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TRIPLE JUNCTION NANOCRACKS IN FATIGUED NANOCRYSTALLINE MATERIALS

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Abstract. A theoretical model is suggested which describes the nucleation and growth of nanocracks (nanoscale cracks) near tips of pre-existent extended cracks in fatigued nanocrystalline materials. In the framework of the model, nanocracks in fatigued nanocrystalline materials nucleate at triple junctions of grain boundaries. The enhanced nucleation and growth of triple junction nanocracks are stimulated by preceding grain boundary sliding and driven by the release of the external stresses and the stresses created by triple junction dislocations and pre-existent fatigue cracks.

1. INTRODUCTION

Nanocrystalline materials exhibit the outstanding mechanical properties that represent the subject of intense fundamental and applied research; see, e.g. [1-5]. For instance, nanocrystalline materials under quasistatic mechanical loading are characterized by very high strength and hardness being several times larger than those of coarse-grained polycrystalline materials with the same chemical composition [1-3]. The unique deformation behavior of nanocrystalline materials under quasistatic loading serves as a basis for the expectations that such materials can show good fatigue characteristics. However, there are large technical difficulties in making fatigue experiments with nanocrystalline materials having very fine grains. The progress in this area has been reached very recently. Hanlon *et al.* [6] and Pao *et al.* [7,8] have reported fatigue characteristics of nanocrystalline materials (produced by electrodeposition and cryomilling methods, respectively) with the mean grain size being in the range from 20 to 40 nm. Following experimental data [6], nanocrystalline materials are characterized by high values of the fatigue endurance limit compared to coarse-grained polycrystalline materials. At the same time, the growth rate of a pre-existent fatigue crack in nanocrystalline materials is several times higher than that in coarse-grained polycrystalline materials [6-8]. In other words, the grain refinement in the nanocrystalline regime hampers fatigue crack initiation, but enhances fatigue crack growth. The former effect is highly desirable for applications of nanocrystalline materials under low amplitudes of cyclic stresses. However, a low resistance of nanocrystalline materials to fatigue crack growth essentially limits their practical utility. In this context, it is very important to understand the mechanisms for fatigue crack growth in the nanocrystalline matter where the nanoscale and interface effects are capable of causing the specific features of fatigue crack propagation. The main aim of this paper is to suggest a theoretical model describing the enhanced generation of nanocracks at triple junctions of grain boundaries near fatigue crack tips in nanocrystalline materials with very small grains. In

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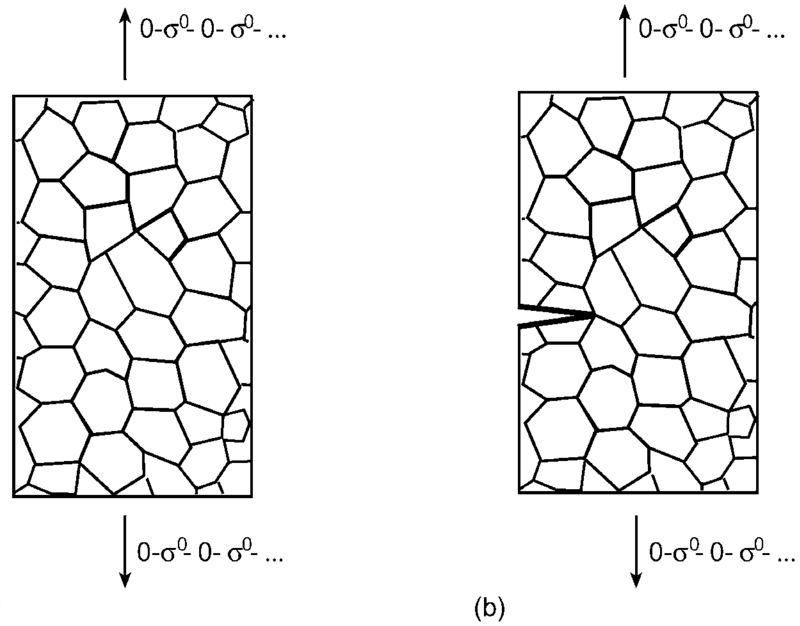

Fig. 1. Nanocrystalline specimen (a) without and (b) with pre-existent fatigue crack under zero-tension-zero fatigue load.

doing so, grain boundary sliding is considered to be the deformation mode crucially contributing to plastic flow in fatigued nanocrystalline materials. The model qualitatively explains experimental data [6-8] on a low resistance to the fatigue crack growth in nanocrystalline materials.

