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14. ABSTRACT

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Final Report for AFRL NO F49620-01-1-0116, Mesoscopic Measurement and Modeling of Slip Transfer Across Boundaries in Anisotropic Metallic Systems

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Abstract

An integrated experimental and theoretical approach to measure and model deformation transfer and microcrack initiation at grain boundaries is being developed. Electron channeling contrast imaging (ECCI) was used to directly image deformation defects associated with strain transfer and/or crack nucleation at grain boundaries. ECCI observations were correlated with mesoscale crystallographic texture information measured by selected area channeling patterns (SACPs), electron backscattered diffraction (EBSD) and x-ray texture measurements. To interpret and model these observed grain boundary deformation and strain accommodation phenomena, a nonlinear variational model of plastic deformation in a bicrystal that couples bulk grain deformation with compatibility enforced at the grain boundary was partially developed.

Research Objectives

The broad objective of this research program is to measure and model the process of deformation transfer at crystal boundaries in anisotropic materials, with a view towards predicting optimal microstructures to enhance materials for Air Force applications. A multidisciplinary group of scientists is: 1) experimentally measuring and quantitatively characterizing dislocation and twin structures at boundaries in polycrystalline metals, 2) determining how crystal/boundary misorientations affect deformation transfer across boundaries, microcrack initiation, and hence, ductility, and 3) developing quantitative 3-dimensional models that describe these deformation processes.

Experimental Approach

The experimental research objectives were pursued using polycrystalline equiaxed near gamma TiAl as a model material. Defect generation and deformation at crystalline boundaries was examined using Electron Channeling Contrast Imaging (ECCI), which allows imaging of defect structures in bulk samples using an FEG-SEM and channeling/diffraction contrast [Simkin, 1999]. Two loading conditions were used. Microcrack *nucleation* was examined at a statistically significant number of grain boundaries under a known global state of stress on the tensile surface of *ex-situ* deformed 4-point bend specimens. Crack *propagation* and re-nucleation was studied using notched 4-point bend specimens deformed *in-situ*. Observations were correlated with the grain-to-grain misorientations and mesoscale microtexture determined using electron back scattered diffraction (EBSD) and selected area channeling patterns (SACPs), allowing determination of the true **c** and **a** directions in the tetragonal TiAl structure. Observations of cracked and intact boundaries were analyzed for all available true twinning and ordinary dislocation systems (neglecting superdislocations) in grains on either side of the boundary, using the Schmid factor, the Burgers vectors, and the stress axis, to obtain a fracture initiation parameter that can be used in computational codes to predict damage nucleation.

Summary of Results

This is the final report for work conducted from 12/14/00 to 12/13/03, with a no cost extension to 8/13/04. During this time, two Ph.D. degrees were earned by B. A. Simkin (2003) and B.C. Ng (Ng will defend his dissertation in early 2005). An additional graduate student, Y. Wang, received support but changed projects. In addition, visiting scholars K. Boyapati and Prof. A. Fallahi were supported to conduct research on this project, and an M.S. graduate student, D. Kumar, was supported to finish analytical work that followed from Simkin's dissertation. In addition to the $375,000 grant from AFOSR, this project had $114,621 in matching funds provided by the MSU Composite Materials and Structures Center.

Brief descriptions of major accomplishments are provided using individual researcher's activities as a focus. Progress reports were provided in July of 2001, 2002, and 2003, and copies of oral presentation power point files presented in August contractors meetings have been provided earlier. A powerpoint file describing progress through October 2004 was submitted on October 21, 2004.

1. Development of a parameter for predicting the propensity for grain boundary microcrack nucleation (B.A. Simkin, A. Fallahi, D. Kumar)

Using the experimental paradigm we developed in this program, we characterized deformation mechanism interactions with grain boundaries. In particular, we found that microcracks nucleate at many boundaries where deformation twins interact with grain boundaries (Figure 1). Close examination revealed that the microcracks can be attributed to specific twins (see dashed arrows). In the example given below, there are two twin systems operating in the upper grain, and one in the lower grain.

