Modeling the mechanics of intergranular crack propagation

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ABSTRACT. *A mechanical model for simulating intergranular crack propagation is presented. In order to understand fracture mechanics and processes that occur in a polycrystalline body it is necessary to accommodate a large number of parameters, including the macroscopic effects of load together with stress state and component geometry. A dislocation analysis based on the boundary element method is introduced to model crack growth through microstructures. Simulated microstructures are generated using the Voronoi algorithm. Each grain is assigned with a set of randomly oriented slip directions in which plastic flow by shear is allowed. A uniform stress is applied that drives the crack, emanating from a free surface, along the grain boundaries. The crack is advanced quasi-statically along a GB path, solving for the distribution of dislocations within plastic zones emanating from the crack tip and the crack opening. The stress intensity factor is calculated at each step. At each triple junction the crack kinks towards the direction of the highest stress intensity. A superdipole (SD) algorithm is introduced to save simulation time without loosing important information and necessary geometric details. At the present time the factors controlling the path taken by a crack are not completely understood. By limiting the crack advancement to grain boundaries and applying the introduced dislocation model, relations between crack advancement, CTOD and stress intensity factors (SIF) can be determined.*

INTRODUCTION

Today, the process of intergranular crack propagation is still not well understood. Statistical analysis of crack growth in a given material may be useful for understanding the phenomenology and mechanisms of intergranular crack propagation. Most approaches dealing with statistical analysis use very simplified fracture models integrated in Monte Carlo simulations to obtain crack trajectories in randomly assigned microstructures.

Arwade et al. [1] analyzed intergranular cracks in polycrystal materials for different crack propagation laws statistically. Their crack propagation heuristic is based on simplified representations of the stress field in a microstructure, generated with the Voronoi algorithm, and GB material resistance. The crack propagates in the direction of maximum circumferential stress or the direction of maximum energy release rate (along

weakest boundary). The rate of variance growth depends strongly on the empirical crack growth direction law that controls the relative importance of the stress acting on a GB and the misorientation at the GB in determining the direction of crack propagation.

A three-dimensional Monte Carlo approach has been done by Kamaya and Itakura [2] using Finite Element Analysis (FEA) in a polycrystalline body generated by Voronoi tessellation. Both the local stress distribution and inclination of the grain boundaries were taken into account in determining crack initiation and propagation based on damage mechanics.

In order to reduce the high computational cost of full FEA simulation, Jivkov et al. [3,4] introduce a two- and three-dimensional mechanical model for simulating intergranular stress corrosion cracking using beam-type FEA. The model accounts for mechanical crack driving force and the formation of ductile bridging ligaments by resistant boundaries as well as branching. Monte Carlo type simulations with randomly distributed susceptible and resistant boundaries as well as resistant boundary failure strengths are performed in a regular hexagonal grain pattern. The model does not account for kinetics.

Another way of modeling crack propagation is the application of dislocation models. Dislocation models can calculate local stress fields accurately, are low in calculation time and flexible in accounting for complex and complicated crack geometries through realistic, irregular microstructures. Most of the recent studies deal with transgranular fatigue crack growth. The work done by Künkler et al. [5], Riemelmoser et al. [6,7,8,9] or Hansen and Melin [10] use a dislocation based Boundary Element Method (BEM) to model transgranular fatigue crack growth. A similar approach of a static discrete dislocation based BEM will be applied in this paper to model intergranular crack propagation.

MODEL DESCRIPTION

General

The following section describes algorithms for simulating the quasi-static propagation of a simple crack emanating from the free surface at an arbitrary angle φ and length a. Plane strain conditions are assumed. The sample dimensions are large compared to the crack of the length a. The free surface is taken to be parallel to the y-axis. The remote loading σ_{app} is characterized by a uniform stress in the y-direction (see Figure 1). Each boundary element in the crack contains a collocation point c_i^e and both a dipole of climb character and a dipole of glide character in order to simulate mode I and mode II displacements respectively. The boundary elements are made gradually smaller the closer to the crack tip they are located so as to guarantee a higher accuracy in that area. The length l_i of boundary elements can be calculated knowing the crack length and the number of boundary elements and follow the geometric progression: $l_i = 1.08 \cdot l_{i-1}$. Uniformly sized boundary elements in the slip planes contain a collocation point c_i^p and a dipole of glide character.

