MODELLING INTERGRANULAR CRACK GROWTH IN 2D AND 3D VORONOIA CELLS

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Intergranular subcritical branching localized at the crack front is simulated by a computer procedure. This process was observed in ultra-high strength low-alloyed (UHSLA) steels during the standard K_{Ic}-test. Branching is controlled by the effective crack driving force corresponding to the I+II mixed mode and takes place in a 2D Voronoia mosaic approximating the real grain boundary network. This 2D model can explain more than 50 pct of the virtual beneficial effect of increasing austenitizing temperature. By means of a 3D model, briefly mentioned in terms of its simple noninteractive variant, a complete elucidation of this effect is expected to be achieved.

INTRODUCTION

Increase in fracture toughness K_{Ic} with increasing prior austenite grain size (austenitizing temperature) in case of martensite UHSLA steels was experimentally observed by many authors during the years 1973-1985 (e.g. Lee et al (1)). Related qualitative interpretation was very inconsistent and unconvincing - improve in matrix chemical homogeneity, more favourable distribution of retained austenite, changes in size and distribution of low tempered carbides, etc. Later works have shown (Pokluda et al (2), Tomita (3)) that the intergranular fracture along prior austenite grain boundaries was the most prevailing surface morphology in case of coarse grained structures. Accompanied shielding effects like subcritical intergranular crack front branching can lead to substantial reduction of the crack driving force (e.g. Surresh and Shih (4)). In order to asses the role of austenite grain size in the fracture process, simple analytical 2D model was developed on the basis of regular hexagonal grain boundary network (Zeman et al (5)). This model has shown that the

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shielding effect increases with decreasing number of grains n inside the zone of subcritical growth which corresponds to the improved K_{Ic}-values of coarse grained steels. This procedure led to a singularity when approaching the case of extremely large grain size. Therefore, a computer procedure of intergranular crack generation was developed within the crack tip zone containing the network of hexagonal grains of log-normal size distribution (Pokluda et al (6)). This analysis has shown that more then 50 pct of the K_{Ic} increment can be explained due to the crack branching. Simultaneously, a negligible effect of the zone shape was verified.

The aim of this paper is to present results of a computer model based on 2D Voronoia cells in a very close approximation to the real grain boundary network in a cross section planes. In addition, some results of a simple 3D variant of simulation are shown.

PRINCIPLES OF 2D MODEL

A subcritical intergranular crack tip branching in a standard CT-specimen during the K_{Ic}-test is to be simulated. For this purpose, following assumptions are accepted:

(i) The main macroscopic plain of the fatigue precrack (length l_0) is perpendicular to the direction of applied stress.

(ii) The fatigue precrack front is assumed to be locally stopped by intergranular facets deviating from the main crack plain by an angle greater than 0.93 rad. This value is a result of a balance between works needed for an elementary extension of a straight crack front segment along an intergranular facet and that of a half-circle shaped segment along the main crack plain.

(iii) Subcritical intergranular crack growth takes place within the butterfly-like process zone at the crack tip (von Mises yielding condition), size of which is independent on the applied austenitization temperature (mean austenite grain size) and much less than that of the apriory fatigue crack ($L \ll l_0$). It is given by the yield stress of martensitic matrix and, consequently, it is of the same value for all equally quenched and tempered steel specimens.

(iv) In each arbitrary selected cross section perpendicular to the fatigue precrack plain, the grain boundary network is simulated by a 2D Voronoia mosaic based on the Poisson point process.

(v) A possible crack path between two Voronoia cells (grains) is explicitly determined by the grain boundary. At a boundary triplet, further crack growth direction is given by the greater value of the effective crack driving force related to possible elementary branches in the I+II mix-mode as (4):

$$G_{ef} = \frac{1-\nu^2}{E}\cos^4(\gamma/2)K_I^2,$$

where ν and E are elastic moduli and γ is the angle between the intergranular segment and the main crack plain.

