beneath the punch. These two initiation spots are due to the bending moment caused by the interaction between the deformation part and the undeformed part of the battery. After the crack propagates along these two paths, the crack in the center appears until the bottom of the batteries, as shown in Figure 14 (c) and (d).

In Figure 15, the fracture path development is shown for the E_{vol} criterion. The prediction of

both the force–displacement response and the failure pattern by Evol criterion show a good agreement with the experiments. The initiation spot of the crack is right at the center of the battery and it is slightly towards the top surface. The crack then quickly propagates upwards to reach the top surface and develops secondary cracks at positions very close to the top surface of the battery. However, the crack does not develop obviously downwards towards the bottom surface of the battery. This inaccurate crack development history is not revealing the physics of the failure under the plane-strain condition and is also limiting the applicability of this criterion to reach an overall prediction for both punch geometries.

Both the CL and JC criteria are the best candidates in terms of both force–displacement response and the failure pattern prediction. Their crack development history plots are shown in Figure 16 and Figure 17. It is noted that they are actually giving very similar results. Different from the Evol criterion, it is seen that the crack is initiated from the middle plane of the battery closer to bottom. Its position in the middle plane is in a very good agreement with the experimental results. The crack is then propagated in both directions to form a completely through-thickness shear fracture.

Figure 14: The crack initiation and propagation history of the Emax failure criterion: (a) crack initiation; (b) second crack initiation; (c) third crack initiation and (d) final crack.

Figure 15: The crack initiation and propagation history of the Evol failure criterion: (a) crack initiation; (b) crack propagation and (c) final crack.

Figure 16: The crack initiation and propagation history of the CL failure criterion: (a) crack initiation; (b) crack propagation and (c) final crack.

Figure 17: The crack initiation and propagation history of the JC failure criterion: (a) crack initiation; (b) crack propagation and (c) final crack.

6 Conclusions

The aim of this study was to perform a systematic investigation of the shear fracture modeling of the battery cells by incorporating seven failure criteria into the Deshpande–Fleck model. During indentation of the cylindrical or hemispherical punch into the battery, there is initially predominant compressive stress. Then, membrane tension develops, so leading to shear loading of material elements and subsequent slat fracture, which is clearly observed in experiments. Out of seven fracture models, three are purely stress-based, two are strain-based, and two are formulated in the mix stress-strain space. It was found that the latter ones captures best the physics of the problem and gave the most accurate prediction. The winning models are the familiar Johnson–Cook and the Cockcroft–Latham model. The accuracy of predicting the crack path in the cylindrical punch indentation tests is unprecedented in the battery-related literature, see Figure 18.

Figure 18: Comparison of the fracture path of experiment and simulation of indentation test with a cylindrical punch of 15 mm diameter.

All fracture models were calibrated using the compression test by a cylindrical punch of 15 mm diameter. Those tests produce the plane-strain loading condition. The validation was performed on a similar test with 28.6 mm diameter, the results of those tests were reported in a previous publication of the present investigating team [23]. Measured in those tests were the load–displacement curve, the peak force, and the punch displacement to fracture. The plane-strain finite element model was established in Abaqus/Explicit, and a number of runs were made to calibrate and validate the plasticity and fracture models. It was shown that the Johnson–Cook and the Cockcroft–Latham fracture models predicted correctly the amount of peak load and the displacement to fracture.

Another very important finding was that both of those fracture models were able to predict correctly the initiation of fracture, the orientation of the fracture plane, and the global through-thickness shear fracture. This is a very remarkable finding because, with the complexity of the discrete structure of cells, it is remarkable that a simple one-parameter fracture model was able to predict the process of initiation and propagation of a crack leading to the electric short circuit. It is expected that a similar good correlation will be obtained for different loading conditions, such as indentations by a hemispherical punch, which is the subject of the current research.

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- Shear fracture of the battery cells is observed in experiments under cylindrical indentation.
- Severn failure criteria are coupled with the Deshpande–Fleck model to predict failure behavior.
- Johnson–Cook model and Cockcroft–Latham model provide the best failure prediction.
- An unprecedented accuracy of predicting the crack path in the cylindrical punch indentation tests is achieved by the two models in the battery-related literature.