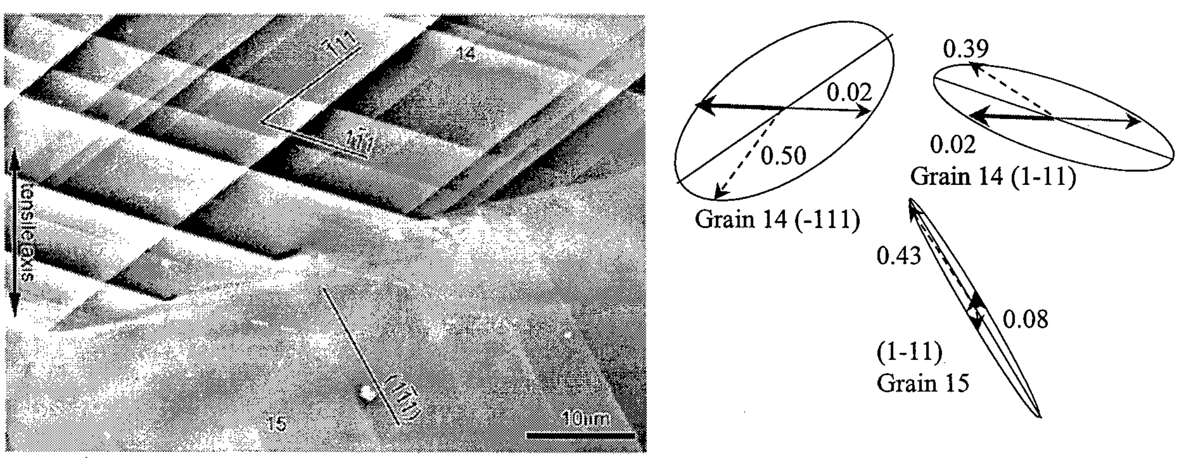

Figure 1: ECCI image of multiply fractured γ-γ grain boundary; arrows show microcracks. The traces of {111} twin planes are indicated for each grain. Ellipses represent unit circles on slip planes, with the major axis representing the plane trace evident on the micrograph. Arrows represent unit vector directions for ordinary dislocation slip (red) or twins (dashed black). Bold arrows have a component out of the plane of the page.

Using trace analysis based on SACP, it is possible to determine the active twinning planes in the grains on either side of a boundary (Figure 1), because the orientation of the grains are known with respect to the macroscopic tensile stress on the surface of the *ex-situ* deformed bend samples. Since there is only 1 twinning direction on each twin plane in TiAl, it is then possible to completely identify the twin systems involved in the microcrack nucleation. The Schmid factors of all of the possible twinning and dislocation slip systems for each grain were determined, along with the true sense of shear for the observed deformation twins (the twinning is unidirectional). The slip plane inclination is shown with the ellipses (see explanation in caption).

Though the Schmid factors are moderately high for all three of the twinning systems identified, the microcracks are associated with the twinning system on the (1-11) plane in grain 14, which has the lowest Schmid factor of the three. However, this is the only twinning system of the three that has a sense of shear that moves mass away from the boundary and causes an opening Mode I type stress on the surface at the grain boundary. This tensile mode I effect on the boundary accounts for nearly every microcrack studied. In every other boundary, the microcracks are associated with the twinning system that has the highest Schmid factor (Figure 1, where the twinning system associated with the microcracks it is the third highest Schmid factor is the only exception). Thus microcrack nucleation is most likely to occur on boundaries that have highly active twinning systems that move mass away from the boundary ***and*** have a high Schmid factor, i.e. a high probability of being active, and hence thicker than other twins, making the sense of grain boundary strain highest.

In a recent TEM study, Gibson and Forwood [2002] found that twin impingement on grain boundaried in γ TiAl is accommodated by ordinary dislocation motion on both sides of the boundary. Based on this observation, Simkin developed a mechanistically based parameter for predicting the propensity for microcrack nucleation, $F_{\max}$, where this factor is the maximum value of the 8 possible values of the parameter F given below (one for each of the 4 possible twin systems on each side of the grain boundary):

$$F = m_{\mathrm{tw}} \left|\hat{\mathbf{b}}_{\mathrm{tw}} \cdot \hat{\mathbf{t}}\right| \sum_{\mathrm{ord}} \left|\hat{\mathbf{b}}_{\mathrm{tw}} \cdot \hat{\mathbf{b}}_{\mathrm{ord}}\right|$$