(vi) When the ratio of effective crack driving forces related to both possible branches lies within the range of $1 < G_{ef1}/G_{ef2} < \psi$, the crack tip can split. The parameter ψ is associated particularly with fluctuations of both the cohesive strength and the surface energy of intergranular grain boundaries.

(vii) A set of more then 1000 independently generated Voronoia networks is substituted for an extreme variety of possible grain boundary networks in real cross sections. A statistical evaluation of subcritical crack growth is performed in this set.

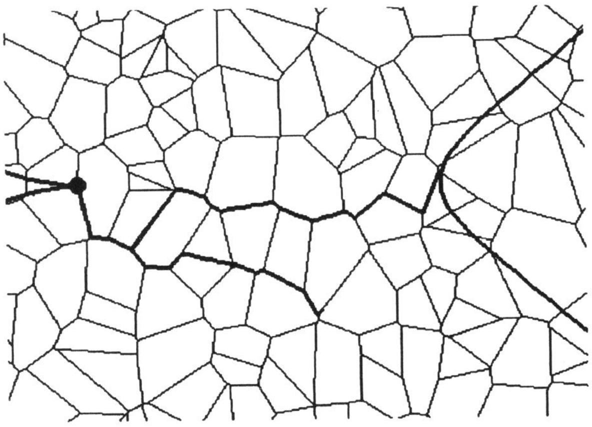

Figure 1: Branched crack in 2D mosaic. Left – precrack, right – zone boundary.

RESULT OF 2D SIMULATION PROCEDURE

An example of the Voronoia mosaic is shown in Fig. 1 where the critical intergranulary branched crack within the process zone is constructed according to the principles given above. It is to distinguish between the apparent driving force G_I related to the idealized straight crack front and the I+II mixed-mode effective driving force G_{ef} related to the branched crack. Ratio of those driving forces is function of the kink (or fork) angles of the branched crack front.

This function can be easily determined by substituting an appropriate configuration of abscissas for elementary kinks or forks (Rooke et al (7)). When a certain dimension is related to Voronoia tessellations, e. g. the standard metallographical grain size number, grain boundary networks of various mean grain sizes can be simulated by a single Voronoia mosaic. For this networks, ratio $G_{efc}/G_{Ic} = K_{efc}^2/K_{Ic}^2$ of critical stress intensity factors as function of the grain size d can be calculated. Clearly, due to the very small size of the process zone, also the critical branches (through the whole process zone as in Fig. 1) can be approximated by appropriate abscissas. As a result, relation K_{Ic} vs. d can be determined under the obvious and experimentally verified assumption that the branching effect can be neglected in structures with superfine grains where $K_{efc} = K_{Ic} = 50$ MPa m$^{1/2}$ (5).

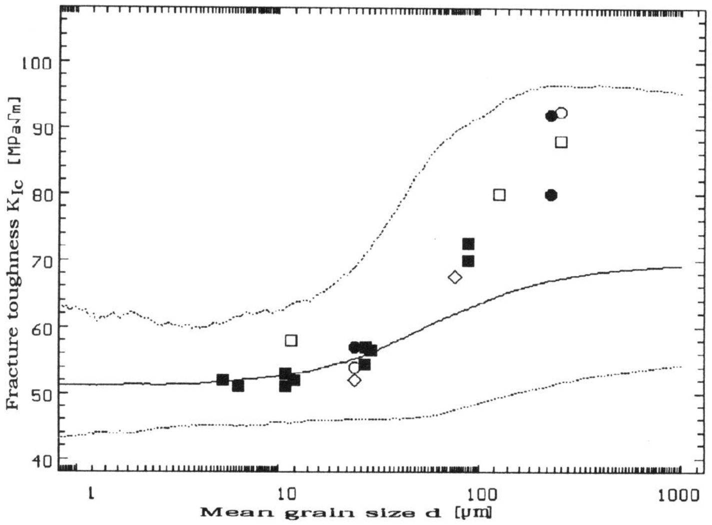

Figure 2: Statistical dependence of fracture toughness on mean grain size.

