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Organisation de Coopération et de Développement Economiques
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NUCLEAR ENERGY AGENCY
COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

NEA/CSNI/R(2001)6
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Technical Report on Micromechanical Versus Conventional Modelling in Non-Linear Fracture Mechanics

English - Or. English

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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

Pursuant to Article 1 of the Convention signed in Paris on 14th December 1960, and which came into force on 30th September 1961, the Organisation for Economic Co-operation and Development (OECD) shall promote policies designed:

- to achieve the highest sustainable economic growth and employment and a rising standard of living in Member countries, while maintaining financial stability, and thus to contribute to the development of the world economy;
- to contribute to sound economic expansion in Member as well as non-member countries in the process of economic development; and
- to contribute to the expansion of world trade on a multilateral, non-discriminatory basis in accordance with international obligations.

The original Member countries of the OECD are Austria, Belgium, Canada, Denmark, France, Germany, Greece, Iceland, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The following countries became Members subsequently through accession at the dates indicated hereafter: Japan (28th April 1964), Finland (28th January 1969), Australia (7th June 1971), New Zealand (29th May 1973), Mexico (18th May 1994), the Czech Republic (21st December 1995), Hungary (7th May 1996), Poland (22nd November 1996), Korea (12th December 1996) and the Slovak Republic (14th December 2000). The Commission of the European Communities takes part in the work of the OECD (Article 13 of the OECD Convention).

NUCLEAR ENERGY AGENCY

The OECD Nuclear Energy Agency (NEA) was established on 1st February 1958 under the name of the OEEC European Nuclear Energy Agency. It received its present designation on 20th April 1972, when Japan became its first non-European full Member. NEA membership today consists of 27 OECD Member countries: Australia, Austria, Belgium, Canada, Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Japan, Luxembourg, Mexico, the Netherlands, Norway, Portugal, Republic of Korea, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The Commission of the European Communities also takes part in the work of the Agency.

The mission of the NEA is:

- to assist its Member countries in maintaining and further developing, through international co-operation, the scientific, technological and legal bases required for a safe, environmentally friendly and economical use of nuclear energy for peaceful purposes, as well as
- to provide authoritative assessments and to forge common understandings on key issues, as input to government decisions on nuclear energy policy and to broader OECD policy analyses in areas such as energy and sustainable development.

Specific areas of competence of the NEA include safety and regulation of nuclear activities, radioactive waste management, radiological protection, nuclear science, economic and technical analyses of the nuclear fuel cycle, nuclear law and liability, and public information. The NEA Data Bank provides nuclear data and computer program services for participating countries.

In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has a Co-operation Agreement, as well as with other international organisations in the nuclear field.

COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

The NEA Committee on the Safety of Nuclear Installations (CSNI) is an international committee made up of scientists and engineers. It was set up in 1973 to develop and co-ordinate the activities of the Nuclear Energy Agency concerning the technical aspects of the design, construction and operation of nuclear installations insofar as they affect the safety of such installations. The Committee's purpose is to foster international co-operation in nuclear safety amongst the OECD Member countries.

CSNI constitutes a forum for the exchange of technical information and for collaboration between organisations which can contribute, from their respective backgrounds in research, development, engineering or regulation, to these activities and to the definition of its programme of work. It also reviews the state of knowledge on selected topics of nuclear safety technology and safety assessment, including operating experience. It initiates and conducts programmes identified by these reviews and assessments in order to overcome discrepancies, develop improvements and reach international consensus in different projects and International Standard Problems, and assists in the feedback of the results to participating organisations. Full use is also made of traditional methods of co-operation, such as information exchanges, establishment of working groups and organisation of conferences and specialist meeting.

The greater part of CSNI's current programme of work is concerned with safety technology of water reactors. The principal areas covered are operating experience and the human factor, reactor coolant system behaviour, various aspects of reactor component integrity, the phenomenology of radioactive releases in reactor accidents and their confinement, containment performance, risk assessment and severe accidents. The Committee also studies the safety of the fuel cycle, conducts periodic surveys of reactor safety research programmes and operates an international mechanism for exchanging reports on nuclear power plant incidents.

In implementing its programme, CSNI establishes co-operative mechanisms with NEA's Committee on Nuclear Regulatory Activities (CNRA), responsible for the activities of the Agency concerning the regulation, licensing and inspection of nuclear installations with regard to safety. It also co-operates with NEA's Committee on Radiation Protection and Public Health and NEA's Radioactive Waste Management Committee on matters of common interest.

Foreword

The Integrity and Ageing Working Group (IAGE WG) of the CSNI deals with the integrity of structures and components, and has three sub-groups, dealing with the integrity of metal components and structures, ageing of concrete structures, and the seismic behaviour of structures. The sub-group dealing with metal components has three mains areas of activity: Non-Destructive Examination; fracture mechanics; and material degradation.

Based on concluding discussions at the International Comparative Assessment Study of Pressurized-Thermal-Shock in Reactor Pressure Vessels (RPV PTS ICAS, report referenced NEA/CSNI/R(1999)3), participants proposed a list of future tasks that could contribute to further refinement of RPV integrity assessment methods:

- Selection of consensus reference solutions that could serve as benchmarks for future qualification of analytical methods. These would provide a valuable tool for the qualification of new analysts on the subject of RPV integrity assessment;
- Study of the implications of the observed scatter in the THM task on deterministic fracture
- mechanics assessments;
- Assessment of the nozzle region of an RPV;
- Assessment of the significance of residual stresses upon RPV integrity;
- Study of crack arrest of a fast running crack in an RPV;
- Study of micro-mechanical modelling of the crack-tip region;

The CSNI Working Group on Integrity and Ageing (IAGE) decided to carry out a report on micro-mechanical modeling to promote this promising and valuable technique. The report presents a comparison with non-linear fracture mechanics and highlights key aspects that could lead to a better knowledge and accurate predictions.

Fracture mechanics reports issued by the group since 1992 are:

NEA/CSNI/R(92)21 Proceedings of IAEA/CSNI Specialists Meeting on Fracture mechanics verification by large scale testing, ORNL, October 1992 (NUREG/CP-0131, ORNL/TM-12413)

NEA/CSNI/R(94)12 FALSIRE Phase I Comparison Report

NEA/CSNI/R(95)1 SOAR on Key fracture mechanics aspects of integrity assessment

NEA/CSNI/R(95)4 Report on Round robin activities on the Calculation of crack opening behaviour and leak rates for small bore piping components

NEA/CSNI/R(96)1 FALSIRE Phase II - Fracture Analyses of Large Scale International Reference Experiments

NEA/CSNI/R(96)4 Proceedings of Workshop on Probabilistic structural integrity analysis and its relationship to deterministic analysis, Stockholm, March 96

NEA/CSNI/R(97)8 Fatigue crack growth benchmark.

