Modelling the Ductile-Brittle Transition Behaviour in TMCR Steels

S. J. Wu[a, d], C. L. Davis[a], A. Shterenlikht[b] and I. C. Howard[c]

[a] Department of Metallurgy and Materials, The University of Birmingham, Birmingham B15 2TT, UK
[b] Materials Science Centre, University of Manchester, Grosvenor Street, Manchester, M1 7HS, UK
[c] Department of Mechanical Engineering, The University of Sheffield, Mappin Street, Sheffield S1 3JD, UK
[d] School of Materials Science and Engineering, Beijing University of Aeronautics and Astronautics, Beijing 100083, China

ABSTRACT

The Charpy impact transition temperature (ITT) is well modelled for hot rolled or normalised steels using empirical equations. However the ITT of inhomogeneous steel microstructures, such as duplex (mixed fine and coarse) grain sizes, and the scatter in experimental Charpy energy values, observed in the transition region, are not accurately modelled. This paper describes research on the microstructure-fracture property relationship and the prediction of the ITT using a cellular automata finite element (CAFE) model in thermomechanically controlled rolled (TMCR) Nb-microalloyed steels. The ferrite grain size distributions for two TMCR steel plates were analysed and used for the prediction of the local fracture stress (σ_F) values based upon the Griffith model. It was found that the coarse grain size distribution could be used to predict the range of σ_F values observed. The CAFE model was used to predict the ITT using the predicted σ_F distribution for a TMCR steel. Results showed that the CAFE model realistically predicted the Charpy ITT;- in particular it was able to reproduce the scatter in values in the transition region. Within the model the percentage of brittle failure and the upper shelf ductile energy were predicted well. However the lower shelf brittle energy was over-estimated due to computational limitations in the commercial finite element software used with the current CAFE model.

Key words: ductile-brittle transition temperature, TMCR steel, grain size distribution, fracture stress distribution, CAFE modelling.

I. INTRODUCTION

Despite many advances made in (sharp crack) fracture toughness testing and assessment procedures over the last thirty years, the vast majority of steel products are released to a specification which is based on energy absorption in the Charpy notched bar impact test, carried out at a prescribed low temperature. Body centred cubic metals, such as mild steels, demonstrate a transition from a ductile fracture mode to a brittle cleavage failure mechanism as the test temperature decreases. The ductile-brittle transition may occur over a temperature range of only a few degrees Celsius, or a wide range of over a hundred degrees, depending upon the microstructure and specimen geometry (thereby the applied stress-strain states in the specimen). Extensive studies have been carried out, over the past 40 years, to determine the quantitative structure-property relationships in steels. As a result, many empirical equations have been proposed to relate the strength and impact behaviour to the microstructure and composition of the steels [1-4]. It is well established for hot rolled or normalised ferrite-pearlite microstructures that the yield strength (σ_y) [5, 6], the critical local fracture stress (σ_F) [7] and the Charpy impact transition temperature (ITT) [8] are a linear function of $(\bar{d})^{-½}$, where $\bar{d}$ is the mean grain size of polygonal ferrite.

The empirical equations, however, can only be applied to materials regarded as "uniform, homogeneous", such as normalised steels, which have a single size distribution of ferrite grains together with small and finely distributed carbides. The fracture properties of such materials are essentially *single-valued functions* within random experimental errors and can be expressed using *average* microstructural parameters such as *mean grain size*. Whereas for inhomogeneous materials, such as steels with a duplex ferrite grain structure, seen in many thermomechanically control rolled (TMCR) steels, the average grain size parameter does not properly represent the microstructure [9], and therefore cannot be used to predict the cleavage fracture stress and ITT. It has been reported that cleavage microcracks form preferentially in the largest polygonal ferrite grains [10], suggesting that the σ_F value should correlate with some measure of the large grains rather than the mean value of the grain size distribution [10-13]. Previous experimental results [14] have shown that there can be a large scatter in σ_F value for TMCR steels, and a *mean* σ_F value has little meaning in describing the fracture behaviour. The distribution of the σ_F values is therefore required to describe the fracture behaviour of these inhomogeneous steels.

In other words, in order to predict the ITT for inhomogeneous steels, one has to simulate the brittle fracture behaviour of a material as that of an ensemble of grains of different sizes, i.e. with different fracture stresses.

Modelling of the ductile to brittle transition behaviour in steels is usually performed with the "local approach" to fracture [15-21]. In this approach, micro-mechanical models for fracture are constructed in which the failure criteria are based on stress, strain and damage levels local to the crack tip. The most widely used model for the local approach to cleavage is that of Beremin [22].

In this model the probability of cleavage P is calculated as:

$$P = 1 - \exp(-\sigma_w / \sigma_u)^m \qquad (1)$$

where σ_w is the "Weibull stress", which is a function of the maximum principal stresses in the plastic zone, σ_u and m are considered to be true material properties, independent of geometry and loading mode, which are calibrated by finite element modelling of the appropriate experimental results at the lower shelf temperatures.

In finite element discretisation σ_w is defined as:

$$\sigma_w = \{\Sigma_i(\sigma_{Ii})^m V_i/V_0\}^{1/m} \qquad (2)$$

where σ_{Ii} is the maximum principal stress in the ith finite element, V_i is volume of the ith element and V_0 is a characteristic volume of material.

By using the distribution for m rather than a single value it is thus possible to simulate the fracture stress distributions within the classical local approach framework. Indeed if the ith finite element is given a randomly generated m_i then the Weibull stress from equation (2) can be rewritten as:

$$\sigma_w = \{\Sigma_i(\sigma_{Ii})^{mi} V_i/V_0\}^{1/m^*} \qquad (3)$$

where m^* denotes the mean value across the finite elements in the plastic zone.

Thus finite elements with higher m_i will contribute more to the Weibull stress and to the probability of cleavage than those with lower m_i. It is therefore logical to relate finite elements with higher m_i to lower fracture stress and those with lower m_i to high fracture stress. The local approach model for cleavage based on the Weibull stress calculated according to equation (3) is thus capable of simulating brittle fracture behaviour of a material composed of grains of different sizes. However, the added level of detail means that the number of calibration simulations have to be increased by an order of magnitude. Indeed, simulations with different parameters for the distribution of m will yield different results, and also the outcome of each run with m values generated from a given distribution will be different.

