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A phase transformation based method to predict fatigue crack nucleation and propagation in metals and alloys

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This paper is dedicated to the memory of Professor Morris E. Fine of the Materials Science and Engineering Department of Northwestern University.

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ABSTRACT

The fatigue failure of metallic materials contains of dislocations, lattice defects accumulation and interactions. Fatigue is a dynamically changing process of the Gibbs free energy, and the change of defects in the materials could be considered to be a generalized form of phase transformation. In the current work, phase transformation theory has been applied to predict fatigue crack nucleation and propagation. An updated fatigue crack nucleation model based on phase transformation theory and micromechanics is developed and compared with experiments. The proposed approach is also extended for predicting fatigue crack propagation in metallic materials. A new energy parameter is proposed and its relationship with the stress intensity factor is studied. The predicted fatigue crack propagation rates are compared with experimental data for different metallic materials, and the results show that the proposed model can predict fatigue crack nucleation and propagation with reasonable accuracy.

1. Introduction

In the past decades, the fatigue crack nucleation and propagation behavior under various fatigue loading [1–6] has been extensively studied. The method used to predict fatigue crack nucleation cycles and propagation rate is not by just using the stress intensity factor but more focused on the physics of the fatigue process. Although many energy-based models [5–10] to predict the fatigue behavior of metals have been proposed, the energy parameters are usually required to be determined numerically. Most of the proposed models used in industry are based on traditional statistical or semi-empirical methods [11–14], and the physical mechanisms behind fatigue damage still requires further research. The main cause of fatigue crack nucleation process of metallic materials are the accumulation and reaction of dislocations and crystal defects: for example, the singular stress field around the crack tip of polycrystalline titanium alloys will change the crystal structure in the local region.

Phase transformations in fatigue are defined as a dissipation process where the internal energy of the solid dynamically changes under cycle loading [4,15,16]. Corresponding to the change of lattice defects structure, fatigue crack nucleation and propagation process can also be regarded as phase transformations process. In fatigue crack nucleation process, Mura [17] showed that fatigue crack nucleation is a process to break through an energy barrier. The energy barrier reflects not only the energy required creating a new surface [18], but also the release of elastic energy into the solid material [17,18] and the energy loss from lattice defects near the crack tip. Fine and Bhat [20,21] utilized phase transformation theory to analyze the nucleation of single crystal iron and compared the result with experiments. Although a model to predict the crack nucleate was proposed, the parameters in the equations were difficult to determine and hardly measurable in the experiments.

Based on Fine and co-worker's work, an energy dynamic equilibrium method to predict crack propagation rate was developed [16]. Fatigue damage is regarded as a phase transformation process and the internal energy in system changes dynamically under cycle loading. In addition to the traditional metals, the phase transformation based theory was also used to study the fatigue behavior of solder alloys [22–24]. Although the predictions agreed well with

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experiments, the dimensionless constant in the model is a statistical parameter and requires a clear physical meaning. In addition, the traditional phase transformation theory did not appear to be applicable to some materials, such as titanium alloys [25].

In the current research, the traditional phase transformation method is improved by combining thermodynamics with fracture mechanics. In the crack nucleation phase, the dislocation movement is considered to predict the cycle numbers to nucleate a crack. In the crack propagation phase, thermodynamics is combined with fracture mechanics to establish the dynamic energy balance equation for crack propagation. A new energy parameter is proposed to consider the physical mechanism of crack propagation. Numerical analysis shows that the proposed parameter is associated with the stress intensity factor. The newly developed parameter has straightforward physical significance and is adapted in phase transformation framework to predict the rate of crack propagation.

2. Generalized phase transformation theory to predict fatigue crack nucleation

For most steel alloys, fatigue cracks usually nucleate in the persistent slip bands at low strain cycling or in the grain boundaries at high strain cycling [20]. The fatigue crack nucleation process can be regarded as the generalized phase transformation, since an energy barrier (energy required to create a new surface) must be overcome. When cracks nucleate, the accumulated lattice defects and the elastic strain energy from the applied load are released. Therefore, as soon as the change of Gibbs free energy ΔW reaches a critical value, the fatigue crack nucleates spontaneously [4]. When a crack of area A is formed, ΔW can be expressed as:

$$\Delta W = -\delta A - \Delta W(e) + \gamma_T A \tag{1}$$

where δA is energy loss of the defect when new surfaces form, A is the virtual crack area, $\Delta W(e)$ is the elastic strain energy release when crack nucleate and γ_T is the total surface energy.

