MODELLING GROWTH OF SMALL CRACKS IN A POLYCRYSTAL

Robert Lillbacka[1,2], Erland Johnson[1], Magnus Ekh[2] and Kenneth Runesson[2]
1, SP Swedish National Testing and Research Institute
Box 857, SE-501 15 Borås, Sweden
robert.lillbacka@sp.se
2, Chalmers University of Technology
Dept. of Applied Mechanics, SE-412 96 Göteborg, Sweden

Abstract

In this contribution we study the microstructurally short crack propagation phase in a grain structure of a duplex stainless steel (DSS). The grains in the DSS are either austenitic or ferritic. In order to take the material microstructure into account in the simulations we generate models of the grain structure using the Voronoi polygonization algorithm. The material behavior of the grains is modelled by crystal plasticity, hence, the crystallographic directions of the grains are modelled explicitly and evolution equations for the plastic slip along each slip-system are defined. Furthermore, the crystal plasticity model is enhanced, in the spirit of the disclocation model proposed by Navarro and De Los Rios [1], to include a crack propagation model taking into account non-local effects of the dislocation density (via the accumulated plastic slip) along a slip direction within a grain. Finally, numerical results are presented which show the influence of material hardening and slip directions on the propagation of a crack in an austenitic grain.

Introduction

In many industrial applications, the life of a structural component is controlled by fatigue. This life could, from the macroscopic point of view, be divided into the so-called crack initiation and propagation phases, see e.g. Suresh [2]. For the crack propagation phase, fracture mechanics at the macroscale provides a tool to handle life predictions. However, for the initiation phase no such evident tool exists.

The macroscopic crack initiation phase consists of, firstly, the small crack initiation (at free surfaces or defects) due to accumulation of plastic deformation along the slip directions (i.e. persistent slip bands) and, secondly, the subsequent propagation in one or several grains. The propagation is affected by grain boundaries and defects that act as stress raisers and as barriers, which introduce sequence and threshold effects on the macroscale e.g. Miller [3]. Therefore, the important characteristica of the material microstructure must necessarily be modelled in order to predict the duration of the initiation phase and the early propagation phase. Models for the propagation are usually based on the assumption that the cracks propagate along slip directions with the expression for the propagation velocity based on dislocation mechanics, see Pippan [4] and Navarro and de los Rios [1, 5, 6]. In the model by Navarro and de los Rios (the ND-model), the propagation velocity is determined by the number of dislocations along a slip line between the crack tip and the grain boundary. Initially, slip is assumed to have developed along a primary slip plane in one grain. During load cycling, the slip length increases in steps of a grain length when the shear stress has reached a critical value in the next unslipped grain. It is assumed that the crack propagates with a speed that is proportional to the current plastic displacement ϕ along the slip band in front of the crack tip, [1],

$$\frac{da}{dN} = f \cdot \phi \tag{1}$$

where N denotes load cycle. The constant f could be interpreted as the fraction of dislocations in the slip band, which participate in the process of crack extension. All grains are assumed to have identical sizes and slip propagation directions.

The model has been modified to include hardening behavior [7] and, more recently, been used for the study of spectrum loading effects [8, 9]. The model can also be used to predict the Hall-Petch effect, and the continuum limit after propagation for a couple of grains.

In the present paper, we will show how it is possible to combine crystal plasticity and a crack propagation law in the spirit of the (dislocation mechanics based) ND-model to study short crack propagation in a grain structure. The key assumption we make, in order to couple the models, is that the accumulated plastic slip in the crystal plasticity model is a measure of the dislocation density that is used as the driving force for the crack propagation. The combined crystal plasticity and crack propagation law is implemented in a model of a microstructure of duplex stainless steel (DSS). In order to illustrate the model capabilities, we conclude the paper by showing results for the short crack propagation in grains with different hardening characteristica and slip directions.