A number of local models for ductile damage exist, of which the most widely used are the Gurson [23, 24] model and that of Rousselier [25, 26]. The CAFE model reported here uses the Rousselier model to represent the development of ductile damage, principally because of its combination of simplicity and realism. However, comparable results could be obtained by encoding the Tvergaard [24] modified Gurson [23] model.

Although the local approach model described above has some potential, it suffers from two well-known problems of pure finite element modelling of the transitional ductile brittle fracture. The first problem is that the microstructurally significant size scales are very different for the ductile and the brittle fracture mechanisms. Therefore it is hard to relate the finite element size to both the ductile and the brittle size scales [15-17, 27]. The second problem is that the size of the finite element mesh in the damage zone is very small, typically 0.05 – 0.5 mm. Thus many finite elements are required to mesh even a small sized sample (e.g. a Charpy specimen). The computation of such a model becomes a challenge in itself.

In this work a recently developed cellular automata finite element (CAFE) model for fracture [27-30] was used instead of the pure finite element local approach analysis. In this model the structural and material parts of the simulation are separated into two entities. The structural changes in the model geometry are simulated with the finite elements, the sizes of which are chosen only to adequately represent the macro strain gradients. All material information is stored and processed in an appropriate number of cellular automata arrays (CA arrays). This model is fast compared to the pure finite element approach because significantly larger finite elements can be used, thus the total number of finite elements is much smaller. Moreover different size scales relevant to the ductile and the brittle fracture mechanisms can be easily employed by using two CA arrays with cells of different size. The CAFE model is described in greater detail elsewhere [27-30]. Some details of particular importance for the present work are given in the experimental section.

The present paper examines the relationship between the local fracture stress and the coarse ferrite grains for two TMCR steels and, using the relationship as input to the CAFE model, attempts to predict their ductile-brittle transition behaviour.

II. EXPERIMENTAL

Two microalloyed TMCR steel plates (Plate-1 and Plate-2) were used in this work. The nominal chemical compositions of the steel plates are listed in Table I. The original/final gauges of the plates are 230mm/40mm for Plate-1 and 230mm/50mm for Plate-2. Full details of the TMCR processing schedule are given elsewhere [31].

The steel plates were characterised on the section normal to the transverse direction (TD). Statistical analyses of the ferrite grain size distributions were carried out, using optical microscopy and image analysis software (ZEISS KS400 3.0), on a minimum of 1200 grains on samples ground, polished and etched with 2% Nital. The grain size is represented by the equivalent circular diameter (ECD) converted from the grain area.

Blunt-notch four-point-bend specimens were chosen to determine the local fracture stress σ_F. The dimensions of the blunt-notch bend specimens were 10×10×60 mm with a 45° notch of 3.3 mm depth and 0.2 mm root radius. The notches were cut along the section normal to the TD. The blunt-notch tests were carried out between –160 °C and –196°C using a 50 kN DMG testing machine with a loading rate of 0.5mm/minute. The stress-strain distribution ahead of the notch root has been analysed using the finite element method (FEM) [32] together with appropriate values of yield strength and strain-hardening rate of the steels.

The model of the Charpy test consisted of the sample, the anvils and the tup, Figure 1a). Of these only the damage zone of the Charpy sample was modelled with the CAFE approach, the rest were simulated with pure FE. The damage zone, i.e. the area where the fracture might take place, was defined as 10 x 10 x 10 = 1000 FE cubes located in the centre of the sample to accommodate any crack propagation path. Figure 1b) shows all modelled bodies at the end of the simulation. The sample has fractured completely save for a 1 FE long remaining ligament which undergone large plastic shear defomation (plastic collapse). The failed FEs are removed from the mesh and are not shown. For the purpose of the present work the CAFE model was constructed as shown in Figure 2 [22]. Each finite element has two CA arrays attached to it, one representing the ductile properties of the steel (the ductile CA array) and the other addressing the brittle properties of the material (the brittle CA array). The Rousselier' ductile damage model [25, 26] was used as a constitutive routine at each FE integration point. Each ductile CA cell is given a randomly generated critical value of the damage variable, β_c, at the beginning of the simulation. The current value of the damage variable, $\beta(t_{i+1})$, calculated at the integration point is sent to the ductile CA array and distributed across all cells according to local strain gradients associated with dead cells.

A dead ductile cell simulates a microvoid, which is a source of local strain concentration. In this CAFE model such strain concentration is implemented by using the ductile strain concentration factor, c_D, in those cells adjacent to a dead one, which lie on the plane perpendicular to the direction of the maximum principal stress. Accordingly the brittle strain concentration factor, c_B, is utilised in the brittle CA array for the same purpose.

The ductile failure criterion at each ductile CA cell is based on the damage variable exceeding the critical value given to this cell. Thus a ductile cell will become inactive at time increment n if the damage parameter $\beta(t_n)$ exceeds its critical value β_c. Each brittle cell is given a randomly generated grain size, d_g, from within a given distribution, and an orientation angle, θ, at the beginning of the simulation. Moreover it is assumed that a fraction of brittle cells have microcracks from the very beginning of the simulation. Only these cells can initiate brittle fracture propagation.

The maximum principal stress at the finite element integration point is redistributed across the brittle CA array. A brittle CA cell is considered to have failed if the maximum principal stress in this cell exceeds the fracture stress for the grain size assigned to this cell. Brittle fracture will propagate from one cell, k, to another, l, only if the misorientation angle for these cells is smaller than the misorientation threshold, i.e. if $|\theta_k - \theta_l| < \theta_F$. It is further assumed that the misorientation threshold is temperature sensitive: $\theta_F = 0$ at temperatures above -20°C; from -20°C to -80°C θ_F is linearly increasing to 60° and $\theta_F = 60°$ at temperatures below -80°C. Such temperature dependence of θ_F promotes fast brittle fracture propagation at the lower shelf temperatures and inhibits or stops it at the upper shelf. The changes in cell state in one CA array, either brittle, $Y_{m(B)}(t_i+1)$, or ductile, $Y_{m(D)}(t_i+1)$, cause some change of the cell states in the other CA array (Figure 1).