Although hysteresis loop area represents the mechanical energy spent pre cycle, most of the energy are dissipated as heat, and only a small part of the energy store in the structure. Therefore, the energy released by crystal defects are given according to hysteresis parameters [21]:

$$\frac{\mathbf{d}\delta}{\mathbf{d}N} = ft\Delta\sigma\Delta\varepsilon_p \tag{2}$$

where $\mathbf{d}\delta/\mathbf{d}N$ is the energy released by defects per cycle; f is a hysteresis factor and could be a constant for specific test conditions [21]. Here, t stands for the general thicknesses of crack each side when the crack forms, $\Delta\sigma\Delta\varepsilon_p$ represents the stress scope and plastic strain scope during one cycle.

Based on Mura's theory [17], the released elastic energy when a penny-shaped crack form can be expressed as:

$$\Delta W(e) = \frac{8(1-\upsilon^2)\sigma^2 a^3}{3E} \tag{3}$$

where υ is Poisson's ratio; E is elasticity modulus; σ is the maximum stress in one cycle; a is penny-shaped crack radius.

Under cyclic loading, dislocation dipoles that move at the persistent slip bands are accumulated at the grain boundary or surface of the specimen. As the loading cycle increases, the accumulated dislocation dipoles will amplify the back stress, which can cause instability of the system energy. As shown in Fig. 1, the experiment of a representative steel X2CrNiMoN22-5-3 reveals the dislocation dipoles accumulate at the grain boundary with fatigue cycles and lead to the crack initiation [26]. The accumulated dislocation dipoles can be regarded as a microcrack and expressed as:

$$a = Nb\rho_{\mathbf{e}} \tag{4}$$

where N is the cycle number; b is Burger vector magnitude; $\rho_{\mathbf{e}}$ is accumulated number of dislocations per cycle and can be expressed as [19]:

$$\rho_{\mathbf{e}} = (\Delta\sigma - 2k)l/2B \tag{5}$$

where k is the dislocation friction stress; l is the grain size; B is a material constant and can be written as: $B = Gb/2\pi(1-\upsilon)$.

Based on Eq. (1)–(4):

$$\Delta W = -ft\pi N^3 b^2 \rho_e^2 \Delta\sigma\Delta\varepsilon_p - \frac{8(1-\upsilon^2)\sigma^2 b^3 N^3 \rho_e^3}{3E} + \gamma_T \pi b^2 N^2 \rho_e^2 \tag{6}$$

When a crack nucleates, the Gibbs free energy reaches an extremum value. Differentiating $\mathbf{\Delta}W$ with fatigue cycle N yields the crack nucleation condition. The crack nucleation number N^* can then be obtained:

$$N^* = \frac{2\gamma_T \pi E}{3ft\pi E\Delta\sigma\Delta\varepsilon_p + 8(1-\upsilon^2)\sigma^2 b\rho_{\mathbf{e}}} \tag{7}$$

Because Eq. (6) is a cubic function of N, to ensure that the Gibbs free energy is the maximum value when a crack nucleates, the additional condition should be satisfied: $\partial^2\Delta W/\partial N^2 < 0$, which gives:

$$N > \frac{\gamma_T \pi E}{3ft\pi E\Delta\sigma\Delta\varepsilon_p + 8(1-\upsilon^2)\sigma^2 b\rho_{\mathbf{e}}} \tag{8}$$

It is noted that Eq. (7) satisfies Eq. (8), which means the system achieves the maximum energy when a crack nucleates. By substituting Eq. (7) into Eq. (4), the fatigue crack nucleation cycle number and the critical length of the crack radius can be obtained. According to Eq. (7), crack nucleation is influenced by experimental parameters (stress and inelastic strain range); material properties (elasticity modulus and Poisson's ratio); and material structure properties (grain size and internal friction). The proposed approach improves the model developed by Fine and Bhat [21], where the influence of microstructure is considered, and the parameters in Eq. (7) have clear physical meaning that can be obtained from experiments.

From Eq. (4) and Eq. (7), the critical radius when the crack nucleates can be obtained:

$$a^* = \frac{2\gamma_T \rho_e \pi b E}{3ft\pi E\Delta\sigma\Delta\varepsilon_p + 8(1-\upsilon^2)\sigma^2 b\rho_e}$$

where a^* is the radius when Gibbs free energy reaches the maximum value.

The fatigue crack nucleation process has a probabilistic nature, where the random distribution of crystal defects cause the nucleation site and the length of nucleated crack could be flexible. The nucleation area is typically not an exact round shape, the hypothesis of a regular shape is adopted to facilitate the calculation. The nucleated area obtained by using a^* ($A^* = \pi a^{*2}$) is the critical area when the Gibbs free energy reaches its maximum value.

Five groups of steel experimental data (Fe-3%Si, A 336 GR5, A 387 GR22, 15HM, A 10) are adopted [27–29] to verify the proposed