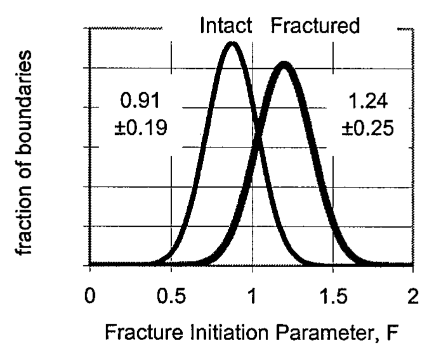

Figure 2: Populations of intact and fractured boundaries

In this factor m_{tw} is the Schmid factor for a specific deformation twinning system under the global stress state, the $\hat{\mathbf{b}}_i$ are unit vectors in the sample coordinate system that describe the Burgers' vector directions for the each twin system *tw* and all 8 of the ordinary dislocation systems in each pair of grains, *ord*.

The rationale behind this parameter is a product of probabilities, i.e. F identifies conditions where slip transfer is highly likely; F is large when twinning is highly likely (large m_{tw}), when the direction of $\hat{\mathbf{b}}_{tw}$ has a significant degree of alignment with the tensile axis such that a mode I opening force is generated in the boundary, and when the twinning vector is reasonably aligned with ordinary dislocation slip directions that can accommodate the twin shear in either grain, i.e. $\cos\kappa = \hat{\mathbf{b}}_{\mathrm{tw}} \cdot \hat{\mathbf{b}}_{\mathrm{ord}}$ as illustrated in Figure 3. This parameter was evaluated to find the maximum value of $F_{\max}$ for each boundary 11 cracked and 11 intact boundarys with microstructurally similar geometric characteristics. The values of $F_{\max}$ for the the two populations were examined using the student t-test, showing that the two populations are statistically distinct with probability > 99.5%, represented schematically in Figure 2 (assuming normal distributions). The fact that fractured boundaries are correlated with a high degree of slip transfer is ascribed to leaving residual slip vectors in the boundary plane that increases boundary strain energy.

Since F consists of parameters that can be evaluated in plasticity based models of microstructures, this result suggests that $F_{\max}$ may predict the propensity of a boundary to develop microcracks and hence provide a mechanistic way to predict damage nucleation in computation models. However, in the form given above, the factor does not take in to account the orientation of the grain bounday relative to the tensile axis, both of which would be exected to play a role in microcrack nucleation. This improvement can be expressed by components that maximize mode I opening components, where $\hat{\mathbf{n}}$ is the grain boundary normal.

$$F_n = m_{\mathrm{tw}} \left|\hat{\mathbf{b}}_{\mathrm{tw}} \cdot \hat{\mathbf{n}}\right| \left|\hat{\mathbf{t}} \cdot \hat{\mathbf{n}}\right| \sum_{\mathrm{ord}} \left|\hat{\mathbf{b}}_{\mathrm{tw}} \cdot \hat{\mathbf{b}}_{\mathrm{ord}}\right|$$

This parameter was evaluated using information obtained from serial sectioning to obtain grain boundary inclinations by Fallahi and Kumar. However, knowing the grain boundary inclination has did not improve the ability of F to separate the boundary populations, which was surprising; this result is examined in more detail in a paper in preparation (Fallahi et. al).

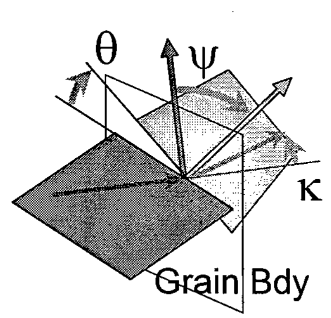

Figure 3 – geometry of strain transfer at grain boundary.