Finally the state variables of the finite element, $Y_a(t_i+1)$, a = 1,2 are calculated and returned back from the CA part of the model to the FE solver. There are two state variables in this model: the integrity of the finite element, Y_1, and the percentage of the brittle phase per finite element, Y_2. At the beginning of the simulation $Y_1(t_0) = 1$, which means that there is no damage. Accordingly $Y_1(t_n) = 0$ means that either the finite element has no load-bearing capacity or that the crack has propagated across the whole of the finite element by time increment n.

This work was aimed at the ITT prediction of the Charpy impact test for TMCR steels. A 3D finite element model of the Charpy test was created in which 900 finite elements located at and near the macroscopic fracture propagation plane (damage zone) were simulated with the CAFE approach [22]. 5 × 5 × 5 cell ductile and 10 × 10 × 10 cell brittle CA arrays were created for each finite element in the damage zone. Thus the ductile damage cell size was 0.2 mm and the brittle damage cell size was 0.1 mm (it should be noted that the shape of the CA array is not linked to the shape of the FE mesh and remains the same throughout the simulation).

III. RESULTS AND DISCUSSION

Microstructural Characterisation: The two TMCR steel plates exhibit a microstructure of ferrite-/-pearlite banded in the rolling direction (Figure 3). Variations in ferrite grain sizes were frequently observed through the thickness with coarse ferrite grain patches studded in a matrix of desirable fine grains resulting in a "duplex" ferrite grain distribution. The duplex grain structure may stem from an inhomogeneous distribution of microalloying element precipitates [9], especially niobium [33, 34]. Segregation of niobium and other alloying elements during solidification results in an inhomogeneous distribution of microalloying precipitates and consequently partial recrystallisation can occur during the TMCR process.

As reported in the literature [10, 11], for steels having a bimodal distribution of polygonal ferrite grains (comprising bands of coarse and fine grains), cleavage microcracks form preferentially in the largest grains. A cleavage microcrack formed in a large grain within a coarse grain patch or band will propagate through the large grains within the band and may carry on to cause catastrophic cleavage failure if the stress intensification resulting from the cleavage crack in the coarse grains exceeds the fracture strength of the surrounding fine ferrite grains. The large grains in the coarse grain patches are therefore regarded as the "weak link" and the dominant microstructural factor in the cleavage fracture process. In this work, the ferrite grains *within* the coarse grain patches were analysed for the two TMCR steels by setting a lower ECD grain size threshold limit of 6μm during quantification. The grain size distributions from through-thickness characterisation are shown in Figure 4. The mean coarse grain size of 12.2μm for Plate-1 is smaller than that for Plate-2 (13.2μm). The average areal proportion of the coarse grain patches is 38.7% and 47.1% for Plate-1 and Plate-2 respectively. Therefore, there is a significant statistical chance of a crack tip sampling a coarse grain patch.

Local Fracture Stress (σ_F): Critical local fracture stress (σ_F) values for both TMCR steels were determined using values of fracture load in combination with a 2D finite element analysis (FEA) of the stress-strain distribution ahead of the notch root under plane strain conditions [32]. The stress-strain distributions were expressed in terms of the ratio of maximum principal stress to yield strength, σ_{mp}/σ_Y, corresponding to the position ahead of the notch tip and the largest value of σ_{mp}/σ_Y at each applied load normalised by the general yield load (P_{app}/P_{GY}). Assuming that the largest maximum principal stress corresponding to the failure load of the specimen is the critical local fracture stress "σ_F", the σ_F values for the two TMCR steels can then be obtained from the failure loads of the blunt-notch four-point-bend specimens and the yield stress values determined through tensile tests at different temperatures.

Figure 5 shows the σ_F values for the two steels tested at different temperatures. It can be seen that the σ_F values are almost independent of temperature and that a large scatter in σ_F values exists for both steels due to the duplexity of the ferrite grain sizes. The mean σ_F value of 1749 MPa for Plate-1 is greater than that of Plate-2 (1666 MPa). This is probably due to the consistently smaller grain size (overall and coarse) and the smaller area fraction of the coarse grain bands in Plate-1.

Prediction of σ_F from grain size distribution: Significant scatter in the σ_F values (Figure 5) is revealed by a very limited number of tested specimens. It can be postulated that the scatter will be larger with more specimens tested. A great number of specimens is required to thoroughly describe the real σ_F distribution that is a crucial input to the CAFE model for the prediction of the ductile-brittle transition temperature. Since experimental tests are time and money intensive, attempts were made to predict the σ_F distribution from the microstructure of the steels.

The well-established empirical expressions for normalised steels may still be applicable to predict the tensile strengths of the TMCR steels using its *mean* grain size because tensile tests average the microstructure (for ductile failure) as the strain field samples a relatively large area compared to the scale of the microstructure. The *mean* grain size for the duplex grains, however, cannot be used to predict the Charpy impact energy and the fracture stress due to the highly concentrated stress and strain ahead of the notch or fatigue-precrack tip. Failure of the notched or precracked specimens is dominated by the intensification of stress and strain within a small area, usually the plastic zone, in front of the notch or crack, which strongly limits the sampling of the microstructure. As a result, a large variation in fracture properties will appear for steels with non-uniform microstructure. A single-valued function obtained from the *mean grain size* is not representative of the fracture properties such as σ_F and ITT for such steels.

