Micro-mechanism on the Metal Materials with the Fatigue Propagation

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Abstract. Low stress failure due to fatigue is one of the most common and common forms of component failure. Especially for aerospace and Aeronautical products, the system structure is complex, the environmental conditions are complex, the application of new technologies and materials is significant, and the investment of a single product is high. Therefore, the abnormal low stress damage of individual structures often causes catastrophic losses. In practice, most of the components with defects are not easy to find because of the stress damage caused by the continuous crack growth under fatigue load. Therefore, the study of fatigue crack and growth rate has great practical significance. In this paper, the general law and microscopic mechanism of crack growth of metal structural materials under normal temperature and transverse fatigue load are studied.

1. Introduction

When metal materials are subjected to fatigue alternating load stress, they will show cracking and other phenomenon, at the same time, metal materials will be deformed from plastic to brittle zone directly. At present, according to, metal materialsfatigue in the engineering industry can be divided into the following categories the external environmental conditions: high-cycle fatigue [1-3], low-cycle fatigue [4], Thermal fatigue [5], corrosion fatigue [6], Contact fatigue [7]. High cycle fatigue denote fatigue with a stress cycle of more than 100,000 weeks under low stress conditions (as we all known the Working stress is usually sated by under the yield limit of the materials, or even below the elastic limit). Low cycle fatigue refers to fatigue with a stress cycle of less than 10,000 to 100,000 weeks under high stress (the working stress is close to the yield limit of the material) or high strain conditions. The main mechanism of fatigue under this cycle load is the plastic strain. Thermal fatigue refers to the repeated effects of thermal stress due to temperature changes, resulting in fatigue damage. Corrosion fatigue refers to the fatigue damage caused by machine parts under the joint action of alternating loads and corrosive media (such as acids, bases, seawater, active gases, etc.) Contact fatigue refers to the contact surface of the machine parts in the repeated action of contact stress, the hemp point peeling or the surface crushing and peeling occurs, resulting in the failure and destruction of the machine parts.

The study on the metal materials' influence mechanism directly converted from plastic zone to brittle material under fatigue loading has also become the focus of attention in recent years. Among them, plasticity refers to the ability of metal materials to produce plastic deformation (permanent deformation) under loading. The plasticity of the polycrystalline material will be improved with the decrease of the grain. In addition, due to the inverse ratio of the grain boundary diffusion creep rate to the cubic size of the grain size, especially during the expansion of the high cyclic fatigue crack, due to the expansion of the grain boundary. The change in creep deformation rate, this leads to an increase in

the rate of crack propagation. In addition, the dislocation movement of the grain boundary is also the reason for the change of the crack propagation rate.

In addition, due to the particularity of the interaction between the twin interface and dislocation, the common lattice boundary also has a special contribution to the strength and plasticity of the material compared to the ordinary bighorn crystal boundary. For example, nano-twinning copper containing high-density growth twins exhibits high tensile strength and good plasticity at the same time. This is mainly due to: On the one hand, the twinning interface [8] Can be as effective as the bighorn crystal boundary to block dislocation through, improve the strength; On the other hand, the twinning interface itself, as a sliding surface, also allows dislocation to slip on it, thereby increasing plasticity. Under cyclic loading conditions, the twin interface also shows different characteristics from the ordinary bighorn crystal boundary. The stress concentration of elastic Anisotropy on both sides of the twin interface makes it easy to start fatigue crack under high cycle fatigue load. Under the low cycle fatigue load, fatigue cracking is more difficult to occur in the larger angular crystal boundary of the twin interface. The understanding of resistance to low cycle fatigue cracking at the higher interface of twin crystal is still unclear. Shenyang Materials Science National (Joint) Laboratory[9-11] the low cycle fatigue cracking behavior of twin interface in face-centered cubic metal was systematically studied by Zhefeng Zhang researcher group of material fatigue and fracture research department. The previous study found that with the reduction of the fault energy of the alloy layer, the tendency of fatigue crack initiation at the twin interface increased. Recently, they also studied the effects of crystal orientation, layer error energy, and slip patterns on the fatigue cracking behavior of twin interfaces in Cu and Cu-Zn and Cu-Al alloys. The results show that under the same fatigue loading conditions, fatigue cracks in several alloy materials can be generated either along the slip zone or along the interface of the twin crystal. This shows that whether fatigue cracks are generated at the interface of the twin crystal depends not only on the external loading. And the material itself, and it is closely related to the specific load conditions of each grain.