Crystal plasticity framework

The applied model is based on crystal plasticity and is thoroughly discussed in, e.g. Asaro [10], Miehe et al. [11] and Ekh et al. [12]. Here we shall only summarize the main ideas. The model is based on the classical multiplicative split of the deformation gradient $\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p$. The kinematic assumption is that the plastic deformation gradient $\mathbf{F}^p$ describes the plastic slip along the slip-systems, whereas the elastic deformation gradient $\mathbf{F}^e$ describes the crystal lattice distortion. The plastic slip on a slip-system ($\mathbf{s}_\alpha, \mathbf{m}_\alpha$) is driven by the the resolved shear (or Schmid) stress τ^α, which is calculated as

$$\tau_\alpha \overset{def}{=} \mathbf{s}_\alpha \cdot \boldsymbol{\tau} \cdot \mathbf{m}_\alpha \tag{2}$$

where $\boldsymbol{\tau}$ is the Kirchhoff stress tensor, and ($\mathbf{s}_\alpha, \mathbf{m}_\alpha$) define the slip-direction and slip-plane normal, respectively, in the slip-system. Hence, the yield function on each slip-system can be defined as

$$\varphi_\alpha = \tau_\alpha - (Y_\alpha + \kappa_\alpha) \tag{3}$$

where κ_α is the drag-stress corresponding to latent hardening, and Y_α is the initial yield stress.

Further, from the principle of maximum dissipation, the plastic velocity gradient (describing the evolution of the plastic deformation gradient) becomes

$$[\dot{\mathbf{F}}^{\mathrm{p}}] \cdot \mathbf{f}^{\mathrm{p}} = \sum_\alpha \dot{\mu}_\alpha ((\mathbf{s}_\alpha \cdot [\mathbf{F}^{\mathrm{e}}]^{-\mathrm{T}}) \otimes ([\mathbf{F}^{\mathrm{e}}]^{\mathrm{T}} \cdot \mathbf{m}_\alpha)), \qquad \mathbf{f}^p = [\mathbf{F}^p]^{-1} \tag{4}$$

Regarding the evolution for the hardening κ_α, we adopt the model proposed by Chang and Asaro [13]. This model takes cross-hardening effects into account.

Short crack propagation model

A new crack propagation model is developed in the spirit of the ND-model. A grain structure with both ferritic and austenitic grains is generated through Voronoi polygonization, Lillbacka et al. [14] (for a description of the algorithm c.f. Cannmo [15]). It is discretized using CST-triangles as illustrated in Figure 1.

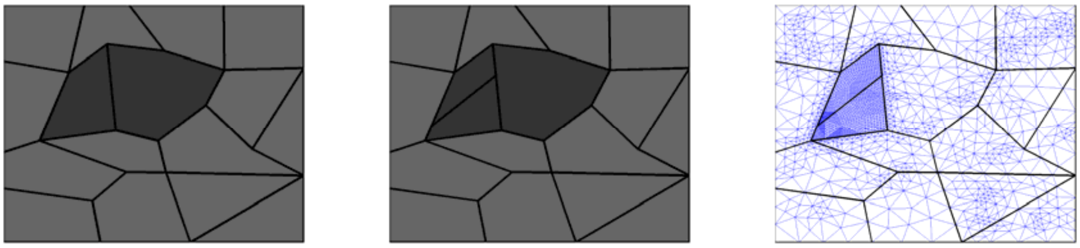

Figure 1. From left to right: initial grain structure with 16 grains (14 ferritic grains (light grey) and 2 austenitic grains (dark grey)) obtained from Voronoi polygonization, grain structure with predefined crack path and a FE- discretized grain structure.

In the numerical examples we will predefine a crack propagation direction (that coincides with a slip plane) inside an austenitic grain of the grain structure, see Figure 1. We will also assume that the crack will initiate at the left grain boundary and then propagate through the centre of that grain in the predefined direction. In order to accomplish crack growth in the FE simulations, double nodes are inserted along the crack path, and a penalty formulation is used to control the crack opening and closure.

In the crystal plasticity model the amount of accumulated plastic slip (μ_α) is calculated in the chosen slip directions. It is possible to obtain a measure of the relative plastic displacement (between two slip planes) in the slip direction as

$$\phi_\alpha = b\tan(\mu_\alpha) \approx b\mu_\alpha \tag{5}$$

where b is the magnitude of a Burgers vector. The mean value of the plastic displacement along the specific slip direction between the crack tip at $x = a$ and the tip of the slip line at $x = c$ is obtained through integration

$$\bar{\phi}_\alpha = \frac{b}{c-a}\int_a^c \mu_\alpha(x)dx \tag{6}$$

This measure is then used together with Eq. (1) to define the crack propagation law.