The ferrite grain size distribution must therefore be used to predict the distribution of the σ_F values. It has been shown [7, 35] that the critical event for cleavage failure in a notched steel specimen is the propagation of a microcrack across the adjacent ferrite/ferrite grain boundary. This will occur when the stress level at the microcrack exceeds the "ferrite grain strength" which is given in terms of the grain diameter d by the equation [7]:

$$\sigma_F = [\pi E \gamma_p / (1-\nu^2) d]^{1/2} \qquad (4)$$

where E is Young's modulus, ν is Poisson's ratio, and γ_p is the effective surface energy. Assuming that the *mean* local fracture stress of the TMCR steels is related to the *mean* ferrite grain size of the grains within the coarse grain patches (since cleavage microcracks will form preferentially in the large polygonal ferrite grains), the γ_p value can then be determined, using equation (4) and ν=0.3, E=208x10^3 MPa. A value of γ_p of 52 J/m^2 is obtained for both TMCR steels, which is in the range reported in the literature [36]. Using equation (4) and the obtained γ_p value, the coarse ferrite grain size distributions in Figure 4 can then be converted into local fracture stress distributions.

The probability of cleavage failure occurring at a certain fracture stress value calculated from equation (4) corresponding to a particular grain size are shown in Figure 6 together with the experimental results of the σ_F values. The reason that there are no test data at the lower value side of the σ_F distributions may be attributed to the limited number of tested specimens and the very low probability of sampling the extremely large ferrite grains due to their rarity. It can be seen that the experimental results fit very well to the predicted σ_F distributions obtained from equation (4) based upon the coarse ferrite grain distributions for the two TMCR steels. This implies that the fracture stress σ_F of a TMCR microalloyed steel can be predicted based on the coarse grain size distributions within the coarse grain bands. This fracture stress distribution can then be used as an input into the predictive CAFE model for ITT.

The ductile part of the CAFE model was tuned using the Charpy test modelling at the upper shelf temperatures, where the model does not exhibit any significant brittle fracture. The strain concentration coefficients were chosen as c_D = 1.4 and c_B = 11 so that the concentration around a failed brittle cell (microcrack) is much higher that that around the dead ductile cell (microvoid).

The experimentally measured grain size distribution for another TMCR Nb-microalloyed steel (nominal composition same as plate-2), with known Charpy DBTT curve, was simulated in the CAFE model using a random number generator based on a Weibull three-parameter probability density function. The parameters of this function were chosen such that the mean, standard deviation and the mode calculated on the generated values are the same as those calculated from the experimental grain size data. Each brittle cell was then assigned a fracture stress calculated with equation (4) for a grain size generated for this cell.

The modelling was performed at 11 temperatures from -80^{o}C to 0^{o}C, with three simulations at each temperature. The resulting total energy absorbed and the percentage of the brittle phase values are shown in Figures 7a) and b) accordingly. Figure 7a) indicates that the lower shelf starts at approximately -50^{o}C to – 60^{o}C. These temperatures can be taken as the energy-based ITT. On the other hand the 50% ITT obtained from the data shown in Figure 7b) is approximately -30^{o}C to -35^{o}C. Although in general the model predicts a higher ITT than observed experimentally, the shape of the transition curve is well reproduced. The scatter in the simulated energy and brittle phase values is due to the fact that each modelling run represents a unique sampling of β_F, θ_F, and σ_F. Therefore each simulation has a unique fracture propagation history.

Figure 7a) shows that the CAFE model over-predicts (approximately 60J) absorbed energies for 100% brittle failure. This is because the present CAFE model cannot simulate crack propagation from one finite element into another due to the restrictions of the Abaqus code

[23, 26]. Consequently brittle fracture has to re-initiate when a crack crosses a finite element boundary. In each run the crack has to cross approximately 100 finite elements (the exact number depends on the actual fracture propagation path). As crack initiation requires plastic deformation, the total absorbed energy becomes high. Further model development will be to allow crack propagation from one finite element to another.

An important feature of the present CAFE model is that temperature-dependent scatter in both the energy and the percentage of brittle phase was achieved. The scatter is caused by the fact that the locations of the brittle CA cells representing larger grains vary randomly from one modelling run to another. It has been argued that in the upper shelf the number of larger grains that can fail is so small that their locations do not matter, as it is extremely unlikely that one such grain will be found in the crack propagation path [27]. Similarly in the lower shelf there are so many grains that can fail that their locations also are not important, as many such grains will be found along any crack propagation path. However, at transitional temperatures, the number of larger grains that can fail is such that their locations become important as different fracture propagation paths will cross a larger grain at different crack lengths, or would not cross any such grain at all. Accordingly the level of scatter is higher in the transition region than in the upper and in the lower shelves. Such modelling behaviour agrees with the experimental observations (Figure 7). In addition it is impossible to achieve this scatter if only the mean grain size (fracture stress) is used in the model.

In summary it has been shown that the observed microstructural inhomogeneity (fine and coarse grain sizes) translates into a distribution of fracture stress values, which can be predicted from the coarse grain size distribution. This fracture stress distribution can be used with a novel modelling approach (CAFE model) to reproduce the scatter seen experimentally in Charpy impact testing and predict the Charpy ITT behaviour.

IV. CONCLUSIONS

A combined experimental and modelling approach to understanding and predicting the scatter in Charpy impact transition temperatures (ITT) for thermomechanically controlled rolled (TMCR) Nb-microalloyed steels has been carried out. The major findings are:

- A significant degree of scatter in experimentally determined fracture stress (σ_F) values exists for the Nb-microalloyed TMCR steels investigated. The σ_F distribution can be predicted, with reasonable accuracy, from the coarse grain size distribution.

- A cellular automata finite element (CAFE) model has been developed using experimental data (fracture stress distribution) as an input. The results from multiple runs of the model showed that a realistic prediction of the Charpy ductile-brittle transition behaviour could be achieved. In addition, the experimentally observed scatter in Charpy energy values in the transition region can be reproduced by the model.

- The CAFE model prediction of the upper shelf ductile energy and percentage brittle failure for the Charpy impact test agrees well with the experimental data. The prediction of the lower shelf brittle energy is not as good due to computational limitations (Abaqus code) of the current CAFE model.

V. ACKNOWLEDGMENTS

The authors would like to thank the Engineering and Physical Sciences Research Council (EPSRC) for financial support and Corus UK Ltd for financial support, provision of test material and data.