2. NANOCRACKS AT TRIPLE JUNCTIONS OF GRAIN BOUNDARIES IN NANOCRYSTALLINE MATERIALS. MODEL

Following current representations on plastic flow in nanocrystalline materials with very fine grains [1-5,9-20], their unique deformation behavior is caused by both suppression of conventional lattice dislocation slip and effective action of alternative deformation mechanisms. These alternative mechanisms are conducted by grain boundaries and include grain boundary sliding [9-12], grain boundary diffusional creep [13-15], triple junction diffusional creep [16] and rotational deformation [17-19] (for a review, see [5,20]). In addition, twin deformation mediated by partial dislocations emitted by grain boundaries has been experimentally observed in nanocrystalline materials [21-24]. In the context discussed, in our theoretical analysis of the fatigue behavior of nanocrystalline materials with very fine grains, we should take into account the active role of grain boundaries in plastic deformation and failure processes.

Let us consider a nanocrystalline sample under one-axis zero-tension-zero fatigue load with the maximum tensile stress σ^0 (Fig. 1a). Following [9-12], we assume that grain boundary sliding crucially contributes to plastic flow of nanocrystalline materials with fine grains. In doing so, as with quasistatic deformation [12], grain boundary sliding in nanocrystalline specimen under fatigue loading gives rise to the formation of sessile dislocations at triple junctions of grain boundaries. These triple junction dislocations provide the strengthening of nanocrystalline materials [12] and, at the same time, serve as 'dangerous' stress sources capable of inducing nanocrack nucleation in vicinities of triple junctions [25].

In the situation where the local stresses created by a triple junction dislocation play the dominant role in the nanocrack nucleation, the nanocrack is characterized by a sole equilibrium length l_{e2} [25]. (Its definition [26] is as follows: the growth of the nanocrack is energetically favorable until its length reaches l_{e2}, whereas the nanocrack growth at $l>l_{e2}$ is energetically unfavorable.) The situation with the dominant role of the triple junction dislocation stresses in the nanocrack generation has been theoretically examined in paper [25]. Here we will focus our consideration on the situation where a macroscale fatigue crack exists (Fig. 1b) which pro-

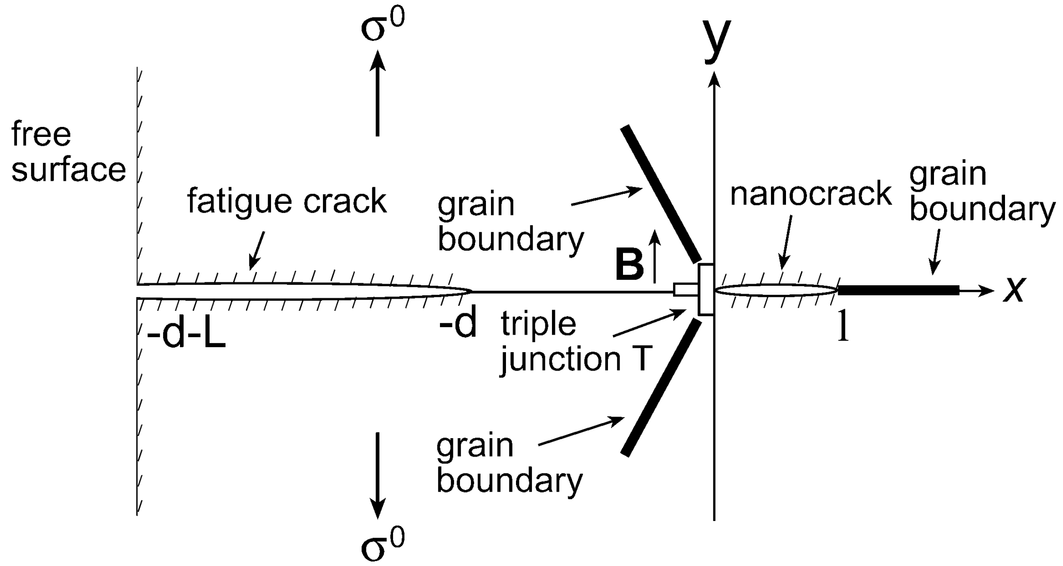

Fig. 2. Nucleation of nanocrack at dislocated triple junction in front of fatigue crack tip.