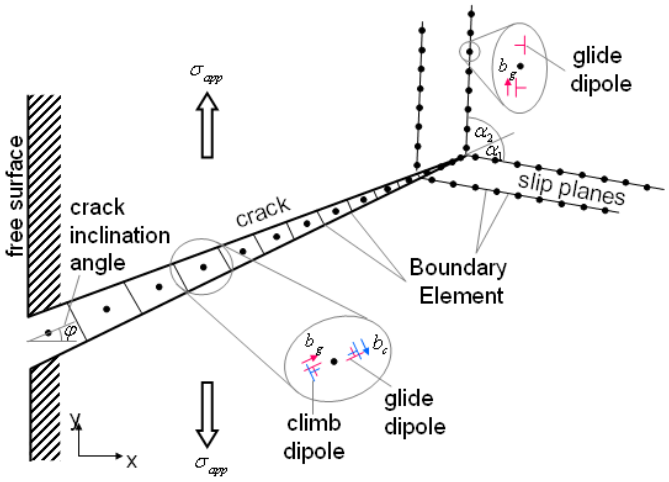

Figure 1. Mixed mode crack at a free surface

At each growth increment an iterative process is used to find a consistent equilibrium solution of the strength of all dislocation dipole elements. A set of simultaneous linear equations is formed in which stresses at each collocation point is given by the (unknown) Burger's vectors of each of the dipoles through a matrix representing the geometric arrangement. Stresses considered are the normal and shear stresses across the crack plane which are forced to zero and the shear stress along the glide dipoles representing plasticity which is forced to a constant critical flow stress in active regions. In the first iteration the stress contributions initially come from the far field applied stress, the dipole elements representing the crack and the stresses from dislocations generated by plastic flow in previous increments. Using this, a solution is found for the Burger's vectors of dipoles representing the crack, and the shear stress is then calculated at all dipoles representing plastic flow. Any plasticity dipole for which the stress is above the critical value is then activated and added to the set of linear equations. The new set of equations is solved, now including some plastic flow, and stresses are recalculated to see if more dipoles need to be included. This process is iterated until the plastic zones have expanded to a point at which stresses are kept at or below the critical level. Active slip planes are considerd to be those radiating directly from the crack tip and the two planes that were generated in the preceding increment. Thus some redistribution of plastic strain is allowed as the slip plane moves behind the crack tip. Dipoles and associated Burger's vectors of older slip planes become fix but still influence crack shape and plasticity in the two active slip planes. More information about how to solve this numerical problem is given in [11].

In this model the kinetics of crack growth are not accounted for. The real time dimension of crack propagation is not determined.

Grain patterns and slip plane systems

The microstructure is a randomly generated Voronoi grain pattern with uniformly distributed seed points. Each grain is assigned with a set of randomly oriented slip

directions in which plastic flow in shear is allowed. Here three directions, each 120º apart are assumed (see Figure 2). The slip direction of highest shear stresses is chosen in each grain. At each triple junction the crack kinks towards the direction of highest K_I and does not stop until it reaches a certain crack length.