VI. REFERENCES

1. B. Mintz, G. Peterson, and A. Nassar: *Ironmaking and Steelmaking*, 1994, Vol.21, pp. 215-222.
2. T. Gladman, D. Dulieu and I. D. McIvor: in *Microalloying 75*. New York, Union Carbide Corp., 1977, pp. 32-55.
3. B. Mintz, W. B. Morrison, and A. Jones: *Met. Technol.*, 1979, Vol.6, pp.252-260.
4. W. E. Duckworth and J. D. Baird: *J. Iron Steel Inst.*, 1969, Vol 207, pp. 854-871.
5. E. O. Hall: *Proc. Phys. Soc.*, 1951, B64, pp. 747-753.
6. N. J. Petch: *J. Iron & Steel Inst.*, 1953, Vol.173, pp. 25-28.
7. T. Lin, A. G. Evans and R. O. Ritchie: *Met. Trans.*, 1987, Vol.18A, pp. 641-651.
8. T. Gladman: *The Physical Metallurgy of Microalloyed Steels*, The Institute of Materials, London, 1997, p.62.
9. C. L. Davis and M. Strangwood: *J. Mater. Sci.*, 37 (2002), pp. 1083-1090.
10. M. T. Shehata and J. D. Boyd: in *Advances in Physical Metallurgy and Applications of Steels*, Proc. Conf., University of Liverpool, TMS, 1982, pp. 229-236.
11. J. H. Chen, L. Zhu and H. Ma: *Acta Metall. Mater.*, 1990, Vol.38, pp. 2527-2535.
12. J. H. Chen, G. Z. Wang, Z. Wang, L. Zhu and Y. Y. Gao: *Met. Trans.*, 1991, Vol.22A, pp. 2287-2296.
13. A. From and R. Sandstrom, *Materials Characterization*, 1999, Vol.42, pp. 111-122.
14. S. J. Wu and C. L. Davis: Presented at ICSMA13, Budapest, 2003, to be published *by Materials Science and Engineering A*.

15. I. C. Howard, Z. H. Li, M. A. Sheikh, A. H. Sherry, D. P.G. Lidbury and D. W. Beardsmore, "Local approach predictions of transition behaviour of specimens and structures", IMechE Seminar, '20 Years of R6', IMechE HQ, London, 20 November 1996.

16. M. C. Burstow, "Local approach analysis of fracture in the transition region", SIRIUS report, Department of Mechanical Engineering, The University of Sheffield, 1998.

17. I. C. Howard, Z. H. Li and M. A. Sheikh, "Modelling the ductile to cleavage transition in steels and structures", Fatigue and Fracture Mechanics: 30th volume, ASTM STP 1360, P. C. Paris and K. L. Jerina, Eds., American Society for Testing and Materials, West Conshohocken, PA, 2000, pp. 152-168.

18. L. Xia, and F. S. Shih, "Ductile Crack Growth - I. A Numerical Study using Computational Cells with Microstructurally-Based Length Scales", Journal of the Mechanics and Physics of Solids, Vol. 43, 1995, pp. 233 - 259.

19. C. Ruggieri and R. H. Dodds, "A Transferability Model for Brittle Fracture Including Constraint and Ductile Tearing Effects- a Probabilistic Approach", *International Journal of Fracture*, Vol. 79, 1996, pp. 309 - 340.

20. L. Xia, and F. S. Shih, "Ductile Crack Growth - III. Transition to Cleavage Fracture Incorporating Statistics", *Journal of the Mechanics and Physics of Solids*, Vol. 44, 1996, pp. 603 - 639.

21. L. Xia, and L. Cheng, "Transition from Ductile Tearing to Cleavage Fracture: a Cell-Model Approach", *International Journal of Fracture*, Vol. 87, 1997, pp. 289 - 306.

22. F. M. Beremin, "A local criterion for cleavage fracture of a nuclear pressure vessel steel", *Metallurgical Transactions A*, 1983, 14, pp. 2277-2287.

23. A. L. Gurson, "Continuum Theory of Ductile Rupture by Void Nucleation and Growth: Part I- Yield Criteria and Flow Rules for Porous Ductile Media", *Journal of Engineering Materials and Technology*, Vol. 99, 1977, pp. 2-15.

24. V. Tvergaard, "Influence of Voids on Shear Band Instabilities under Plane Strain Conditions", International *Journal of Fracture Mechanics,* Vol. 17, 1981, pp. 389-407.

25. G. Rousselier, J. C. Devaux, G. Mottel and G. Devesa, "A methodology of ductile fracture analysis based on damage mechanics: an illustration of a local approach of fracture", in J.D. Landes, A. Saxena and J. G. Merkle, eds, 'Nonlinear fracture mechanics: Volume II – Elastic Plastic Fracture', 1983, ASTM STP 995, Philadelphia, pp. 332-354.

26. G. Rousselier, "Ductile fracture models and their potential in local approach of fracture", *Nuclear Engineering Design*, **105**, 1987, 97-111.

27. A. Shterenlikht, "3D CAFE modelling of transitional ductile-brittle fracture in steel", PhD Thesis, 2003, Sheffield University, Mechanical Engineering Department.

28. J.H. Beynon, S. Das, I.C. Howard and A. Chterenlikht, Extending the Local Approach to Fracture: Methods For Direct Incorporation of Microstructural Effects into Finite Element Models of Fracture. In: Brust FW (Ed.), New and Emerging Computational Methods: Applications to Fracture, Damage and Reliability, The American Society of Mechanical Engineers, 2002, pp. 229 – 237.

29. Beynon JH, Das S, Howard IC, Palmiere EJ and Chterenlikht A, The combination of Cellular Automata and Finite Elements for the Study of Fracture; the CAFE Model of Fracture. In: Neimitz A, Rokach IV, Kocanda D, Golos K (Eds.), ECF14, Fracture Mechanics Beyond 2000, EMAS Publications, Sheffield, UK, 2002, pp. 241 – 248.

30. A. Shterenlikht and I. C. Howard: Cellular automata finite element model for transitional ductile brittle fracture, in preparation.

31. S. J. Wu and C. L. Davis, Paper was presented at the 10th EBSD Conference, Swansea, UK, 2003 and *J. Microscopy*, 213, 2004, pp. 262-272.