Numerical examples

In the numerical examples plane strain is assumed, and the twenty-four slip systems in the ferrite and austenite grains are reduced to planar double and triple slip systems, respectively, c.f. McDowell et al [16]. In the case of hardening, the actual material parameter values from calibration of a duplex stainless steel were used. Moreover, one of the slip systems is aligned with the crack direction, thus allowing for the calculation of the plastic displacement along the crack path from Eq. (6). The loading on the microstructure is a prescribed cyclic uniaxial strain ε in the range $0 \le \varepsilon \le 0.25\%$ along the vertical axis, leading to an almost elastic (macroscopic) response.

A parameter study was conducted with respect to the choice of the crack angle and the influence of hardening. These results are shown in Figures 2 and 3. The crack growth is comparatively high when the crack starts to propagate from a grain boundary while it is decelerated as it approaches the next grain boundary, *c.f.* right Figure 2. The crack angle 45 degrees results in higher shear stress (due to the applied loading) and, thus, higher crack growth rate than does 40 degrees. Comparing the crack growth rate vs. crack length with the same type of curves for the ND-model e.g. Navarro and de Los Rios [1, 5, 6], we note that the growth rate is not as smooth in our model as in the ND-model. This is an effect of the fact that we really calculate a fluctuating plastic displacement, whereas in the ND case this is assumed to be constant across the grain. As to the influence of hardening, the obvious result that reducing hardening promotes crack growth was confirmed.

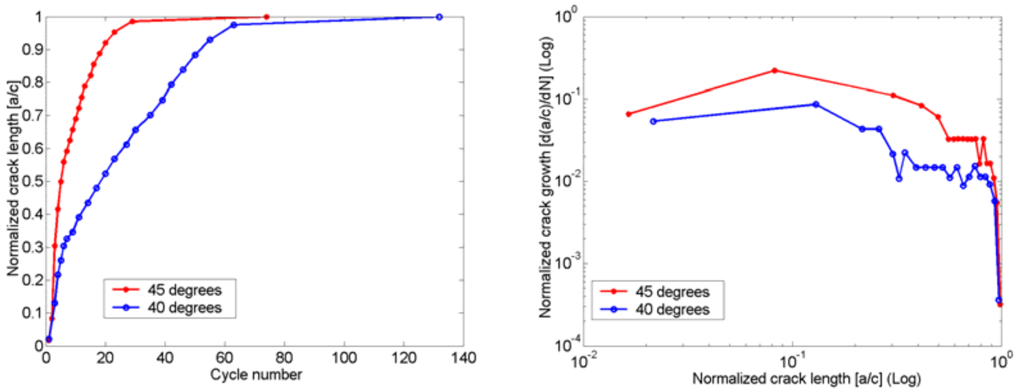

Figure 2. Left figure shows normalized crack length vs cycle number for a crack that is inclined 40 and 45 degrees against the horizontal axes. Right figure shows normalized crack growth vs normalized crack length for the same cases.

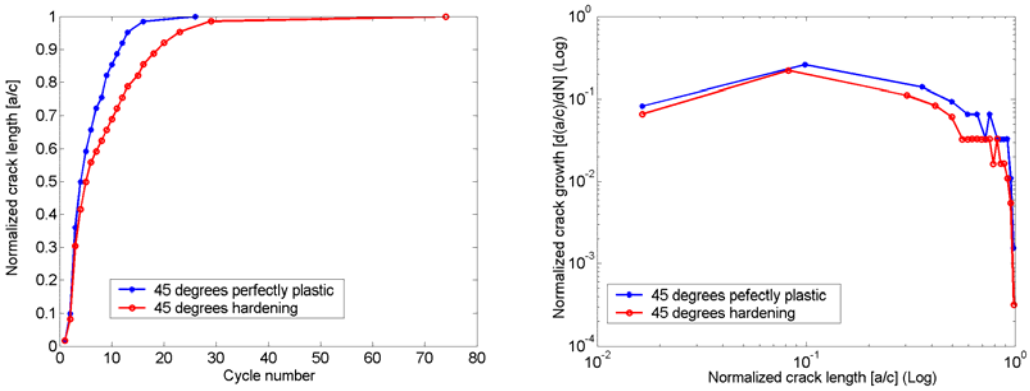

Figure 3. Left figure shows normalized crack length vs cycle number for a crack with 45 degrees alignment against the horizontal axes for perfectly plastic and hardening material behavior. Right figure shows normalized crack growth vs normalized crack length for the same cases.

Furthermore, the crack extension and effective plastic slip field, which is the “driving force” behind the crack propagation law are shown in Figure 4.