Deepak Kumar has further explored a large number of variations of the fracture initiation parameter to examine what combination of factors can best separate the cracked and intact grain boundary populations. He examined how misalignment of slip planes affects the propensity for slip transfer which was not considered in prior models. Ashmawi and Zikry used a parameter to quantify this misalignment, that can be expressed as, $\cos\theta = \hat{\mathbf{n}}_{tr,tw} \cdot \hat{\mathbf{n}}_{tr,ord}$, the degree that the traces of the slip planes of ordinary dislocations are aligned with the trace of the twin plane on the boundary plane which has been used as and additional accomodation factor as follows, and this version of F has been the most successful in distinguishing between fractured and intact boundaries. This result is described further in a paper by Kumar et al., that is in preparation.

$$F_{2\max} = \max(m_{tw} \,|\, \hat{\mathbf{b}}_{tw} \cdot \hat{\mathbf{t}} \,|\, \sum_{ord} |\, \hat{\mathbf{b}}_{tw} \cdot \hat{\mathbf{b}}_{\ ord} | \sum_{ord} |\, \hat{\mathbf{n}}_{tr,tw} \cdot \hat{\mathbf{n}}_{tr,ord} \,|)$$

Elastic anisotropy also plays an important role on the stress in a grain boundary region. This was examined in symbolic triple junctions using the known three dimensional stiffness ($\mathbf{C}_{ijkl}$) in each grain, as illustrated in Figure 4. So far, we have estimated $\hat{\mathbf{t}}$ as uniaxial tension, but the traction acting on the boundary is likely to be somewhat different from the global stress state. To find the local stress tensor at a boundary

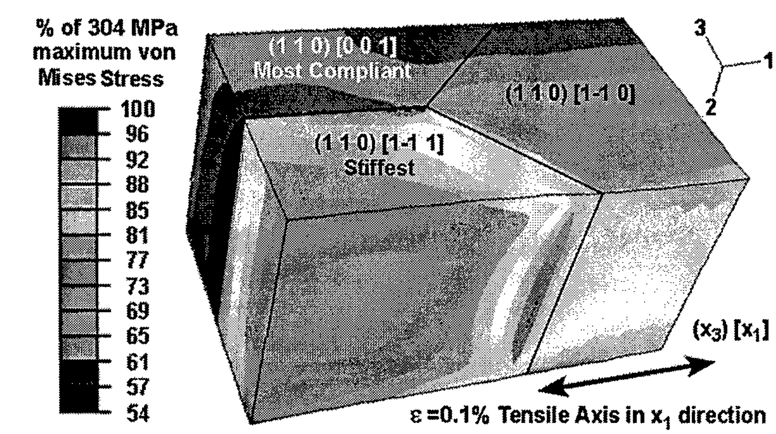

Figure 4 Full 3-D elastic anisotropic finite element analysis of von Mises stress distribution in a TiAl tri-crystal, (calculation provided by A. Zamiri and F. Pourboghrat)

requires elasto-plastic modeling of actual microstructures, which is beyond the scope of this program. With knowledge of the local traction, we expect the distribution depicted in Figure 2 to be narrower.

2. Prediction of crack path using a fracture propagation parameter (Ng)

Ng adapted the ideas introduced by Simkin to develop a crack propagation parameter. He identified cracked and intact boundaries in the notched 4-point bend specimen in Figure 5, where the initial crack propagated and arrested. In this study, the role of twinning as a deformation accommodation mechanism in grain B due to twinning deformation in grain A was examined, because crack growth involves strain gradients. This requires consideration of directionality, since slip transfer by twinning requires that the *absolute* direction of the twinning shear is not opposed to twinning in the neighboring grain. Directionality is also relevant to the process of crack propagation, because a crack approaching grain A before grain B will cause more deformation in grain A than B. Thus, slip transfer is more important from grain A to B than B to A. A crack propagation parameter can be expressed as

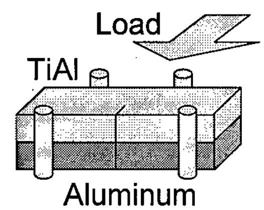

Figure 5 Notched crack growth specimen

$$F_{A\to B} = m_{Atw}\left|\hat{\mathbf{b}}_{Atw}\cdot\hat{\mathbf{t}}\right|\left(\sum_{Bord=1}^{2}\left|\hat{\mathbf{b}}_{Atw}\cdot\hat{\mathbf{b}}_{Bord}\right| + \sum_{Btw=1}^{4}\hat{\mathbf{b}}_{Atw}\cdot\hat{\mathbf{b}}_{Btw}\Big|_{if>0}\right)$$