32. S. J. Wu, and J. F. Knott, Proc. Conf. on Structural Integrity in the 21st Century, Eds. J. Edwards et al, EMAS Publishing, 2000, pp. 247-255.

33. B. Dutta and C. M. Sellars, *Mat. Sci. and Tech.*, 3, 1987, pp. 197-206.

34. A. C. Knessi, G. Posch, C. I. Garcia and A. J. Deardo, in Proc. of Int. Symp. on Low-Carbon Steels for the 90's, Pittsburgh, USA, edited by R. Asfahani & G. Tither, TMS 1993, pp. 113-119.

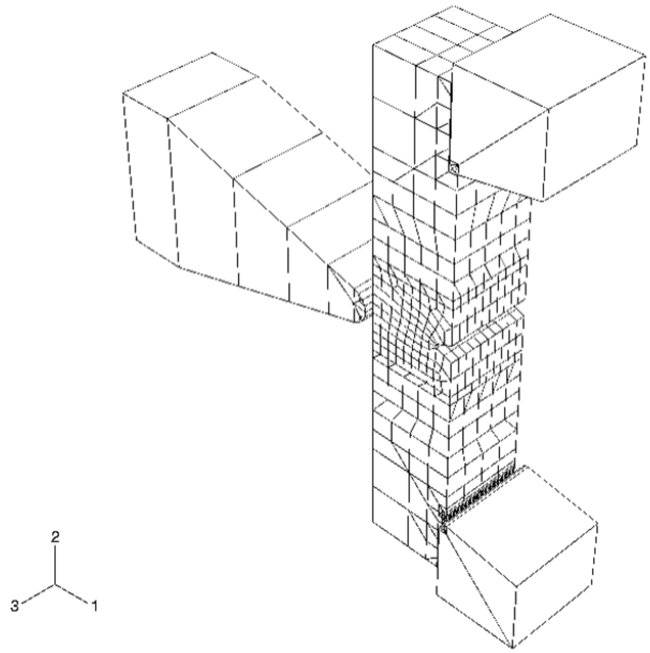
35. R. O. Ritchie, J. F. Knott and J. R. Rice, *J. Mech. Phys. Solids*. 21, 1973, pp. 395-410.

36. W. W. Gerberich and E. Kurman, *Scripta Metall.*, 19, 1985, pp. 295-298.

Table I. Nominal chemical compositions (wt%) of the steel plates used.

	C	Si	Mn	P	S	Cr	Ni	Al	Cu	Nb	N	Ti	V
Plate-1	.11	.31	1.39	.010	.003	.03	.32	.037	.033	.024	.006	.002	.045
Plate-2	.11	.30	1.43	.011	.003	.023	.30	.039	.013	.040	.005	.003	.063

a)



b)

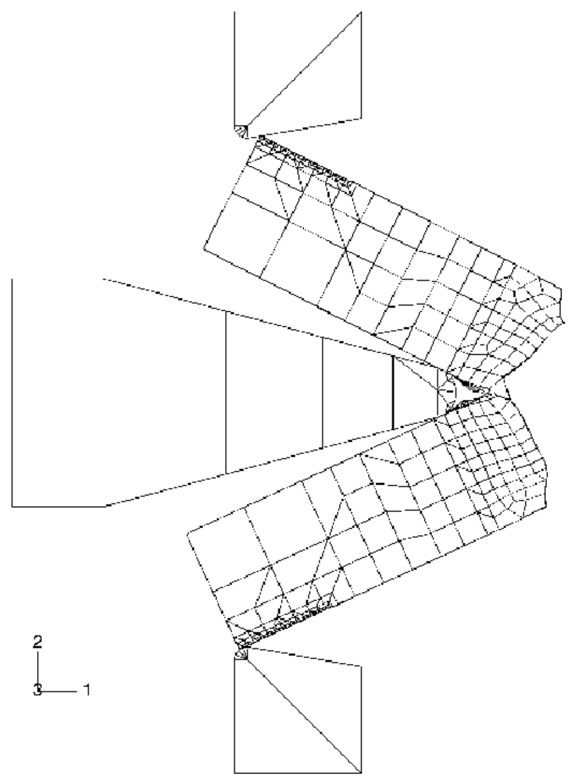


Figure 1. FE model of the Charpy test, a) before and b) at the end of the simulation.

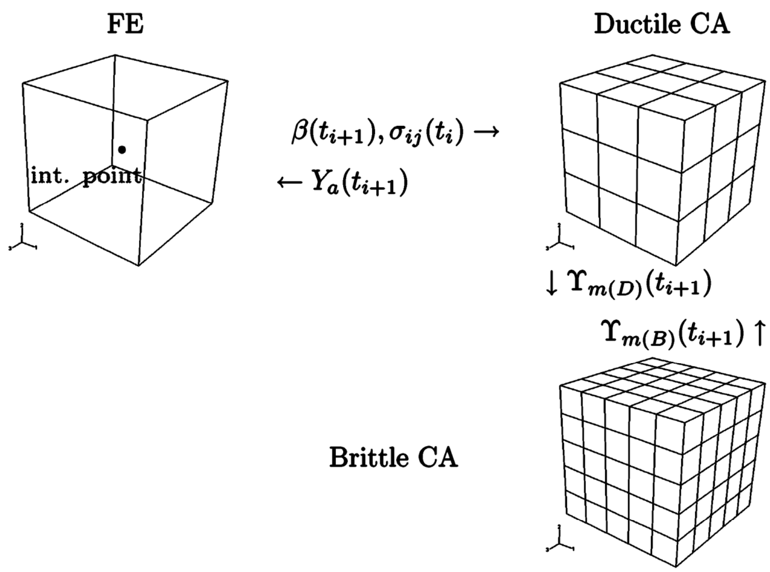


Figure 2. Representation of the cellular automata arrays for ductile and brittle failure associated with each FE cell in the CAFE model.

Figure 3. Microstructure of the TMCR microalloyed steel showing coarse and fine grain sizes.