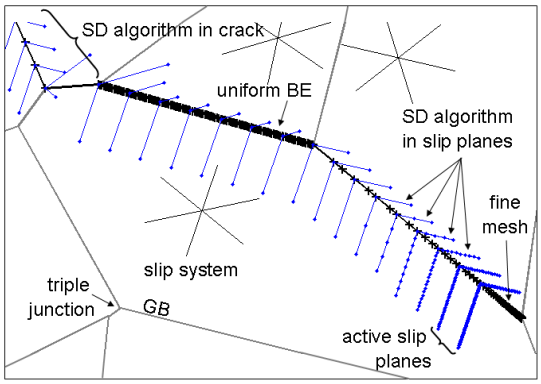

Figure 2. Example for advancing crack in Voronoi microstructure and applied SD algorithm in slip planes and crack

SD algorithm

The simulation of a growing crack requires the investigation of the effect of the dislocations which are left behind along the crack wake, since these are responsible for the plasticity induced crack closure, see [7]. As the crack tip moves away from the first slip plane pair, its influence on dislocations in crack tip vicinity decreases. After a certain crack extension the interaction force between the pre-existing slip planes and the dislocations on the new slip planes at the crack tip is small enough to apply a SD approach. This gradually bundles up dislocation dipoles on old slip planes to reduce the size of the numerical problem, see [6], and so keep the calculation time down, see [12]. From simulation step 3, after the crack has grown two growth increments, further plastic flow in the oldest slip plane pair is no longer allowed but the effect of those dislocations must be retained. This is where the SD algorithm applies:

Every two dipoles on a slip plane become one SD with a mean value of their Burger's vectors. This approach is used in every simulation step so that gradually more and more dipoles of old slip planes will be bundled up the further away from the crack the slip plane is located. The algorithm applies until there is only one SD left on each slip plane. One superdislocation is located right at the crack flank and the other one at the end of the plastic zone (see Figure 2). The associated Burger's vector is the mean value of all initial Burger's vectors of the slip plane dipoles.

A modified SD algorithm is also applied to the crack dipoles. Once the growing crack moves onto a new GB, the boundary segment that has just fractured is remeshed to have dipoles of uniform width. When the crack advances onto a third GB the penultimate GB will be subject to a SD algorithm. Each position of a dislocation is prediscribed by the position of a slip plane. So the number of crack dipoles of one GB is eventually reduced to the number of emanating slip planes from that GB (see Figure 2).

The SD algorithm is very important to reduce calculation time when the numerical system becomes very complex due to a kinking and branching crack. It has been shown by Brandinelli and Ballarini [13] that crack growth in random media is largely independent of the details of the crack trajectory and that the stress intensity factors depend almost entirely on the geometry of the final kink in the crack path and this is where the highest accuracy is achieved in the model introduced in this paper. Comparison of SIFs calculated with and without application of the SD algorithm for a crack of length 400 μm obtained in 79 simulation steps gives a mean deviation of less than 6%. In this particular example the application of the SD algorithm saves 78% of calculation time.

RESULTS

The simulation parameters used are representative of sensitized stainless steel: Young's modulus E = 206 GPa, Poisson's ratio $\nu = 0.3$, yield strength $\sigma_y = 205$ MPa and a initial remote stress $\sigma_{app} \approx 0.5 \cdot \sigma_y$ [5,6]. The average grain size of the randomly generated homogeneous grain patterns is 50 μm.

The following sections present the results of a Monte Carlo type simulation and statistical evaluation of crackpath, CTOD and SIFs. All results presented in this section are based on 20 crack trajectories as a result from conducting crack growth within 20 different random microstructures using the simulation parameters just introduced. In order to get information about the standard deviation of the crack path, all crack trajectories were shifted in *y*-direction so as to initiate from (0,0). In every of the following diagrams one data set is highlighted which belongs to the same set of input parameters in order to show relations between crack path, CTOD and SIFs for one particular crack.

Crack path and CTOD

Figure 3 shows 20 different crack paths of length 400 μm. A crack of this length in a grain pattern of 50 μm average grain size fractures 16.3 GBs on average.

As expected, the mean values fluctuate around zero while the standard deviation is slowly growing in a square root of crack length dependence as the crack extends (see red line in Figure 3). Crack initiation points are chosen randomly at the left boundary of the generated microstructure. This describes the very steep inclination angle of one of the crack paths which is not likely to occur in reality.