The three parts of this parameter are explained: m_{Atw} is the maximum Schmid factor for a reference twin system in grain A; $\hat{\mathbf{b}}_{Atw}\cdot\hat{\mathbf{t}}$ identifies how well the reference twin Burgers vector is aligned with the tensile traction unit vector $\hat{\mathbf{t}}$ (for simplicity, in the direction of tensile loading); the two sums of the dot products in large parentheses describe how well the Burgers vector of this most highly stressed twin system in grain A is aligned with the Burgers vectors for ordinary dislocations and twins in grain B. Also, using a clever synthesis of EBSP and ECCI measurements, Ng was able to characterize crystal orientations for more than twice as many grain boundaries as Simkin. The histogram in Figure 6 shows that microcracking is unlikely when $F_{A\to B} < 1.0$, but is more likely when $F_{A\to B} > 1.0$. From a t-test analysis (using a non-pooled and unequal variance mean comparison, assuming the underlying populations are approximately normal), the mean value of $F_{A\to B}$ for the cracked population, μ_{ABc}, exceeded the intact population mean, μ_{ABi}, with 99.9% confidence. Thus, this parameter may be used to predict a path for crack propagation (i.e., grain boundaries with $F_{A\to B} > 1.0$ are prone to fracture while boundaries with lower values are not).

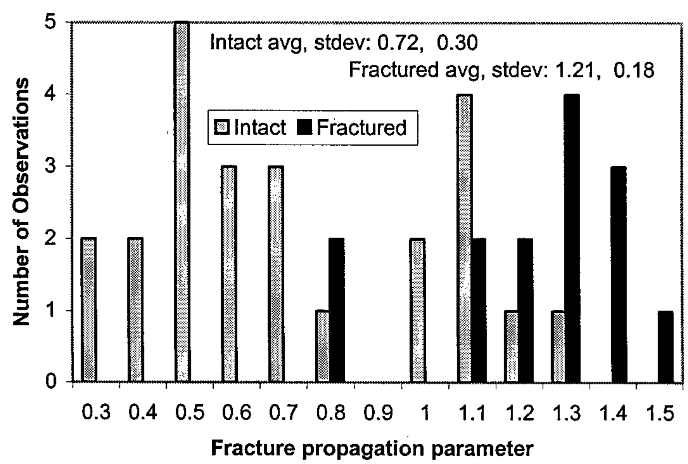

Figure 6 – Histogram of intact and cracked boundaries using $F_{A\text{-}B}$.

Figure 7 shows a comparison of the mapped microstructure ahead of the arrested crack with the specimen after the crack was grown with additional loading. Use of the $F_{A \to B}$ to identify strong and weak boundaries are indicated in Figure 7 with black lines for weak boundaries. The effectiveness of this parameter is illustrated by the fact that the crack path connected regions of weak boundaries. Also, intergranular cracking occurred in boundaries that did not have a Mode I opening force, but were weak. It is notable that strong boundaries prevented crack propagation and that an annealing twin boundary was oriented to be a weak boundary where the crack jogged parallel to the tensile axis. This shows that grain boundary character can also be defined in terms of its slip characteristics.

It is remarkable that grain boundary deformation character on the surface affects the fracture path as much as it does; suggesting that microcracking on the free surface may be more likely than beneath the surface (consistent with the geometry of twins that move mass away from the grain boundary identified above). Some 3-D Anisotropic elastic finite element simulations of deformed TiAl tri-crystals show the highest stress concentrations at boundaries on the surface.