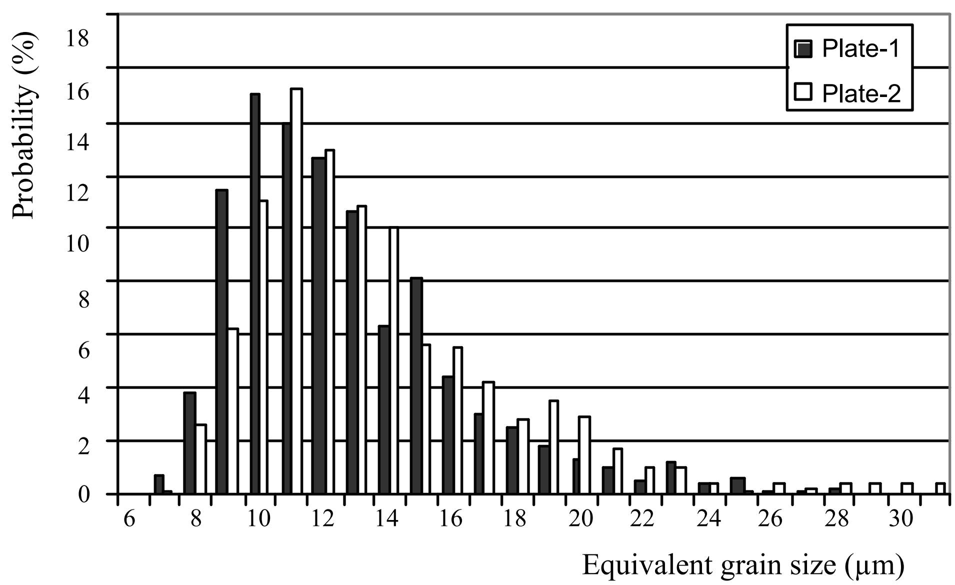
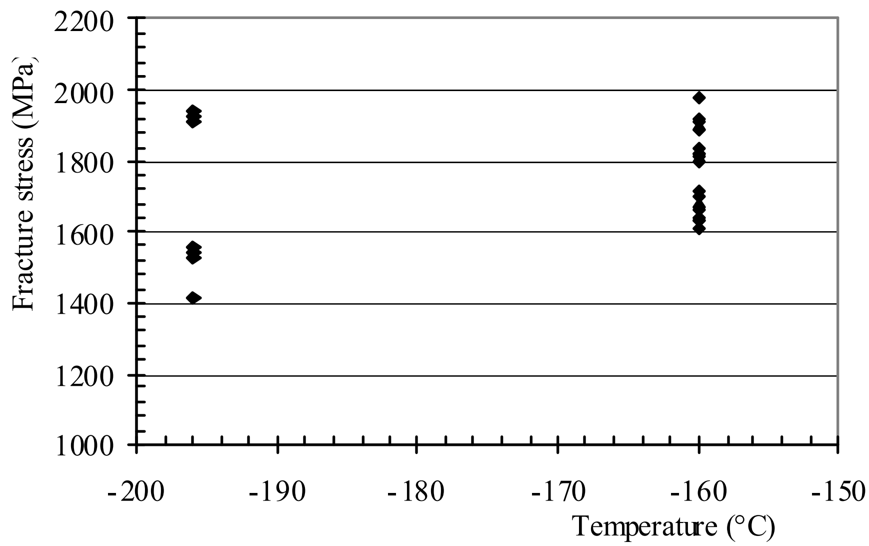


Figure 4. Equivalent ferrite grain size distributions for the large (>6 μm) grains located within the coarse grain bands of the two TMCR microalloyed steels.

a)



b)

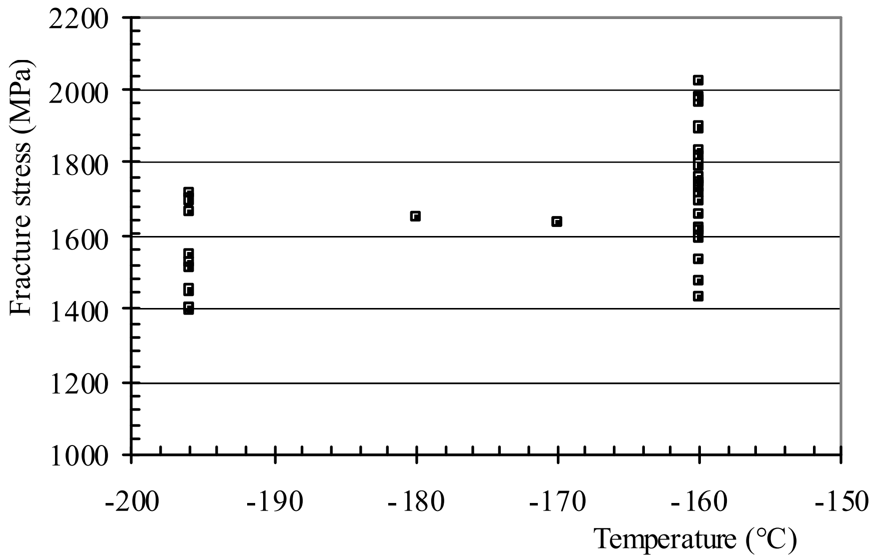
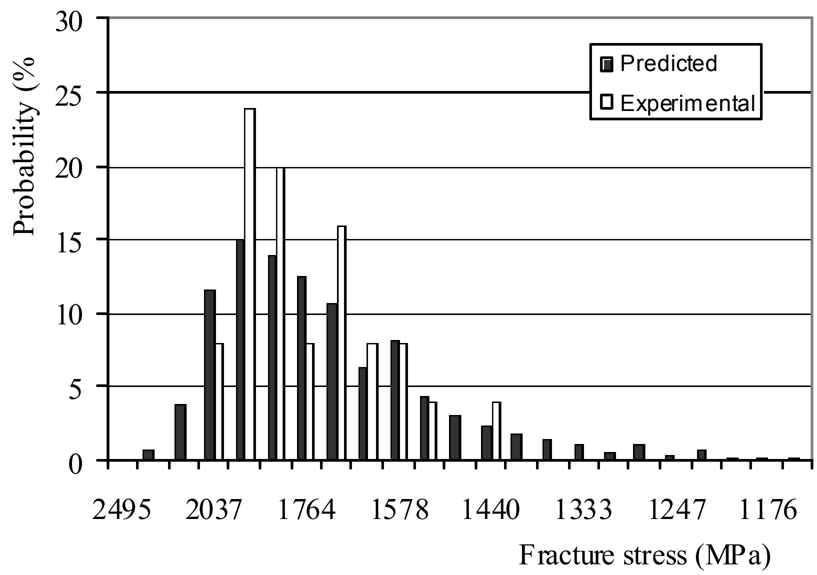