NEA/CSNI/R(99) 3 Comparison report of RPV pressurized thermal shock international comparative assessment study (PTS ICAS)

NEA/CSNI/R(2001)14 Technical report on the fatigue crack growth benchmark based on CEA pipe bending tests

The complete list of CSNI reports, and the text of reports from 1993 on, is available on http://www.nea.fr/html/nsd/docs/

Current activities include a benchmark on Probabilistic Structural Integrity of a PWR Reactor Pressure Vessel and a benchmark on crack propagation under thermal loading. An other activity is related to bullet 1 above and is aiming towards the completion of the compendium of large PTS tests.

Acknowledgement

Gratitude is expressed to Professor Fred Nilsson of the Department of Solid Mechanics with the Royal Institute of Technology (KTH), Sweden for carrying out this report.

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MICROMECHANICAL VERSUS CONVENTIONAL MODELLING IN NON-LINEAR FRACTURE MECHANICS

1. Introduction

The possibility of a fracture of a reactor pressure vessel has always been considered as a problem of central concern and has indeed been one of the driving forces behind the development of fracture mechanics. Fracture events in other components are also of significant interest although less critical than a pressure vessel failure. As nuclear reactors age these concerns may increase due to irradiation embrittlement and the possible occurrence of service induced defects. Although the fracture mechanics methodology has experienced tremendous advance during the last two decades, still a number of problems remains to be solved. One group of problems falls mainly under the general heading of whether *transferability* can be relied upon. The goal of fracture mechanics is to enable predictions of initiation and propagation of growth of existing or postulated cracks of given configurations in structures of arbitrary shapes. It should be possible to base a prediction on results from experiments performed on specimens of the same material, but with a geometry that differs from the one under consideration. It is here to be understood that the environmental conditions such as for instance temperature should remain the same. This concept of transferability of fracture mechanics results is central to the success of fracture mechanics. If we can rely on the transferability, results from experiments conducted on small laboratory specimens can be used to predict the fracture behaviour of a large structure for which an assessment is desired. Complicated, occasionally impossible, full scale testing is thus avoided.

The load carrying material in a reactor pressure vessel and in several other components is a ferritic steel. It is well known that the temperature has important effects on the fracture behaviour of such materials. At high temperatures (upper shelf) crack growth occurs by a wholly ductile mechanism either through void growth and coalescence or through shear localisation. For these mechanisms continued crack growth requires increasing loads. At low temperatures (lower shelf) the fracture mode is cleavage which is a highly unstable event. In an intermediate temperature region, the transition region, the incipient growth and propagation can often be identified with fibrous rupture. Fracture may then occur as a ductile fracture or an unstable event of the cleavage type. Characteristic for the loss of stability due to cleavage is that it can not be explained within the framework of J_R-philosophy based on experimentally measured resistance curves on the macro level, since a change of micromechanism occurs. Obviously, both ductile and cleavage micro-mechanisms are operative and competitive. This behaviour is more marked in the upper transition region and has been recognised in a large variety of experiments over the years. While mechanistic explanations of this type of behaviour have been developed, a full understanding of the temperature transition problem is still lacking. It is the object of the present report to provide an overview of the methods available to perform predictions of crack growth either by ductile or cleavage mechanisms.

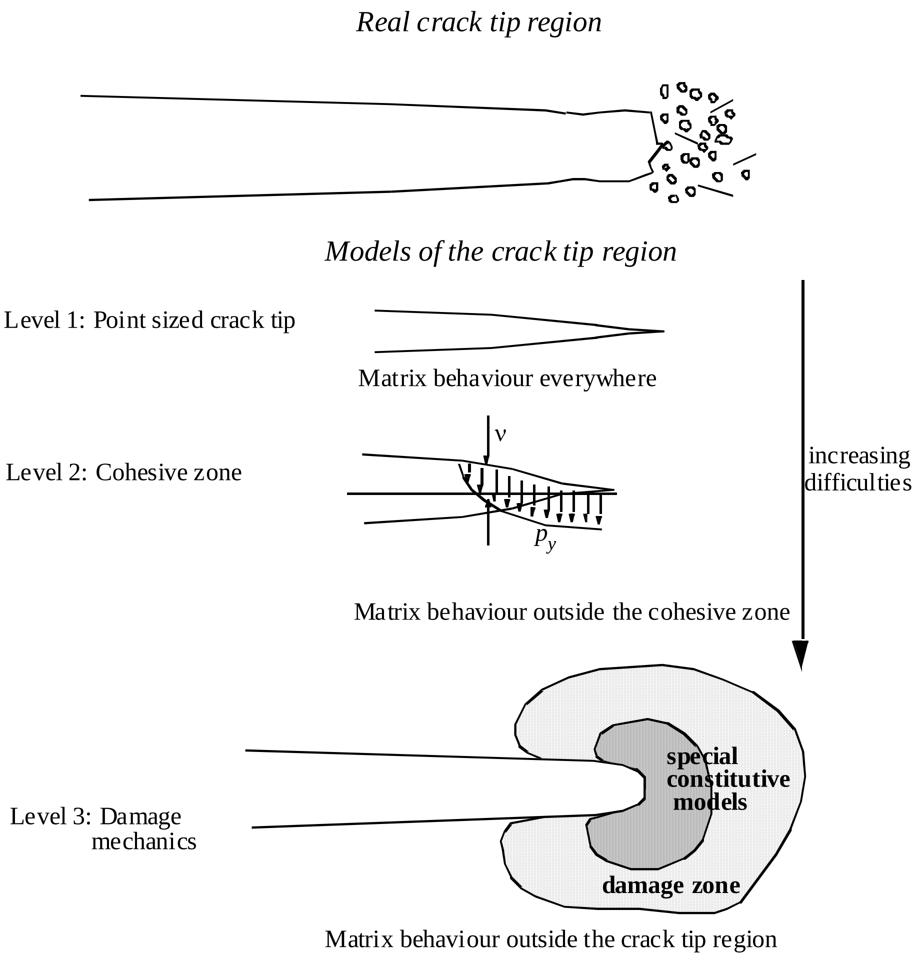

Fig. 1. Different levels of modelling the crack tip region.

Depending on which type of problem that is under consideration different ways of modelling can be employed. The state of a loaded crack tip in reality is complicated and any more detailed modelling of the structure and the processes is in general not possible. Fracture mechanics modelling can be divided into different levels according to Fig. 1. At the highest level (1) the crack tip is assumed to be a point and no special assumptions of the material behaviour apart from those of the matrix material are made. The bulk of current fracture mechanics theory is at this level including linear elastic fracture mechanics (LEFM) and non-linear fracture mechanics using for instance *J*-type description. As will be discussed this type of modelling works well in many cases but there are some problems that can not be analysed at this level of modelling.