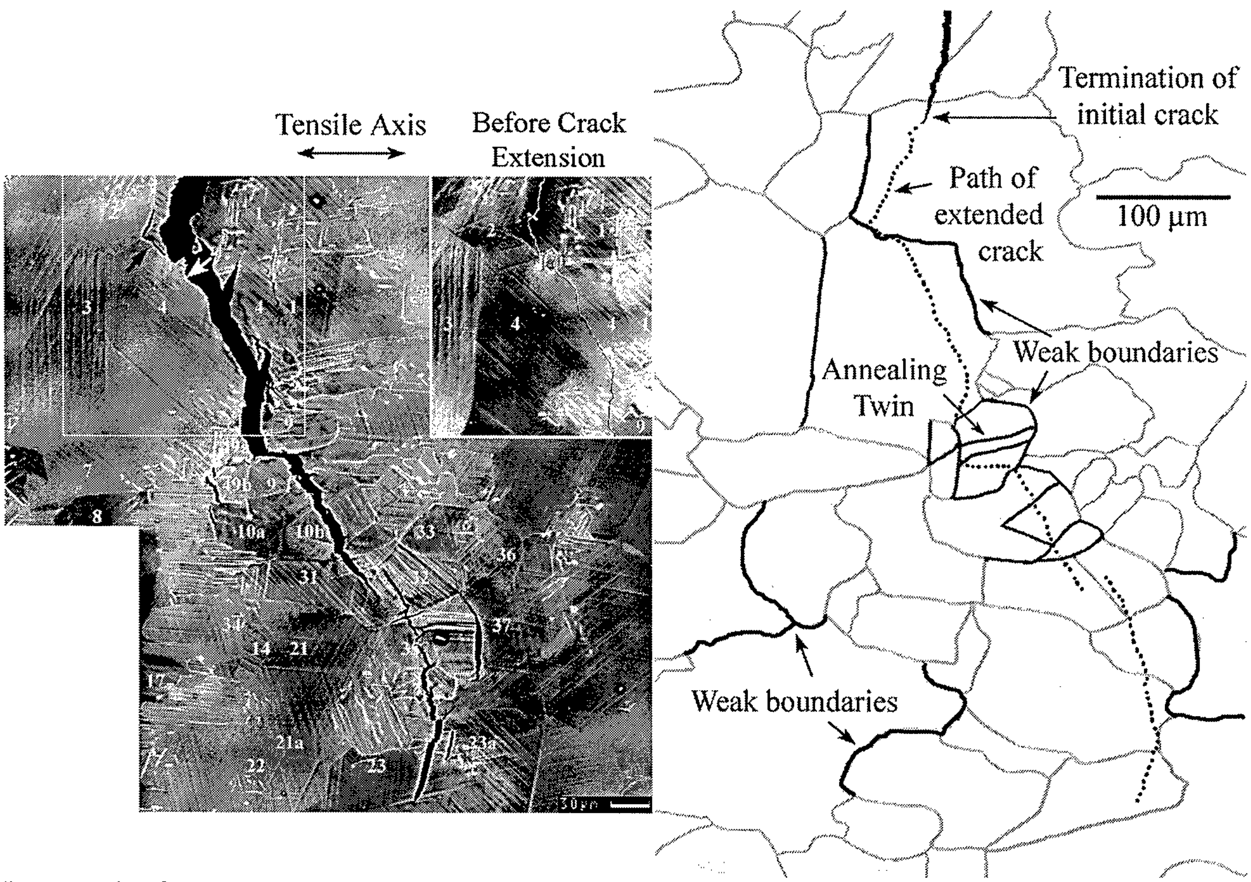

Figure 7 Crack propagation and map of microstructure ahead of initial crack tip. Bold lines represent weak boundaries, and dotted line represents actual crack path. Not all weak boundaries cracked, see Figure 6.

3. *Modeling of Slip Transfer in a Bi-Crystal (Mason)*

Darren Mason's contributions to this effort have been important, though less visible. His time available for this effort was affected by his moving to Albion College during the course of this project. Much of the analytical work needed to accomplish the tasks described above were made possible by Darren's development of software that accelerated microscopic analysis. In addition to this practical contribution, he also developed a foundation for modeling slip based grain boundary deformation in the form of a variational model. No further progress occurred in this effort since Summer 2003, and the state of this model development is repeated from the 2003 progress report:

To begin, we summarize briefly the kinematical/kinetic structure of this problem. Let $\Omega^{(j)}$, $j = A, B$ correspond to two bounded regular three-dimensional regions with piecewise smooth boundaries that represent the reference configuration of each grain in the bi-crystal. The deformation of each grain is modeled by a smooth mapping $\mathbf{y}^{(j)}$ so that the domain occupied by the deformed grain is $\omega^{(j)} = \mathbf{y}^{(j)}(\Omega^{(j)})$. The material is endowed with a Helmholtz bulk free energy $\psi := \psi(\mathbf{F}^{(j)}, \gamma^{(j)})$ as well as an interfacial energy density $\chi(\mathbf{H}, \mu)$ representing an energetic contribution resulting from lattice incoherence / distortion at the grain boundary. Here $\gamma^{(j)}$ and μ correspond to vectors of internal variables and $\mathbf{H}=[\mathbf{F}^{(2)}]^{-1}\,[\mathbf{F}^{(1)}]$ denotes the relative deformation gradient evaluated at the grain boundary (*cf.* [Cermelli, Kinderlehrer]).

Within this framework, given a deformation history $\mathbf{F}^{(j)}(t)$ at a fixed material point, we require that the defect state $\gamma^{(j)}(t)$ in the material evolve along a path of minimal work W, where

$$W = \int_{t}^{t_2} \frac{\partial \psi}{\partial \mathbf{F}} \cdot \dot{\mathbf{F}}\, dt + \int_{t_1}^{t_2} \frac{\partial \chi}{\partial \mathbf{H}} \cdot \dot{\mathbf{H}}\, dt.$$

Integration by parts at any material point yields

$$W^j = \psi^j \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{\partial \psi^j}{\partial \boldsymbol{\gamma}} \cdot \dot{\boldsymbol{\gamma}}\, dt + \chi \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{\partial \chi}{\partial \boldsymbol{\mu}} \cdot \dot{\boldsymbol{\mu}}\, dt$$

so that calculation of $\delta W = 0$ at a point *away* from the grain boundary for variations is equivalent to that found in [Ortiz].

On the other hand, consideration of points *on* the grain boundary requires more care. One approach is to consider the framework outlined in Figure 8. Here, $B^j(h)$ represents the pre-image of a neighborhood of the boundary point in reference grain j. The energy associated with that point then becomes

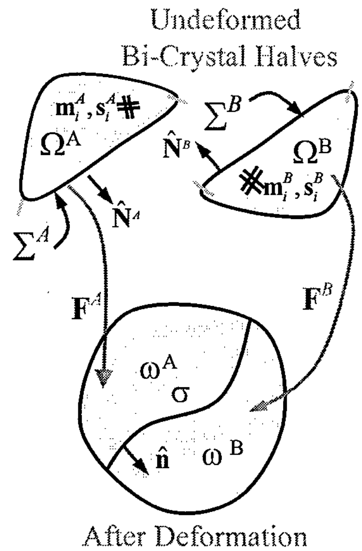

Figure 8. Schematic image of reference and deformed bi-crystal configuration for grain boundary model framework.

$$\begin{aligned} W^j &= \lim_{h\to 0}\left[\sum_{j=A,B} \frac{1}{\left|B^j(h)\right|_3} \int_{B^j(h)} \int_{t_1}^{t_2} \frac{\partial \psi^j}{\partial \mathbf{F}} \cdot \dot{\mathbf{F}}\, dt\, dV + \frac{1}{\left|B^A(h)\cap \Sigma^A\right|_3} \int_{B^j(h)} \int_{t_1}^{t_2} \frac{\partial \chi^j}{\partial \mathbf{H}} \cdot \dot{\mathbf{H}}\, dt\, dV \right] \\ &= \delta W_\psi + \delta W_\chi \end{aligned}$$

Variational analysis of this energetic expression for *compatible* deformations of the grains yields the equilibrium equation