Figure 5. Variation of the local fracture stresses with temperature for the two TMCR steels (a) Plate-1 and (b) Plate-2.

a)



b)

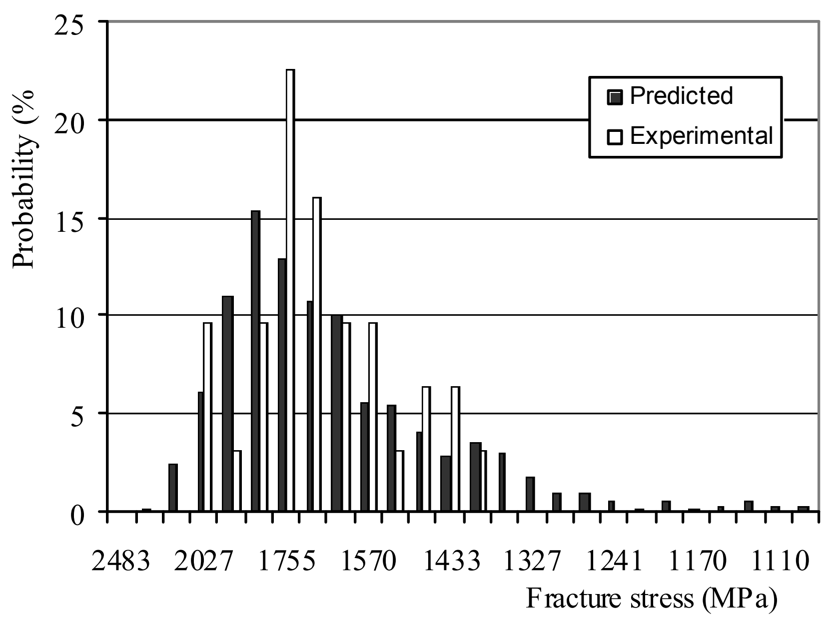
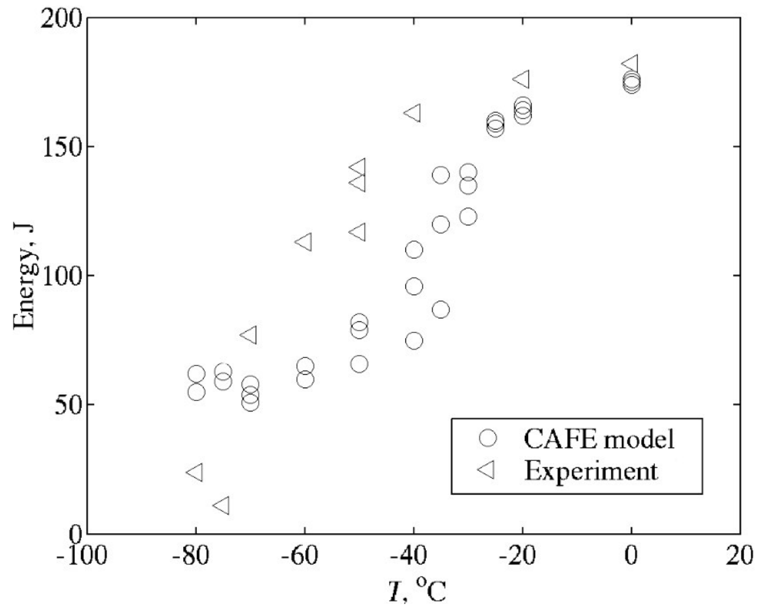


Figure 6. Comparison of the local fracture stress distribution predicted from the coarse grain size distribution with the experimental data. (a) Plate-1 and (b) Plate-2 steel.

a)



b)

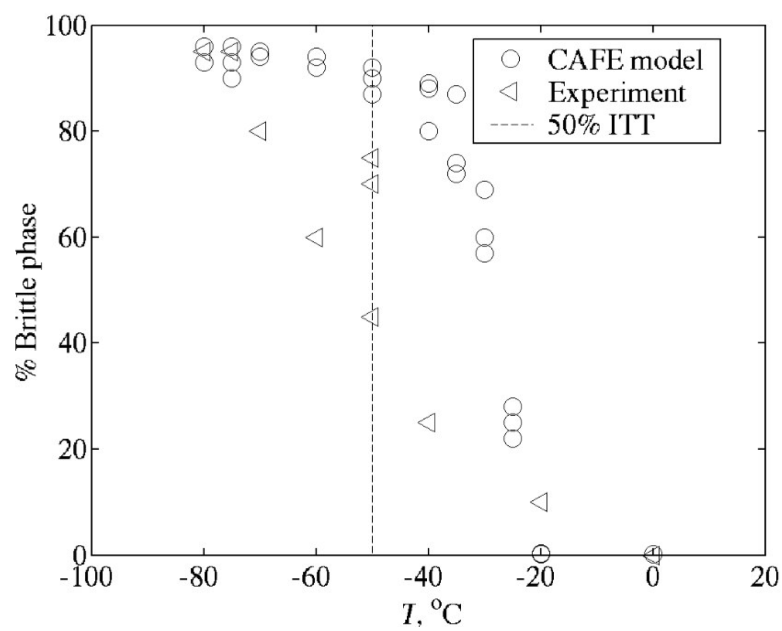


Figure 7. CAFE model results for a) total energy absorbed and b) percentage brittle phase versus temperature compared to the experimental results for TMCR Nb-microalloyed steels.