If we want to model the decohesive processes explicitly the simplest way (level 2 in Fig. 1) is to use a cohesive zone model. Here it is assumed that the crack surfaces start to separate if some measure of stress or strain exceeds a critical level. Usually this is assumed to be the normal stress perpendicular to the prospective crack plane in a mode I case. Behind the front end of the zone, tractions are assumed to act across the partly opened crack surfaces. The constitutive properties of the zone are embodied in a functional relation between these tractions and the crack surface separation. Once this relation has been established the motion of the front and rear ends of the zone can be calculated and no further fracture criterion is needed.

In certain situations even the cohesive zone models are not sufficient to describe the crack tip region behaviour. Decohesive processes and other forms of damage may occur out of the crack plane whereby some kind of volumetric modelling is necessary. For this purpose so called *damage mechanics* constitutive laws have been used (level 3 in Fig. 1). In addition to the normal constitutive laws these equations contain state variables that describe the deterioration of the material. Considerable success in modelling ductile fracture processes has been achieved by use of the so called Gurson law. The distinction between cohesive zone models and damage mechanics models is sometimes not sharp.

2. Concepts of non-linear fracture mechanics with point crack tip modelling

In fracture mechanics theories at this level it is assumed that the state at a point of the crack front can be described by one or few scalar parameters. In the current methodology of non-linear fracture mechanics these are the *J*-integral complemented by some constraint parameter. For three-dimensional cases the *J*-value at a point along the crack front can be formally defined by the following expression (cf. Carpenter *et al* [6])

$$J(s;C) = \int_C \left(w\delta_{1j} - \sigma_{ij}u_{i,1}\right)n_j \mathrm{d}C - \int_{A_s} \frac{\partial\left(o_{ii3}u_{i,11}\right)}{\partial x_3}\mathrm{d}A \qquad (1)$$

Here the co-ordinate system is defined as sketched in Fig. 2 . C is a closed curve in the x_1-x_2 plane ending on the crack surfaces and is the area that is enclosed by this curve. w is the deformation work density, u_i the displacement vector and the stress tensor.

In numerical evaluation of the *J*-integral one often employs other formulations than the line integral. These are the so called domain integrals which are part of for instance the ABAQUS Code [1]. Faleskog and Nordlund [10] compare the different formulations under both proportional and non-proportional loading and found the differences between the two *J* evaluation methods insignificant.

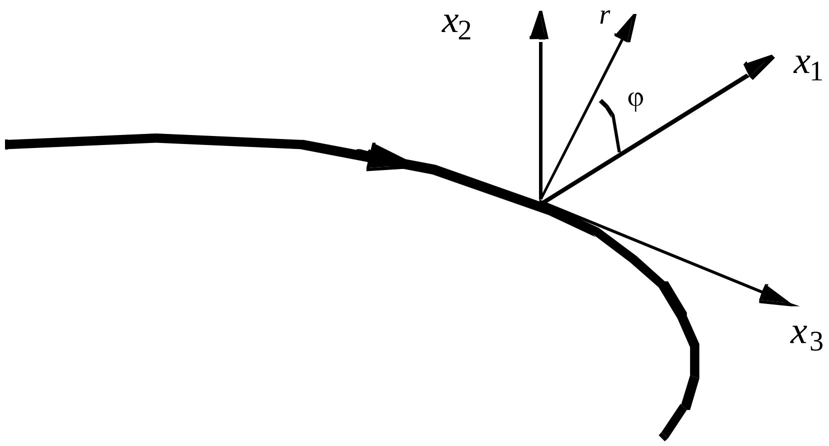

Fig. 2. Definition of co-ordinate system at a curved crack front.

The *J*-integral is for a stationary crack directly related to the strength of the singular field. Except for large deformation effects in the very near tip vicinity, the HRR-singularity (Hutchinson [20], Rice and Rosengren [27]) prevails in hardening materials. The extent of the singularity region is, however, in many cases too small for a pure one parameter description.
The observation made by O'Dowd and Shih [25]-[26] leads to the following approximate and simple form for the stress field ahead of a crack tip.

$$\sigma_{ij} = \left(\sigma_{ij}\right)_{\mathrm{SSY}} + Q\sigma_{\mathrm{Y}}\delta_{ij} \tag{2}$$

Here $\left(\sigma_{ij}\right)_{\mathrm{SSY}}$ is the stress-field that results from a standard small scale yielding (SSY) analysis and is thus directly related to the *J*-integral, σ_{Y} denotes the yield stress and Q is the scaled deviation in hydrostatic stress from the SSY-solution. It is claimed by some authors (*cf*. Betegon and Hancock [3], Hancock *et al* [19]) that Q can be practically uniquely related to the so called *T*-stress, *i.e*. the second term of elastic crack tip stress field expansion.

For a *stationary* crack front the *J*-integral is usually reasonably independent of the integration region if the global loading conditions are reasonably near proportional loading. For a *growing* crack tip in a material that behaves according to an incremental plastic constitutive law, the loading state is very far from proportional in the crack front region. In fact, the order of the singularity for a growing crack in such a material is of such an order that an integration path taken infinitesimally close to the tip would yield a zero value for the *J*-integral. In order to obtain integration region independent values the integration path must be taken so remotely from the tip that proportional loading conditions prevail. A *J*-integral value evaluated in this way is termed J_{F} (far-field *J*). A common approach is instead to neglect the non-proportionally deforming region and calculate the *J*-integral assuming the tip has been stationary at its instantaneous position during the loading process. The *J*-integral value so obtained is termed J_{D} (deformation theory *J*). In a numerical investigation by Nilsson [23] the question whether J_{D} and J_{F} are approximately equal is examined for two-dimensional conditions. This turns out to be the case and has also been confirmed by other investigations.

Based on the above discussion it can be assumed that crack growth locally along the crack front is governed by

$$J(s;P,a) = J_{\mathrm{R}}\left(\Delta a(s), \beta(s), T\right). \tag{3}$$

P is here a measure of the applied load, $\beta(s)$ is some constraint parameter such as Q and J_{R} is a material function depending on the crack growth increment, Δa, and the current constraint. In fully three-dimensional cases it is assumed that Eq. (3) holds locally at every point along the crack border. The fracture resistance may also depend on the temperature T which is indicated explicitly in Eq. (3) .Conventional fracture theory does give any way of finding this dependence except for experimental determination. The criterion is also the same for cleavage as well as ductile conditions and the distinction between mechanisms is only given by the value of the resistance,

For a propagating crack the question of a suitable constraint concept becomes more involved than for stationary crack. Whether the fields in the vicinity of a growing crack in a elastic-plastic material can be written in a form analogous to Eq. (2) is not known and it appears uncertain that such an expression should hold. Instead, a constraint parameter Q corresponding to the J_{D} concept can be considered, *i.e. Q* is calculated for a stationary crack of the current length subjected to the same loading history. The same type of arguments as for the crack tip characterising capacity of *J*-integral could be put forward to justify such an approach. In a recent article by Trädegård *et al* [31] this question is examined and it turns out that a characterisation with J and Q from analyses of stationary cracks serves reasonably well for growing cracks at least at up to moderately high load levels.