The CTOD of a crack is simply the Burger's vector of the innermost climb dipole of the crack. As the crack propagates, the CTOD fluctuates considerably but the mean value $CTOD^{\mu}$ gives a clear tendency of growth while the standard deviation grows for very short cracks but seems to fluctuate around a constant value later on (see Figure 4). To get a definite answer whether the $CTOD^{s}$ rises or is constant for an extending crack, the Monte Carlo type simulations would have to be carried out for a larger maximum crack length. Each peak in the highlighted CTOD trajectory indicated a change of direction in crack growth.

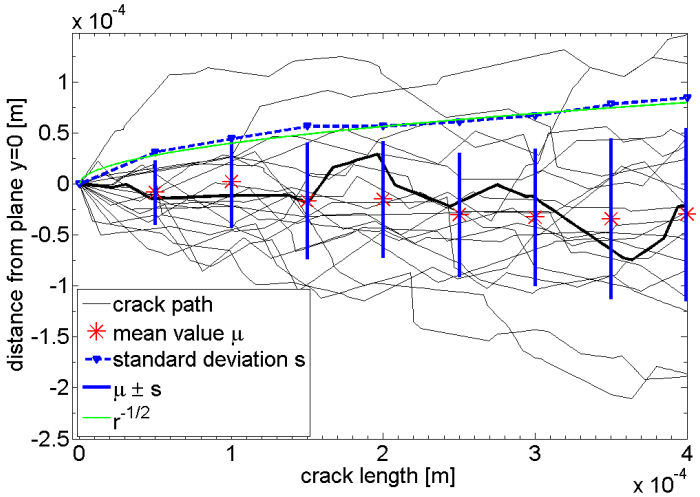

Figure 3. Geometry of 20 crack paths

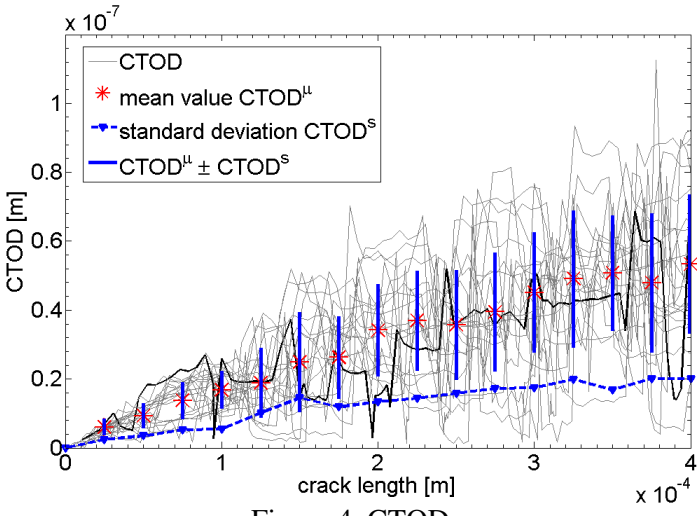

Figure 4. CTOD

SIF

SIFs are of fundamental interest to characterise the stress state at the tip of a crack and to correlate with crack growth data. In this paper SIFs have been calculated fitting the stress field equations

$$\sigma_{yy}^{I} = \frac{K_I}{\sqrt{2\pi r}} \ , \ \sigma_{xy}^{II} = \frac{K_{II}}{\sqrt{2\pi r}}$$

to the stress σ_{yy}, σ_{xy} ahead of the crack.

The stress distribution ahead of the crack follows a $1/\sqrt{r}$ behavior, with r the distance from the crack tip, when disregarding the region very close to the crack tip $r \leq 0.1$ nm. This is a reasonable thing to do, because close to the crack tip the discrete nature of the

simulation tends to stresses that are dominated by the dislocations at the crack tip and do not reflect the crack as a whole. The outer limit of the fitting region is chosen at $r = 10\ \mu m$ because only in this region the stresses σ_{yy}, σ_{xy} resemble the $1/\sqrt{r}$ behaviour.