$$\begin{aligned} \delta W &= \delta W_\psi + \delta W_\chi = 0 = \\ &= \sum_{j=A,B} \int_{t_1}^{t_2} \frac{\partial \psi^j}{\partial \mathbf{F}^j} \cdot \mathbf{G}^j \Bigg|_{t=t_2} + \int_{t_1}^{t_2} \sum_{j=A,B} \left[\frac{d}{dt}\left(\frac{\partial \psi^j}{\partial \boldsymbol{\gamma}^j} \right) \cdot \boldsymbol{\xi}^j \right] - \left(\frac{\partial^2 \psi^j}{\partial \mathbf{F}^j \partial \boldsymbol{\gamma}^j} \cdot \mathbf{G}^j + \frac{\partial^2 \psi^j}{\partial \boldsymbol{\gamma}^{j2}} \cdot \boldsymbol{\xi}^j \right) \cdot \dot{\boldsymbol{\gamma}}^j dt \\ &+ \sum_{j=A,B} \int_{t_1}^{t_2} \frac{\partial \psi^j}{\partial \mathbf{H}^j} \cdot \delta \mathbf{H} \Bigg|_{t=t_2} + \int_{t_1}^{t_2} \left[\frac{d}{dt}\left(\frac{\partial \chi}{\partial \boldsymbol{\mu}} \right) \cdot \boldsymbol{\kappa} \right] - \left(\frac{\partial^2 \chi}{\partial \mathbf{H} \partial \boldsymbol{\mu}} \cdot (\mathbf{F}^{B-1}\mathbf{G}^A - \mathbf{F}^B \mathbf{G}^B \mathbf{H}) + \frac{\partial^2 \chi}{\partial \boldsymbol{\mu}^2} \cdot \boldsymbol{\kappa} \right) \cdot \dot{\boldsymbol{\mu}}\, dt \end{aligned}$$

where $\mathrm{G}^{\,j}$, ξ^j, and κ respectively represent arbitrary admissible variations of the grain deformation gradient, bulk and grain boundary internal variables.

The experimental determination of a fracture initiation parameter described above suggests that boundaries that are not good at transferring slip are less likely to crack. This physical result is highly compatible with the variational modeling approach, where the deformation necessary to maintain the boundary compatibility must be accomplished by deformation within the grain and not across the grain boundary. When this variational model is embedded within a homogeneous surrounding medium deforming under the influence of the boundary conditions, the local stresses and strains in the boundary region near each grain can be evaluated accurately. This model will generate strains near the boundary that will differ from the grain interior, as observed in microscopy. Since the boundary in the variational model has an energy associated with it, it will be possible to investigate and incorporate fracture energy criteria that lead to separation. Thus, this variational model has the potential to provide a physically and microstructurally based damage initiation condition that can be incorporated into a larger scale continuum damage mechanics FEM computation. With this stage of development, practical tools for design of materials for critical applications will be available to enhance the Air Force's ability to introduce advanced materials with confidence.

Summary

Our investigation of microcrack nucleation has resulted in identification of a class of fracture initiation parameters that are based upon slip activity in adjacent grains. This parameter can be used to identify conditions for damage nucleation in computational micromechanical models. Thus, we have identified a slip based definition of grain boundary character that is capable of predicting damage nucleation and the crack propagation path that is based upon the physics of micromechanical deformation.

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Kris Boyapati	Visiting Scholar
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Benjamin A. Simkin, *Tensile Crack Initiation in γ-TiAl*, 2003, (advisor, M.A. Crimp)
Boon-Chai Ng, *Crack Propagation Prediction in γ-TiAl*, 2005, (advisor, T.R. Bieler)

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B.-C. Ng, . T.R. Bieler, M.A. Crimp, D.E. Mason, "Prediction of Crack Path Based on Grain Boundary Misorientation and Stress in a Near-gamma TiAl Alloy", Jounal to be determined.

B.C. Ng, T.R. Bieler, M.A. Crimp, D.E. Mason, "Combining SACP and EBSP diffraction methods to obtain crystal orientations in TiAl alloys", to be submitted to *Ultramicroscopy.*

D. Kumar, T.R. Bieler, M.A. Crimp, "A Slip Based Definition of Grain Boundary Character", to be submitted to *Acta mater.*

B.A. Simkin, B.C. Ng, M.A. Crimp, T.R. Bieler "Crack Opening Due to Deformation Twin Shear at Grain Boundaries in Near-γ TiAl" to be submitted to *Scripta Mater.*

A. Fallahi, D. Kumar, T.R. Bieler, M.A. Crimp, D.E. Mason, "The effect of grain boundary normal on fracture initiation parameters for duplex TiAl", manuscript in preparation for *Mater. Sci. and Engr.*

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