The applicability of the approach implied by Eq. (4) has been studied in several experimental investigations of ductile crack growth. Faleskog and co-workers ([18], [24], [9], [11]) perform studies on a pressure vessel steel with large surface cracked specimens under combined bending and tension as well as on conventional specimens. They find that both ductile crack initiation and propagation can be described by a combined J-Q-theory. The ductile initiation is relatively insensitive to the constraint (Q) level while the J-levels for continued growth decrease with increasing Q. Similar results are also found by Garwood [16] and Hancock *et al* [19]. The modelling with a point sized crack tip can not explain such effects and without micromechanical modelling the only way is empirical observations to evaluate the effects of constraint.

In some of the experiments performed in [8], [24], [9], [11] cleavage fracture occurred immediately upon initiation or after some amount of ductile growth. Again, it is not possible to predict the ductile-cleavage transition without some micromechanical modelling. The only way within the conventional type of modelling is the empirical approach, which is to perform experiments under different combinations of J and Q and observe whether cleavage or ductile crack growth results. In the cited articles and also in others it is found that the cleavage fracture propensity increases with increasing Q. How this can be understood with the aid of micromechanical modelling is discussed below.

3. Micromechanical models for cleavage fracture

For initiation of *cleavage fracture* several micromechanical models have been proposed. Many of these models share the common feature that no modification of the normal bulk constitutive laws is performed. It is thus assumed that cleavage fracture occurs before any material degradation due to void growth etc. has taken place. When treating problems of transition from ductile to cleavage fracture combination of cleavage and degradation models is necessary as will be evident below.

The micromechanical model of Ritchie *et al* [28], hereafter referred to as RKR, predicts trans-granular cleavage fracture if the largest principal stress reaches a critical value, σ_{c}, at a critical distance, r_{c}, ahead of the crack tip. A model for the effect of constraint can be obtained by applying the RKR criterion to the field according to Eq. (2). The ratio between the critical J-value in a finite body where Q is nor zero to the critical J-value in an infinite body (fully constrained body, Q=0) is

$$J/J_0 = \left(1 - Q\sigma_{\mathrm{Y}}/\sigma_{\mathrm{c}}\right)^{\eta}. \qquad (4)$$

Here η is equal to n+1, where n is the hardening exponent in the power hardening law. It is seen that decreases with increasing Q.

The inherently random nature of cleavage fracture has prompted many developments of statistical models of fracture. Most of these are based on the so called weakest link assumption which leads to the following expression for the probability of fracture.

$$p_{\mathrm{f}} = 1 - \exp\left(- \int_V g\left(\sigma_{\mathrm{m}}\left(x_j\right)\right) \frac{\mathrm{d}V}{V_{\mathrm{ref}}} \right), \qquad (5)$$

where V is the volume where plastic deformation has occurred. The function $g(\sigma_{\mathrm{m}})$ expresses the probability of failure of an infinitesimal volume element according to

$$\mathrm{d}p_{\mathrm{f}} = g(\sigma_m)\frac{\mathrm{d}V}{V_{\mathrm{ref}}}, \tag{6}$$

where σ_{m} is the maximum principal stress.

It is shown by Wallin [34] that under one-parameter crack tip control in terms of or alternatively J under more widely spread plasticity the fracture probability is given by

$$p_{\mathrm{f}} = 1 - \exp\left(-\frac{B}{B_0}\left(\frac{J}{J_0}\right)^2\right), \tag{7}$$

or equivalently in terms of the stress-intensity factor

$$p_{\mathrm{f}} = 1 - \exp\left(-\frac{B}{B_0}\left(\frac{K_{\mathrm{I}}}{K_0}\right)^4\right), \tag{8}$$

This expression results irrespective of the form of the g-function, provided that the integral in Eq. (6) exists. This means that one-parameter controlled experiments can not be used to determine this function. Some implications of this fact are discussed by Gao *et al* [14]. These authors also discuss the problem of estimation of the parameters in the probabilistic assumptions.

When the one-parameter control no longer prevails Eq. (7) loses its applicability and the functional form of may influence the resulting probability. In most studies it is then assumed the following form for the g-function

$$g = \left(\frac{\sigma_{\mathrm{m}} - \sigma_{\mathrm{th}}}{\sigma_{\mathrm{u}}}\right)^m \tag{9}$$

It should be pointed that there is no fundamental basis for the form (9) . It is simply a convenient mathematical expression that can be fitted to some experimental results by varying the material constants. A function based on more fundamental principles is of interest. There is for instance some evidence that plastic deformation should in some way influence the propensity for cleavage fracture.

Wang [33] performs calculations for crack tip stress fields controlled by K_{I} and T, so called modified boundary layer (MBL) conditions. The trend of the mean value is very similar to the behaviour of the RKR-model, Eq. (4). Since the effect of constraint (measured as T or Q) essentially results in a hydrostatic stress field the plastic zone is not much affected. The effect of the additional stresses is nearly the same as shifting the threshold stress and thus the same type of distribution as in the one-parameter case results, at least approximately.

A number of investigations show that under one parameter controlled situations deviations from the theoretical result Eq. (8) occur. The deviations are most noticeable at low fracture toughness levels and therefore a lower limit has been suggested. Thus, for instance, Anderson *et al* [2] suggest that

$$p_{\mathrm{f}} = 1 - \exp\left(-\frac{B}{B_0}\left(\frac{K_{\mathrm{I}} - K_{\min}}{K_0 - K_{\min}}\right)^4\right), \tag{10}$$

Here $K_{\min}$ is a constant and it has been suggested that it should be assigned the value 20 MPa for ferritic steels. Similar expressions have been suggested by other authors. It has to be pointed that Eq. (10) is purely empirical and there is no fundamental theory behind the expression. Various explanations have been given as to there should exist a definite lower limit value of toughness. One reason for the existence of a minimum value is that a cleavage event initiated at some point such as an inclusion does not necessarily lead to a total cleavage fracture. The cleavage crack must also be able to propagate through the interface between the inclusion and the matrix and grow further into the matrix material. Narström and Isacsson [22] perform experiments in the upper part of the transition region. They observe that the number of cleavage initiation sites increase with temperature even though the general character of the fracture becomes increasingly ductile, which supports the view that arrest of cleavage attempts is a phenomenon that contributes to the transition behaviour.