vides the external stress concentration strongly influencing the nanocrack generation in vicinities of triple junctions. In this situation, the combined action of the dislocation stresses, the external stresses and the fatigue crack stresses play an important role in inducing the nucleation and growth of a triple junction nanocrack. Notice that the role of the external fatigue load is maximum when the external tensile stress reaches its maximum value σ^0. Therefore, for simplicity, we will focus our further consideration on the nanocrack nucleation and growth at the tensile stress σ^0. In doing so, the fatigue character of the external load is indirectly taken into account in the Burgers vector magnitude *B* that characterizes the triple junction dislocation and evolves (increases) with rising the number of load cycles.

In general, the existence of the external stress modifies the previously revealed [25] conditions for the nanocrack nucleation and growth. More precisely, with the external stress taken into account, besides the equilibrium length l_{e2}, another equilibrium length l_{e1} ($l_{e1}>l_{e2}$) of the triple junction nanocrack comes into play. In doing so, the nanocrack growth is energetically favorable in the following ranges of the nanocrack length l: $l<l_{e2}$ or $l>l_{e1}$. In the situation discussed, the triple junction dislocation is able not only to provide the nanocrack growth until the length $l=l_{e2}$ but also to enhance the thermal-fluctuation-assisted growth of the nanocrack from its length $l=l_{e2}$ to its length $l=l_{e1}$. More than that, as it will be demonstrated below, a triple junction dislocation with a large Burgers vector is capable of causing the energetically favorable generation and growth of a nanocrack of any length along a grain boundary. In terms of the equilibrium lengths, it is the case of $l_{e1}=l_{e2}$.

In the situation where a macroscopic fatigue crack is located near a dislocated triple junction, the external stress concentration at the tip of the fatigue crack can essentially enhance the nanocrack nucleation and growth at the triple junction. This effect of a fatigue crack reduces the critical level of the external stress at which the growth of a nanocrack with a specified length occurs near the triple junction. In the next section, we will examine this effect in more detail.

3. GENERATION AND GROWTH OF TRIPLE JUNCTION NANOCRACK IN VICINITY OF FATIGUE CRACK TIP

Let us consider a flat fatigue crack with the length *L* and the plane being perpendicular to the tension axis (Figs. 1b and 2). Also, let us consider a dislocated triple junction T distant by *d* from the fatigue crack tip (Fig. 2). The triple junction dislocation is characterized by the Burgers vector ***B*** oriented as shown in Fig. 2. The combined action of the dislocation stresses, the fatigue crack stresses and the external stress causes the nanocrack nucleation. In the coordinate system shown in Fig. 2, the nanocrack is located in the plane y=0 and has the x-coordinate in the range: $-L-d<x<-d$. The triple junction dislocation is located at the line x=y=0.

Let us calculate the conditions at which the nanocrack growth is energetically favorable. In doing so, for simplicity, we assume that one of grain boundaries adjacent to the triple junction is located in the plane y=0 at x>0. In this case, the nanocrack growth along this boundary plane is most favorable (compared to other directions of nanocrack growth). In order to calculate the equilibrium lengths, l_{e1} and l_{e2}, that characterize the nanocrack, we will use the configurational force method [26] effectively exploited in analysis of the generation of plane cracks in the stress field of superdislocations [25,26], dislocation pile-ups [26], disclination loops [27], lamellar terminations in eutectics [28] and wedge line disclinations [29]. Following [26], the configurational force F is defined as the elastic energy released when the crack moves over a unit distance. In the situation with the plane strain state of an elastically isotropic solid, examined in this paper, F can be written in its general form as follows [26]:

$$F = \frac{\pi(1-\nu)l}{4G}\left(\bar{\sigma}_{yy}^2 + \bar{\sigma}_{xy}^2\right), \tag{1}$$

where G is the shear modulus, ν is the Poisson ratio, and $\bar{\sigma}_{yy}$ and $\bar{\sigma}_{xy}$ are the mean weighted values of the stress tensor components σ_{yy} and σ_{xy}, respectively. These mean weighted stress tensor components are calculated using the following formula [26]:

$$\bar{\sigma}_{my} = \frac{2}{\pi L}\int_0^l \sigma_{my}(x, y=0)\sqrt{\frac{x}{l-x}}dx,\quad m = x, y. \tag{2}$$

The equilibrium length l_e of the nanocrack is derived from the balance $F=2\gamma_e$ between the release F of the elastic energy and the formation of two new nanocrack surfaces characterized by the surface energy γ_e per unit area. This energy is given as: $\gamma_e = \gamma - \gamma_b/2$, where γ_b is the surface energy per unit area of the free surface, and γ_b is the energy of the grain boundary (per its unit area). The nucleation of the triple junction nanocrack (Fig. 2) is energetically favorable, if $F>2\gamma_e$, and unfavorable, if $F<2\gamma_e$.