In addition, the most commonly used method for the simulation analysis of the fatigue crack propagation process of metal materials is the molecular dynamics method, such as:

Based on studying the special crystallographic relationship between the interface of twinning crystal and the starting sliding system, the most common method for the study of the micro-influence mechanism of metal material in the process of fatigue crack propagation is to carry out the method of determining the grain orientation directly through the sliding morphology. To accurately describe the effect of grain orientation on the fatigue cracking behavior of the twinning crystal interface, the parameter Schmid factor difference($\Delta\Omega$) was introduced to describe the relationship between shear stress and dislocation density during plastic deformation. In addition, to accurately describe the number of dislocation of the product at the surface of the twin boundary due to stress incoordination on both sides of the twinning interface, combined with Schmid's law, the number of dislocation is determined to be

$$n_{\Delta\Omega} = \frac{L(\sigma-\sigma_0)}{KGb}\Delta\Omega \tag{1}$$

The critical stress required for dislocation operation is approximately equal to the yield strength. On the other hand, the extension dislocation needs to be clustered to a certain critical width (Rc) when passing through the twin interface, and the extension width of this dislocation is determined by the layer error energy. Therefore, according to the definition of layer fault energy and the property of dislocation plug product, the relationship between the number of dislocation product and layer fault energy at the twin interface can be determined:

$$n_{RSE} = \frac{M/R_c-\gamma}{\tau_0} \tag{2}$$

M is the repulsive force of two extended dislocations, and$\tau 0$ is the piston force provided by a fault in a stop-fault group.

In addition, can also according to the above about the crystal orientation and dislocations that can place dislocation of the twin boundary surface accumulation of objective influence, coupled with the dislocation slip way influence on twin boundary cracking, they established differential Schmid factor

(ΔΩ), fault (gamma), sliding way and the twin boundary surface cracking critical criterion semi-quantitative equation:

$$\Delta\Omega = \frac{KGb}{L(\sigma-\sigma_0)}\left(\frac{n_c}{\eta} - \frac{M/R_c-\gamma}{\tau_0}\right) \quad (3)$$

The nc for the twin boundary surface cracking need critical product number of dislocation, the approximate constant can be thought of a material, η to consider the parameters of the dislocation sliding way and introduce, K, G, b, M for material constant, and L, Rc, σ0andτ0 to a certain group of materials also haven't changed much. Boundary cracking zone facing the above analysis shows that the twin boundary is Δ Ω and piecewise linear equations of eta: with the change of the dislocation sliding mode (η), Δ Ω and gamma of the linear relationship between the slope will also change. Based on the above model, they use 6 kinds of alloy with different fault can (γ) material in the statistical analysis of a large number of Schmid factor poor relations with the twin boundary surface fatigue cracking or not experimental evidence, the results show that with the wrong alloy material layer can increase and the decrease of the twin boundary surface Schmid factor difference on both sides, twin boundary surface fatigue cracking is becoming more and more difficult, and with the dislocation slip way gradually by Cu wavy slip into Cu-16% et. Al plane slip, the influence of the two is more and more obvious, as shown in figure 1.