A fairly ambitious attempt to compare numerical simulation to experiments is reported by Gao *et al* [15]. These authors apply weakest link modelling to fully 3-dimensional cases of plates with semi-elliptic surface cracks. In their analysis they utilise the following version of the weakest link approach.

$$p_{\mathrm{f}} = 1 - \exp\left(- \left(\frac{\sigma_{\mathrm{w}} - \sigma_{\mathrm{w\,min}}}{\sigma_{\mathrm{u}} - \sigma_{\mathrm{w\,min}}} \right)^{\prime 4} \right), \tag{11}$$

where $\sigma_{\mathrm{w\,min}}$ is a constant and

$$\sigma_{\mathrm{w}} = \left(\frac{1}{V} \int_V \sigma_{\mathrm{m}} \left(x_j \right)^m \frac{\mathrm{d}V}{V_{\mathrm{ref}}} \right)^{1/m} . \tag{12}$$

Under two-dimensional conditions these expressions reduce to Eq. (10) and are thus three-dimensional versions of that expression. Gao *et al* [15] find that their model is able to capture constraint effects.

4. Micromechanical modelling of ductile crack growth

Ductile crack growth in steels proceeds by one of two mechanisms. The first one which dominates at least in modelling, if not necessarily in the real case, is when the crack grows through void nucleation, growth and subsequent coalescence. The second one is shear localisation of plastic flow. The first mechanism is typical for materials with a high degree of hardening, while the latter occurs for high strength materials with a low degree of hardening. As mentioned the bulk of micromechanical modelling aims at the first type of mechanism and there is very little concerning the second mechanism. The shear localisation process is also dependent on voids formation in the material but of another size scale and in other directions than the void growth and coalescence mechanism.

When considering crack growth due to the void mechanism it unrealistic to perform full calculations with the voids explicitly modelled. Instead homogenised models, so called damage constitutive relations are relied upon. A variety of such laws exist in the literature. They do not differ very much and the by far mostly used one is the Gurson-Tvergaard (GT) law (Gurson [18], Tvergaard [32]). The yield condition for this model is

.
$$\Phi = \frac{\sigma_{\mathrm{e}}^2}{\sigma_{\mathrm{f}}^2} + 2 q_1 f \cosh\left(q_2 \frac{3\sigma_{\mathrm{h}}}{2\sigma_{\mathrm{f}}} \right) - \left(1 + q_1^2 f^2 \right) = 0 . \tag{13}$$

Here $\sigma_{\mathrm{h}} = \sigma_{kk}/3$ is the hydrostatic stress and σ_{e} the effective (von Mises) stress of the homogenised material. This yield condition applies to an isotropically strain hardening material. In Eq. (13) *f* is the current void volume fraction which in this case is the damage variable, and is the current flow stress of the matrix material. A calibration of q_1 and q_2 for a strain hardening material is developed and described by Faleskog *et al* [12] by matching the response of a GT-cell with a cell containing one explicitly modelled void.

The plastic strain rate is given by

$$\dot{\varepsilon}_{ij}^{\mathrm{p}} = \frac{1}{\kappa}\frac{\partial\Phi}{\partial\sigma_{ij}}\frac{\partial\Phi}{\partial\sigma_{kl}}\dot{\sigma}_{kl}\,, \tag{14}$$

where $\dot{\sigma}_{kl}$ is the Jaumann rate of the Cauchy stress, see for instance [18] for further detail, and κ a hardening parameter. The void growth rate is obtained using the plastic incompressibility condition of the matrix material as

$$\dot{f} = (1-f)D_{kk}^{\mathrm{p}}\,, \tag{15}$$

where D_{kk}^{p} is the plastic part of the deformation rate tensor. The voids quantified by f are either initially present or nucleated by the deformation process. In the latter case some void nucleation law has to be specified. Chu and Needleman [7] propose the following law which includes the growth law (16), a strain-controlled initiation mechanism and also a stress-controlled one.

$$\dot{f} = (1-f)D_{kk}^{\mathrm{p}} + A\dot{\varepsilon}_{\mathrm{e}}^{\mathrm{p}} + B(\dot{\sigma}_{\mathrm{e}} + \dot{\sigma}_{\mathrm{h}})\,, \tag{16}$$

where for strain-controlled initiation

$$A = \frac{f_{\mathrm{N}}^{\mathrm{n}}}{s_{\mathrm{N}}^{\mathrm{n}}\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{\varepsilon_{\mathrm{e}}^{\mathrm{p}} - \varepsilon_{\mathrm{N}}}{s_{\mathrm{N}}^{\mathrm{n}}}\right)^2\right],\ B\text{=0 for } \dot{\varepsilon}_{\mathrm{e}}^{\mathrm{p}} > 0\,, \tag{17}$$

and for stress-controlled initiation

$$B = \frac{f_{\mathrm{N}}^{\mathrm{sn}}}{s_{\mathrm{N}}^{\mathrm{s}}\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{\sigma_{\mathrm{e}} + \sigma_{\mathrm{h}} - \sigma_{\mathrm{N}}}{s_{\mathrm{N}}^{\mathrm{s}}}\right)^2\right],\ A\text{=0 for } \dot{o}_{\mathrm{e}} + \dot{o}_{\mathrm{h}} > 0\,. \tag{18}$$

Here $f_{\mathrm{N}}^{\mathrm{n}}$ and $f_{\mathrm{N}}^{\mathrm{s}}$ are the volume fractions of void nucleating particles, $s_{\mathrm{N}}^{\mathrm{n}}$ and $s_{\mathrm{N}}^{\mathrm{s}}$ are the standard deviations. The superscripts *n* and *s* denote the strain- and stress-controlled nucleation, respectively. ε_{N} is the mean nucleating strain and σ_{N} the mean nucleating stress *i.e.* material properties like the standard deviations. In this way a number of additional constants is introduced which increases the possibility of fitting the model to data, but on the other hand complicates the parameter identification process.

When f is equal to $1/q_1$ the material loses its load bearing capacity. One fundamental problem with the GT-law and similar constitutive laws is that at the crack tip with its strain singularity the damage parameter approaches this critical value at any finite load. This means that crack growth would commence immediately upon any load application, however small. The only way to mitigate this problem is to introduce a characteristic length in some way. Preferably this should be done by modifying the constitutive law, but a far more common way is to limit the strain levels by letting the elements in a finite element mesh have a certain size. The size of the elements in the crack tip vicinity is thus equivalent to a constitutive assumption. This fact seems to have escaped some of the investigators in this area..