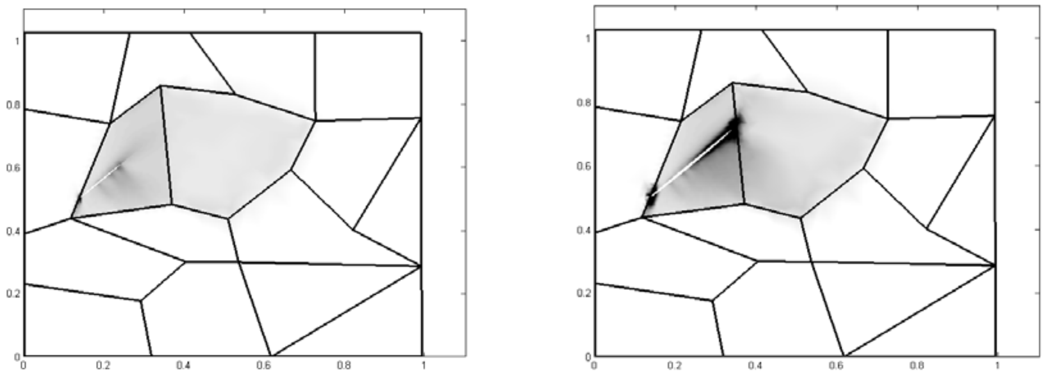

Figure 4. Crack growth through the first grain in the grain structure for a 45 degree crack with hardening. Crack and effective plastic slip field after the fifth and the final cycle from left to right (dark areas indicate high levels of plastic slip).

Conclusions and outlook

In this paper we have exploited the ND-model in the context of crystal plasticity in order to predict the propagation of short cracks in a grain of a polycrystalline material. Preliminary FE simulations have shown that (for constant load amplitude) the propagation rate decreases as the crack approaches the next grain boundary.

Future developments would have to include provision for the crack to extend to the neighbouring grains with a new direction determined by the appropriate crystallography. Moreover, a restriction of the present approach is that Dirichlet boundary conditions are applied to the microstructure. Hence, the crack can never extend to the boundary of the microstructure. To circumvent this drawback, other types of variational settings may be utilized.

Acknowledgements

Part of the support for this work was provided by Sandvik Materials Technology which is gratefully acknowledged.

References

1. Navarro, A. and de los Rios, E.R., *Fatigue Fract. Engng Mater. Struct.*, Vol. **10**, 169-186, 1987.

2. Suresh, S., *Fatigue of materials,* Cambridge University Press, Cambridge, 2001.

3. Miller, K.J., *Fatigue Fract. Engng Mater. Struct.,* Vol. **16**, 931-939, 1993.

4. Pippan, R., *Acta metall. mater,* Vol. **39**, 255-262, 1991.

5. Navarro, A. and de los Rios, E.R., *Fatigue Fract. Engng Mater. Struct.,* Vol. **11**, 383-396, 1988.

6. Navarro, A. and de los Rios, E.R., *Phil. Mag.,* **A57**, 15-36, 1988.

7. de los Rios, E.R. and Navarro, A., *Proc. R. Soc. (London),* **A272,** 304, 1963.

8. James, M.N. and de los Rios, E.R., *Fatigue Fract. Engng Mater. Struct.*, Vol. **19**, 413-426, 1996

9. Wei, L.W., de los Rios, E.R. and James, M.N., *Int. J. Fatigue*, Vol. **24**, 963-975, 2002.

10. Asaro, R., *Adv. Appl. Mech.*, Vol. **23**, 1-115, 1983.

11. Miehe, C., Schröder, J., and Schotte, J., *Comput. Methods Appl. Mech. Engrg*., Vol. **171**, 387-418, 1999

12. Ekh, M., Lillbacka, R., and Runesson, K., *Int. J. Plast*, Accepted, 2002.

13. Chang, Y.W., and Asaro, R.J., *Acta Metall*, Vol. **29**, 241-257, 1981

14. Lillbacka, R., Ekh, M., Johnson, E. and Runesson, K., *In Proceedings of Fatigue 2003*, edited by M.R. Bache, P.A. Blackmore, J. Draper, J.H. Edwards, P. Roberts and J.R. Yates, Engineering Integrity Society, Cambridge, 2003, 475-484.

15. Cannmo, P., *PhD thesis*, Chalmers University of Technology, 1997

16. Morrissey, R., Goh, C. and McDowell, D.L., *Mech. of Mat*., Vol. **35,** 295-311, 2003