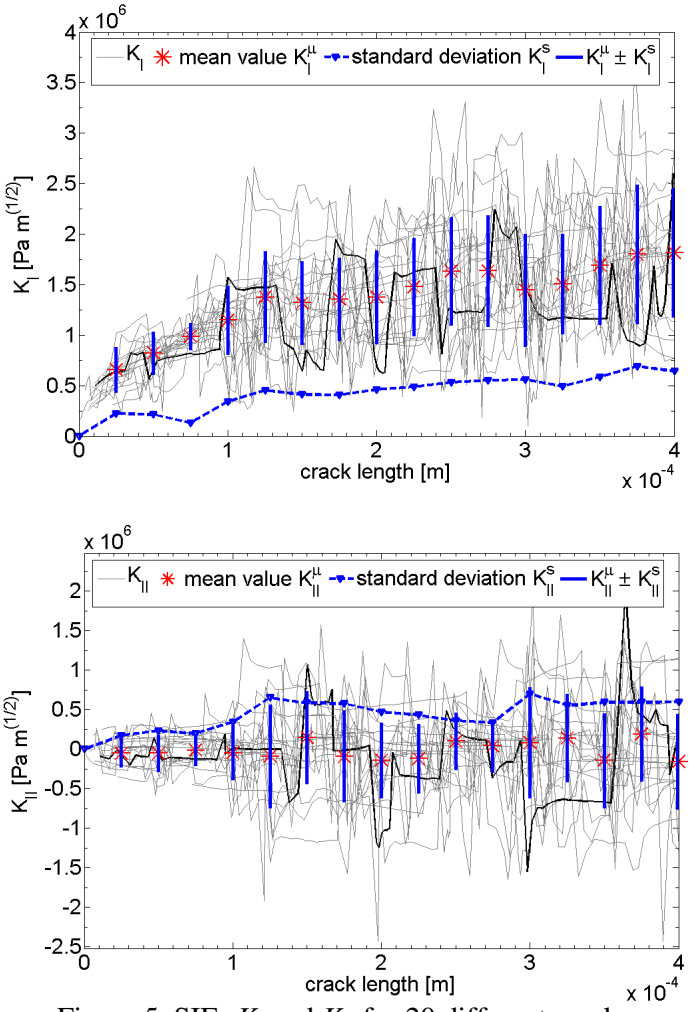

Figure 5. SIFs K_I and K_{II} for 20 different cracks

Figure 5 shows K_I and K_{II}. K_I^μ grows slowly with increasing crack length while K_{II}^μ fluctuates around 0. For both K_I and K_{II} it can be seen that the standard deviation increases for an initiating crack but settles down to a constant value for a longer crack.

The highlighted curves show that every change of direction of crack propagation has a severe influence on SIF. Whenever the crack kinks, K_I and K_{II} peak but mostly settle back down to a genereally increasing (for K_I) or constant (for K_{II}) distribution. There is a tendency for K_{II} to be above zero for a positive crack inclination angle and below zero for negative angles.

SUMMARY

We have presented a dislocation model that allows simulation of difficult and complex crack geometries. It is set up in a very general way and allows a crack to grow along any not curved GB geometry. This generic approach has a wide range of applications such as fatigue cracking as well as intergranular stress corrosion cracking.

A method of reducing calculation time has been developed. Bundling dislocations up in SDs is an efficient way to save calculation time without a significant loss of accuracy. Close to the crack tip the SD algorithm does not influence the model accuracy.

Calculation of SIF K_I and K_{II} is possible without difficulty and gives information about the stress state at the crack tip as the crack propagates through a grain pattern.

Monte Carlo type simulations have been conducted to obtain statistical information about the behavior of crack paths, CTOD and SIFs. All four of the just mentioned simulation output parameters are closely related. Whenever a crack reaches a triple junction and needs to change direction, CTOD, K_I and K_{II} trajectories peak severely but settle down quickly as the crack propagates along the new GB.

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