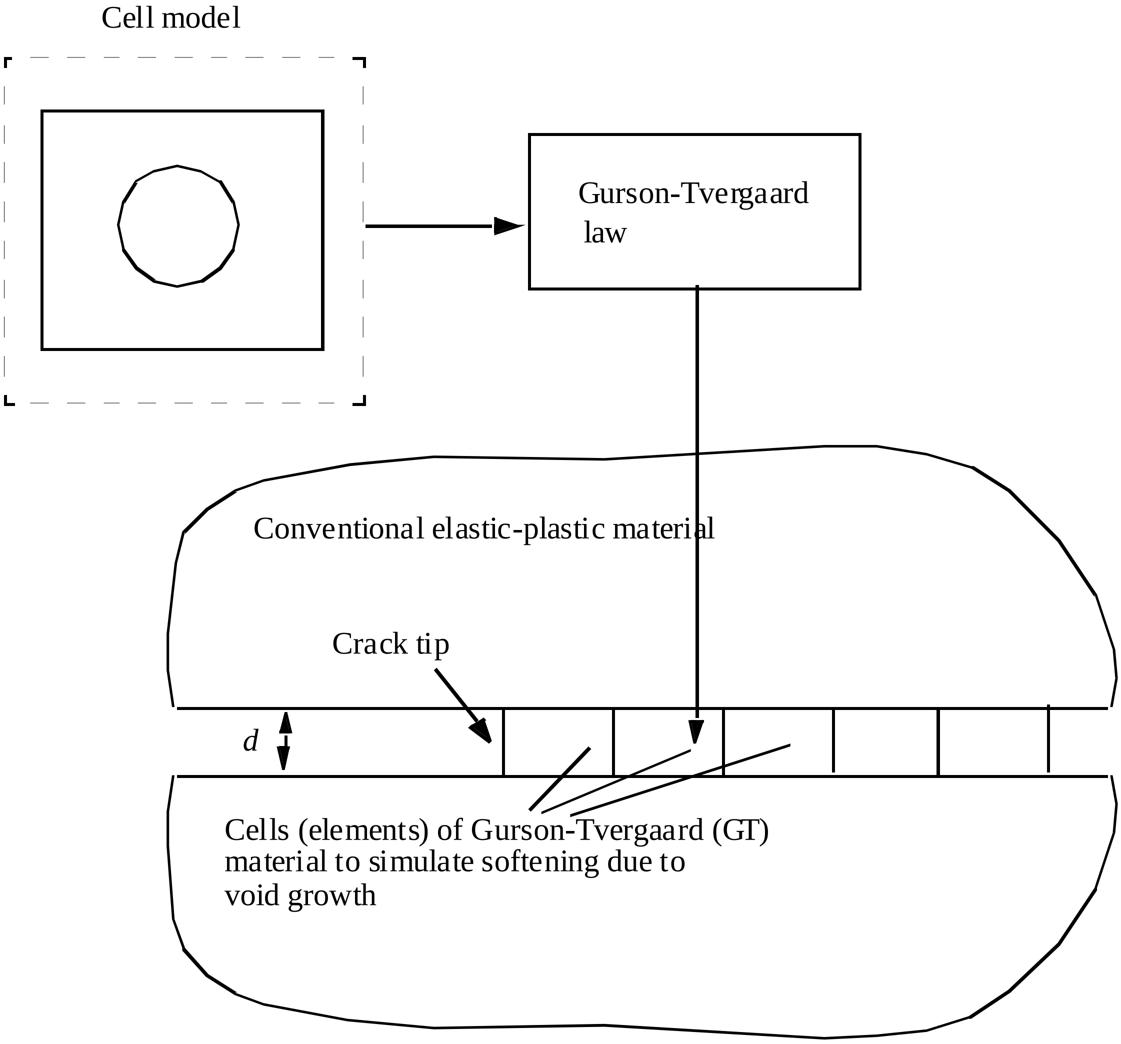

Fig. 3 . Principal strategy for modelling of ductile crack growth.

There are many contributions to this subject. Thus for instance Xia and Shih [35] suggest the strategy sketched in Fig. 3..First the GT-law is calibrated with respect to a model where a cell with an initially spherical void is subjected to applied strains and the resulting average stresses are recorded. The behaviour of the GT-material will in addition to the parameters of the matrix material be dependent on the initial void volume f_0 all voids are assumed to be initially present so any nucleation model is not needed. The behaviour of a cell in the crack model will also depend on the geometrical parameter *d*. In the analysis of experimental data f_0 and *d* are considered as free parameters to be used to fit the predictions to the data. They are however to be kept fixed for different cases of a specific material. Gao *et al* [13] apply this type of analysis to both nominally two-dimensional tests as well as to the tests with surface cracks performed by Faleskog and co-workers ([8], [9], [11]). The results are very encouraging and the crack advance is in all the considered cases well predicted by the methods. It is less accurate in predicting the onset of ductile

crack growth. Several similar analyses of experiments have been performed (cf. Rousellier [29], Bilby *et al* [4], Brocks *et al* [5]).
As mentioned the quantities f_0 and d have to be determined from a fracture mechanics experiment. It would of course be desirable that these or similar quantities could be directly related to physical properties observed by other types of tests, but this has not yet proved possible. One reason is that the presently used models either discard the process of void nucleation entirely or in the cases when this process is modelled, the proposed nucleation laws are not particularly well developed.

The computational problems with the presented type of modelling are not trivial. In a recent article by Gullerud *et al* [17] investigate the numerical aspects and conclude with a number of recommendations in order to obtain reliable results. Among other things they derive requirements on the load step length.

Which advantages have then been gained by using micromechanical modelling for prediction of ductile crack growth? Obviously there is no longer any need to use crack growth criteria like Eq. (3) and possible constraint effects are automatically accounted for. It should, however, be realised that the outlined scheme is still an over-simplified model. The initial void volume f_0 should not for instance be interpreted as any observable physical parameter. Much research is currently performed to increase the precision and applicability of the damage modelling. It may of course be questioned whether ductile crack growth theory needs to be developed much further. The currently used models provide an accuracy that from a safety point is probably quite sufficient for the problem of ductile crack growth. The real challenge to micromechanical modelling is to predict the transition phenomenon as discussed below.

This rather satisfactory state of affairs for modelling of ductile crack growth applies to the mode I situation. Mixed mode cases have not been investigated to same degree of understanding. Experimental studies indicate that the shear localisation mechanism becomes increasingly important as the amount of other modes than mode I are present.