Let us calculate the stress tensor components, σ_{yy} and σ_{xy}, figuring in formula (2). In general, the component σ_{ii} can be written as follows:

$$\sigma_{ij} = \sigma_{ij}^0 + \sigma_{ij}^d + \sigma_{ij}^c. \tag{3}$$

Here $\sigma_{ij}^0=\sigma^0\delta_{ij}$ denotes the external stress, σ_{ij}^d the stress created by the triple junction dislocation, and σ_{ij}^c the stress created by the fatigue crack. The stresses σ_{my}^d (x,y=0) are given in the following form [30]: σ_{xy} (x,y=0)=0, σ_{yy}(x,y=0)=$GB/[2\pi(1-\nu)x]$. In order to estimate the stresses created by the fatigue crack, we assume that $|\sigma_{yy}(x=-\sigma, y=0)| << \sigma_0$, that is, $d >> GB/[2\pi(1-\nu)]\sigma_0$,]. In this situation, the elastic interaction between the triple junction dislocation and the fatigue crack is negligibly small. Also we suppose that $d+l << L$. This allows us to describe the stress σ_{ij}^c as being given by asymptotic expressions [30] for the stress field of a fatigue crack in vicinity of its tip. In these circumstances, we have: $\sigma_{xy}^c(x,y=0)=0$, and $\sigma_{yy}(x,y=0)=(1/2)\sigma^0\sqrt{L/(d+x)}$.

Thus, the expressions for the stresses $\sigma_{my}(x,y=0)$ are as follows:

$$\sigma_{xy}(x, y=0),$$
$$\sigma_{yy}(x, y=0) = \sigma^0 + \frac{GB}{2\pi(1-\nu)x} + \frac{\sigma^0}{2}\sqrt{\frac{l}{d+x}}. \tag{4}$$

With (4) substituted into formula (2), we find:

$$\bar{\sigma}_{xy} = 0,\quad \bar{\sigma}_{yy} = \sigma_e + \frac{GB}{\pi(1-\nu)l}. \tag{5}$$

In formula (5), $\sigma_e=\sigma^0(1+\sqrt{L/(4d)})$ is the effective stress taking into account the external stress concentration at the fatigue crack. When the fatigue crack is absent (L=0), $\sigma_e=\sigma^0$. Thus, in analysis of nanocrack growth, the effect of the fatigue crack is equivalent to the increase of the external stress by the factor $1+\sqrt{L/(4d)}$.

4. CRITERION FOR THE ENERGETICALLY FAVORABLE GROWTH OF TRIPLE JUNCTION NANOCRACK

With formulas (1) and (5) substituted into the inequality $F>2\gamma_e$, we find the criterion for the energetically favorable growth of the triple junction nanocrack. More precisely, if $\sigma_e B>2\gamma_e$, the