Calculations of this kind were performed and statistically evaluated for nearly 1300 various Voronoia mosaics. The result for $\psi = 1.2$ is shown in Fig. 2 together with succesible experimental data after (6). The full line represents the mean value and the dotted lines demarcate the 90 pct confidence intervals. Here, the process zone size at the onset of unstable fracture is considered to be a one half of the von Mises plastic zone corresponding to $\sigma_y = 1400$ MPa. This result suggests, in agreement with previous more simple models, that even the I+II mix-mode shielding effect explains the increase of K_{Ic}-values for coarse grained steels to appreciate extend.

REMARKS TO 3D MODEL

In order to asses both the mode III and the irregular crack front length contributions to the shielding effect, the 3D model is to be developed. Two basic problems are to be solved:

(i) computer procedure for creation of 3D Voronoia tessellation consisting of sufficient number of polyedric cells (10^6) completed by fast procedures performing all necessary geometric analysis;

(ii) new model for kinetics of initiation, coalescence and final fracture of spatial intergranular crack network.

The first task was successfully solved using the Pentium PC. In the Fig. 3, one polyedric cell of such mosaic is shown rotating round the vertical axes in five different spatial positions.

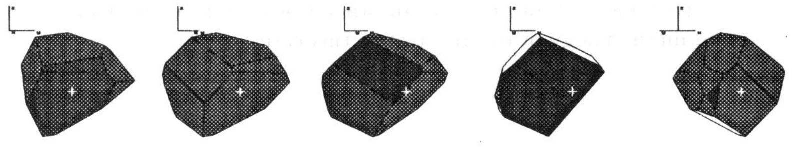

Figure 3: 3D Voronoia cell in five spatial positions.

Up to now, only a simple „noninteractive“ model of intergranular damage is developed. This model deals with the balance between a drop of the elastic energy of given cells with cracked walls and an increase in both the thermal energy and the work done for creation of new surfaces in a way similar to Okabe et al (8). Breaking of cell walls is assumed to be controlled by local effective driving force related to the critical nucleating defect within the cell wall, size

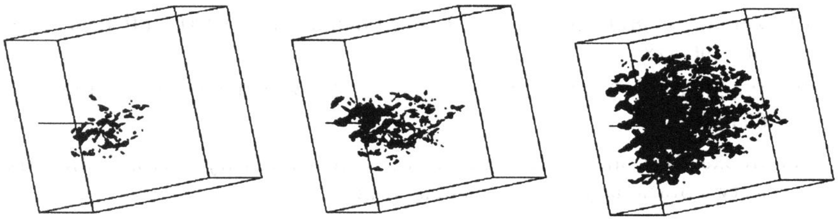

Figure 4: Development of intergranular damage at the crack tip within a 3D Voronoia mosaic (r_{BT} = 0.5, 2, 10 pct).

of which is proportional to that of the wall. In order to involve stress concentrations near cracked walls, rules for redistribution of elastic energy between neighbouring cells are added. No short- or long range interactions between those cracks are considered. As an example, three spatial configurations of cracked cell walls around the main crack front are illustrated in Fig. 4 for three various ratios r_{BT} of broken and total number of cell walls.

CONCLUSION

Results of the 2D model based on Voronoia mosaics confirmed that even the mode I+II of intergranular shielding contribution can, to sufficient extend, interpret an increase in K_{Ic}-values for coarse grained UHSLA steels. It is to be expected that a complete elucidation can be achieved by involving both the mode III and the irregular crack front length shielding contributions. This means that the improved fracture toughness of coarse grained steels has pure geometric (not metallurgic) reason. In other words, it is a result of a wrong evaluation methodology of the K_{Ic}-test in this case.

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