It is likely that the micromechanical methods developed for ductile crack growth of the type described above may be used with success for other crack growth mechanisms. Intergranular fracture is often regarded as a quasi-brittle process. Fracture in these cases develops as decohesion of relatively weak material along the grain boundaries. This may be a highly ductile process while the grains themselves experience little plastic deformation. In fact cohesive zone models or cell models of the type described can presumably be used provided that the material behaviour of the grain boundaries is well modelled.

Micromechanical modelling of ductile fracture has mainly been focused onto ferritic steels. There is no particular reason why for instance ductile crack growth in austenitic materials should not be considered by the same type of methods. Again, since crack growth in austenitic materials mostly commences after considerable overall plastic deformation the need to formulate micromechanical models has not been very urgent.

5. Transition behaviour

A main feature of ferritic steels is that they exhibit a transition from ductile to cleavage behaviour as the environmental temperature is lowered and/or the applied loading rate is increased. It has also been realised since long that the transition is also dependent of the geometry of the body. In general small specimens have a ductile behaviour while the large structure may fracture in a cleavage mode at the same temperature. Thus tests which usually are performed on small specimens may be misleading.

All models of the transition phenomenon are based on the idea of competing mechanism. Thus both the cleavage and the ductile processes are modelled and the critical event is determined by the mechanism that is most favourable under the actual conditions. Most success has been achieved about the influence of geometry on the transition behaviour at a constant temperature. A simple model can be obtained as follows. Assume that ductile initiation occurs when the *J*-level reaches $J_{\mathrm{c}}^{\mathrm{duct}}$ and that cleavage fracture follows Eq. (4). Then cleavage is expected to happen if

$$J_{\mathrm{c}}^{\mathrm{duct}} = J_0 \left(1 - Q\sigma_{\mathrm{Y}}/\sigma_{\mathrm{c}}\right)^{\eta}. \qquad (19)$$

In this relation the geometry effect enters through *Q*, and clearly increasing values of this parameter promote cleavage fracture. More ambitious models of the same problem but also incorporating ductile growth before a possible cleavage fracture can be obtained by combining the cell models discussed above with weakest link modelling according to Eq. (5). This is the topic treated by Xia and Shih [36] among others. These studies generally show that the probability of cleavage fracture increases with crack growth. The quantitative predictions are however difficult to verify by experiments, since a large amount of tests is usually needed to support probabilistic statements. While the geometry effects can be successfully modelled, the effect of temperature is still insufficiently understood. The models that are found in most text books basically ascribe the problem of temperature transition to a decrease of the yield stress. This is clearly not adequate since the change of yield stress is generally too small to furnish an explanation. The temperature transition occurs over a relatively narrow temperature interval. Conventional constitutive properties do not change appreciably over this temperature interval nor does the structure of material *i.e.* grain size, inclusion density etc. It thus remains to understand which changes in the material behaviour that are responsible for the transition behaviour. Since the transition is strain rate sensitive it is likely that these changes are to be found in materials response to the loading rate.

While purely empirical methods to describe the transition through the so called master curve are successful, insignificant steps have been taken in order to understand why there is such a transition behaviour common to most ferritic steels. The remarkable fact that it is indeed possible to construct a master curve should tell us lot about the causes of the transition behaviour. This remains an area of real challenge to a micromechanical modelling scientist.

6. Further problem areas

In the application of fracture mechanics to nuclear technology there are further problem areas in addition to basic ones outlined here. In connection with certain types of accidental conditions the possible benefits of so called warm prestressing (WPS) have received attention in the past. By the term is meant that the loading of the cracked structure at a high temperature may enhance its fracture properties at a lower temperature to some extent. Basically this effect is a consequence of the introduction of residual stresses and thus any micromechanical modelling is not needed to describe the effect. It can however be envisioned that ductile damage can be initiated in the crack tip region at the high warm loading level which may counteract the positive effects of the residual stresses. This may be an area where micromechanical modelling may be of use in determining the limits of the WPS argument. Likewise, micromechanical modelling can be used to assess the probability of a cleavage fracture at the lower temperature. Presumably, the methods of micromechanical modelling as sketched above can be used for this purpose with the additional difficulty to determine the material response at different temperatures.

Repeated load applications up to near critical levels *i.e.* the initiation level for ductile growth, where material damage occurs and accumulates with the load cycles is a topic that has not been very much studied. It borders on the research of fatigue problems, but for such high load levels the mechanisms are more like those of ductile crack growth than those typical of fatigue crack growth. In a study by Kaiser [21] crack growth due to cyclic loading in this regime is considered by use of conventional non-linear fracture mechanics. Again micromechanical modelling could be an attractive way of approaching the problems. The main challenge in this respect seems to be the formulation of laws for development of plastic deformation and damage under cyclic loading.

7. Concluding remarks

While conventional fracture mechanics is capable of predicting crack growth behaviour if sufficient experimental observations are available, micromechanical modelling can both increase the accuracy of these predictions and model phenomena that are inaccessible by the conventional theory such as the ductile-cleavage temperature transition.

A common argument against micromechanical modelling is that it is too complicated for use in routine engineering applications. This is both a computational and an educational problem. That micromechanical modelling is unnecessarily complicated is certainly true in many situations. The on-going development of micromechanical models, computational algorithms and computer speed will however most probably diminish the computational problem rather rapidly. Compare for instance the rate of development of computational methods for structural analysis. Meanwhile micromechanical modelling may serve as a tool by which more simplified engineering methods can be validated.

The process of receiving a wide acceptance of the new methods is probably much slower. This involves many steps. First the research community must be in reasonable agreement on the methods and their use. Then the methods have to be implemented into computer software and into code procedures. The development and acceptance of conventional fracture mechanics may serve as an historical example of the time required before a new methodology has received a wide usage (*cf*. Rossmanith [30]).

8. References

[1] ABAQUS User’s and Theory manuals, version 5.7. (1997): Hibbitt, Karlsson & Sorensen, Inc., (HKS), Pawtucket, RI, USA

[2] T. Andersson, D. Stienstra and R. H. Dodds, “A theoretical framework for addressing fracture in the ductile-brittle transition region, *Fracture Mechanics*: *Twenty-Fourth Volume, ASTM STP 1207*, Ed. by J. D. Landes, D. E. McCabe and J. A. Boulet, American Society for Testing and Materials, West Conshohoken, Pa., 1994, 186-214.

[3} C. Betegon and J. W. Hancock, “2-parameter characterization of elastic-plastic stress fields”, *Journal of Applied Mechanics* 58, 1991, 104-110.

[4] B. A. Bilby, I. C. Howard and Z. H. Li, “Prediction of the first spinning cylinder test using ductile damage theory”, *Fatigue and Fracture of Engineering Materials and Structures* 16, 1993, 1-20.