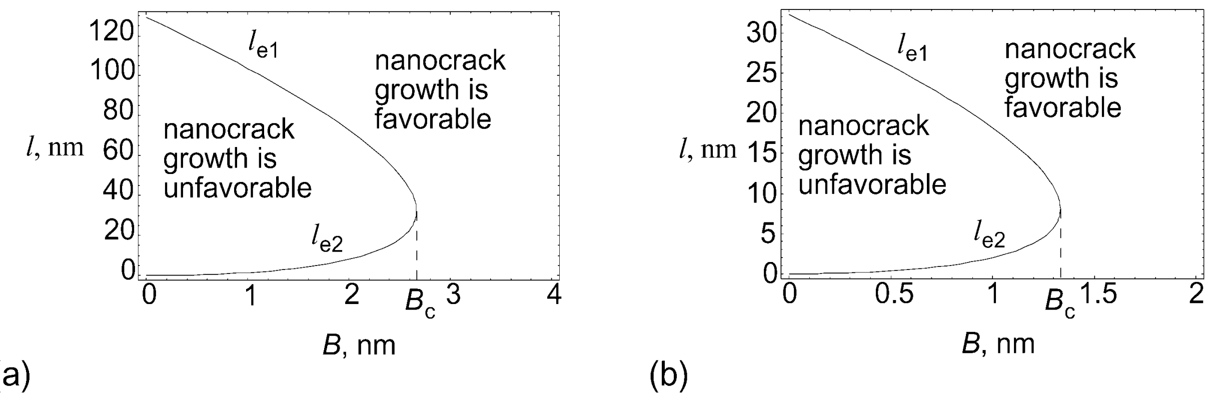

Fig. 3. Dependences of equilibrium lengths l_{e1} and l_{e2} on Burgers vector magnitude B of triple junction dislocation, for G=40 GPa, σ^0=0.75 GPa, γ_e=1 J/m^2 and ν=0.3, in the cases where (a) fatigue crack is absent and (b) fatigue crack with length L=4d is present.

nanocrack growth is energetically favorable in the following range of the nanocrack length l: $l > l_{e1}$ or $l_e < l_{e2}$. Here the equilibrium lengths l_{e1} and l_{e2} are given as:

$$l_{e1,2} = \frac{G}{2\pi(1-\nu)} \frac{4\gamma_e \sigma_e B \pm \sqrt{8\gamma_e (2\gamma_e - \sigma_e B)}}{\sigma_e^2}. \quad (6)$$

The dependences of l_{e1} and l_{e2} on the Burgers vector magnitude B (that characterizes the triple junction dislocation) are shown in Fig. 3, for G=40 GPa, σ^0=0.75 GPa, γ_e=1 J/m^2 and ν=0.3, in the cases where (a) the fatigue crack is absent, and (b) the fatigue crack with the length L=4d is present. As follows from Fig. 3, l_{e1} decreases, and l_{e2} grows with rising B. As a corollary, when B increases, the difference l_{e1}-l_{e2} decreases and becomes equal to zero ($l_{e1}=l_{e2}$) at some critical value $B_c=2\gamma_e/\sigma_e$ of the Burgers vector magnitude. With further increase of B ($B>B_c$), the nanocrack growth is energetically favorable at any length l_e of the nanocrack. Comparison of the dependences shown in Fig. 3a and 3b allows us to conclude that the pre-existent fatigue crack essentially enhances the nanocrack generation in vicinity of its tip.

5. CONCLUDING REMARKS

In this paper, it has been theoretically revealed that the nucleation of nanocracks in fatigued nanocrystalline materials can effectively occur at triple junctions of grain boundaries (Fig. 2). The nanocrack nucleation and growth are driven by both the release of the elastic energy associated with the storage of dislocations at triple junctions and the action of the external stress and the pre-existent fatigue crack. Following our theoretical analysis, in the situation where the Burgers vector magnitude B of the triple junction dislocation is not large ($B<B_c$), the growth of a triple junction nanocrack is energetically favorable, if the nanocrack length l is in the following range: $l < l_{e2}$ or $l > l_{e1}$. When B is large ($B>B_c$), the growth of the triple junction nanocrack of any length is energetically favorable. The existence of the initial fatigue crack (Figs. 1b and 2) in a nanocrystalline specimen enhances the nucleation and growth of triple junction nanocracks in vicinity of the fatigue crack tip. The effect of the pre-existent fatigue crack on the nucleation of triple junction nanocracks (distant by d from the fatigue crack tip) is equivalent to the increase of the external stress by the factor $1+\sqrt{L/(4d)}$, where L is the fatigue crack length. As illustrated by the dependences $l_{e1}(B)$ and $l_{e2}(B)$ presented in Fig. 3, the pre-existent fatigue crack essentially enhances the nanocrack nucleation and growth in vicinity of its tip. As a consequence, the further growth of the fatigue crack is enhanced through its convergence with triple junction nanocracks generated in vicinity of the fatigue crack tip. This effect qualitatively explains experimental data [6-8] on enhanced growth of fatigue cracks in nanocrystalline materials, compared to that in their coarse-grained counterparts, because nanocrystalline materials contain high-density ensembles of triple junctions playing the role of nanocrack nucleation centers.

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