[5] W. Brocks, D. Klingbeit, G. Kunecke and D. Z. Sun, “Application of the Gurson model to ductile tearing resistance”, *Constraint Effects in Fracture: Theory and applications: second volume, ASTM STP 1244*, Ed. by M. Kirk and A. Bakker, American Society for Testing and Materials, West Conshohoken. 1995, 232-252.

[6] W. C. Carpenter, D. T. Read, and R. H. Dodds, “Comparison of several path independent integrals including plasticity effects”, *International Journal of Fracture* 31, 1986, 303-323.

[7] C. C. Chu and A. Needleman, “Void nucleation effects in biaxially streched sheets”, *Journal of Engineering Materials and Technology*, 102, 1980, 249-256.

[8] J. Faleskog, K. Zaremba, F. Nilsson and H. Öberg, “An investigation of two-and three-dimensional elasto-plastic crack growth initiation experiments”, in *Defect Assessment in components - Fundamentals and Applications*, ESIS/EGF9, ed. by J. G. Blauel and K. H. Schwalbe, Mechanical Engineering Publications, London, 1991, 333-344.

[9] J. Faleskog, “An experimental and numerical investigation of ductile crack growth characteristics in surface cracked specimens under combined loading”, *International Journal of Fracture* 68, 1994, 99-126.

[10] J. Faleskog, and P. Nordlund, “Near-tip field characterization and *J*-integral evaluation for nonproportional loads”, *International Journal of Solids and Structures* 31, 1994, 1-26.

[11} J. Faleskog, “Effects of local constraint along three dimensional crack fronts - A numerical and experimental investigation”, *Journal of the Mechanics and Physics of Solids* 43, 1995, 447-493.

[12] J. Faleskog, X. Gao and C. F. Shih, “Cell model for nonlinear fracture analysis-I. Micromechanics calibration”, *Journal of the Mechanics and Physics of Solids* 89, 1998, 355-373.

[13} X. Gao, J. Faleskog, C.F. Shih and R. H. Dodds, “Ductile tearing in part-through cracks; Experiments and cell-model predictions”, *Engineering Fracture Mechanics* 59, 1998, 761-777.

[14] X. Gao, C. Ruggeri and R. H. Dodds, “Calibration of Weibull stress parameters using fracture toughness data”, *International Journal of Fracture*, 92, 1998, 175-200.

[15] X. Gao, R. H. Dodds, R. L. Tregoning, J. A. Joyce and R. E. Link, “A Weibull stress model to predict cleavage fracture in plates containing surface cracks”, *Fatigue and Fracture of Engineering Materials and Structures* 22, 1999, 481-493.

[16] S. J. Garwood, “Measurement of crack growth resistance of A533 B wide plate tests,”, *Fracture Mechanics: Twelfth Conference, ASTM STP 700*, American Society for Testing and Materials, Philadelphia, 1980, 271-295.

[17] A. S, Gullerud, X. Gao, R. H. Dodds Jr and R. Haj-Ali, “Simulation of ductile crack growth using computational cells: numerical aspects”. *Engineering Fracture Mechanics* 66, 2000, 65-92.

[18] A. L. Gurson, “Continuum theory of ductile rupture by void nucleation and growth: Part I-yield criteria and flow rules for porous ductile materials”, *Journal of Engineering Materials and Technology* 99, 1977, 2-15.

[19} J. W. Hancock, W. G. Reuter and D. M. Parks, “Constraint and toughness parameterized by T”, *Constraint Effects in Fracture, ASTM STP 1171*, American Society for Testing and Materials, West Conshohoken, 1993, 21-40.

[20] J. W. Hutchinson, “Singular behaviour at the end of a tensile crack in a hardening material”, *Journal of the Mechanics and Physics of Solids* 16, 1968, 13-31.

[21] S. Kaiser, “On the relation between stable crack growth and fatigue”, *Journal of Fatigue of Engineering Structures and Materials* 6, 1983, 33-48.

[22] T. Narström and M. Isacsson, “Microscopic investigation of cleavage initiation in modified A508B pressure vessel steel”, *Materials Science Engineering* A271, 1999, 224-231.

[23] F. Nilsson, “Numerical investigation of J-characterization of growing crack tips”, *Nuclear Engineering Design* 133, 1992, 457-463.

[24] F. Nilsson, J. Faleskog, K. Zaremba and H. Öberg, “Elastic-plastic fracture mechanics for pressure vessel design”, *Fatigue and Fracture of Engineering Materials and Structures* 15, 1992, 73-89.

[25] N. P. O’Dowd and C. F. Shih, “Family of crack-tip fields characterized by a triaxiality parameter—II. Fracture applications”, *Journal of the Mechanics and Physics of Solids* 40, 1992, 939-963.

[26] N. P. O’Dowd and C. F. Shih, “Two-parameter fracture theory: theory and applications”. *Fracture Mechanics*: *Twenty-Fourth Volume, ASTM STP 1207*, Ed. by J. D. Landes, D. E. McCabe and J. A. Boulet, American Society for Testing and Materials, West Conshohoken, Pa., 1994, 21-47.

[27] Rice, J. R. and G. Rosengren, “Plane strain deformation near a crack tip in a power-law hardening material”, *Journal of the Mechanics and Physics of Solids* 16, 1968, 1-12.

[28] R. O. Ritchi, J. F. Knott, and J. R. Rice, “On the relationship between critical tensile stress and fracture toughness in mild steel”, *Journal of the Mechanics and Physics of Solids* 21, 1973, 395-410.

[29] G. Rousselier, “Ductile fracture models and their potential in local approach”, *Nuclear Engineering Design* 105, 1987, 97-111.

[30] H. P. Rossmanith (ed), *Fracture research in retrospect*, A. A. Balkema, Rotterdam, 1997.

[31] A. Trädegård, F. Nilsson and S. Östlund, “J-Q characterization of propagating cracks”, *International Journal of Fracture* 94, 1998, 357-369.

[32] V. Tvergaard, “Influence of voids on shear band instabilities under plane strain conditions”, *International Journal of Fracture* 17, 1981, 389-407.

[33] Y. Wang, “*A two-parameter characterization of elastic-plastic crack tip fields and applications to cleavage fracture*”, PhD-thesis, MIT, 1991.

[34] K. Wallin, “The scatter in -results”, *Engineering Fracture Mechanics* 19, 1984, 1085-1093.

[35] L. Xia and C. F. Shih, “Ductile crack growth. - I. A numerical study using computational cells with microstructurally based length scales”, *Journal of the Mechanics and Physics of Solids* 43, 1995, 223-259.

[36] L. Xia and C. F. Shih, “Ductile crack growth. - III. Transition to cleavage fracture incorporating statistics”, *Journal of the Mechanics and Physics of Solids* 44, 1996, 603-639.