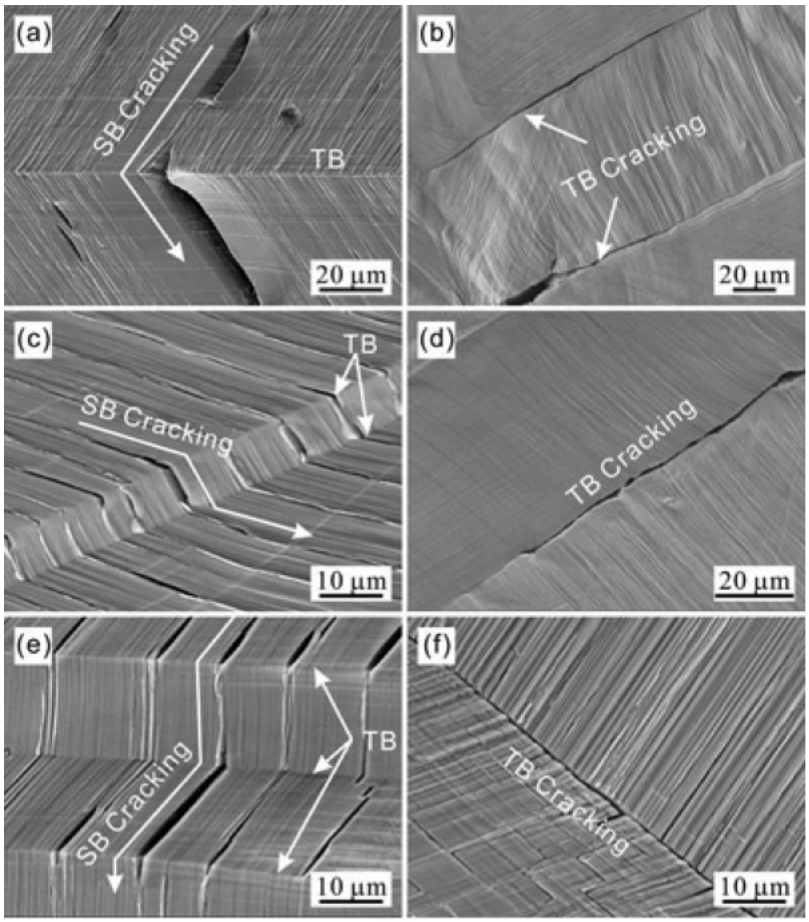

Fig.1 Slip Band Cracking and Twin Boundary Cracking Behavior of different materials Cu (a,b), Cu-10at. %Zn (c,d) &Cu-32at.%Zn (e,f)

2. Molecular Dynamics Simulation Method

Molecular dynamics method is a computer simulation experimental method. This technique can not only obtain the trajectory of atoms, but also observe various microscopic details of the process of

atomic motion. It is a powerful supplement to theoretical calculation and experiment. Because molecular dynamics research is not limited by sample preparation and testing techniques, it is helpful to understand the relationship between microstructure and properties of materials. It is widely used in material science, biophysics and drug design.

In 1957, some research firstly used molecular dynamics to study the equation of state of gas and liquid under the hard ball model, which set a precedent for studying the macroscopic properties of matter by molecular dynamics simulation. In 1972, the method and extended the non-equilibrium system with velocity gradient has been developed. Andersen et al. created the method of constant pressure molecular dynamics in 1980. Method to non-equilibrium systems with temperature gradient is developed. Andthus, forming a molecular dynamics method system for non-equilibrium systems. The creation of thermostatic molecular dynamics is developed. In 1985, the first principle molecular dynamics method, which organically combines electron theory with molecular dynamics method, was proposed for semiconductor and metal Car, etc., which are difficult to model potential function. In 1991, a molecular dynamics method of giant regular systems for the treatment of adsorption problems has been further proposed. In the late 1980s, the rapid development of computer technology, coupled with the proposal and development of multi-body potential function, is a further development of molecular dynamics simulation technology.

The particle motion of the treatment system in MD obeys Newton equation is that:

$$\vec{F_i}(t) = m_i \vec{a_i}(t)$$

In the formula, the force acting on particle $\vec{F_i}(t)$ is the mass of particle m_i and the acceleration of particle $\vec{a_i}(t)$. The force acting on particle $\vec{F_i}(t)$ is the first derivative of the potential energy function to the coordinates, that is, the mass of particle m_i and the acceleration of particle $\vec{a_i}(t)$.

$$\vec{F_i}(t) = -\frac{\partial u}{\partial r_i}$$

$$m_i \frac{\overrightarrow{\partial v_i}}{\partial t} = \vec{F} = -\frac{\partial U}{\overrightarrow{\partial r_i}} + \cdots \frac{\partial U}{\overrightarrow{\partial r_n}}$$

$$\vec{r}(t) = \vec{v}(t)$$

Generally, numerical solutions of these equations need to be carried out by numerical methods. These numerical solutions generate a series of positions and velocities of$\{x_n, v_n\}$, n represents a series of discrete times, $t = n\,\Delta t$, Δt represents the time step. To solve the equations, the initial coordinates and velocities of each particle must be given.

3. Conclusion

In this paper, the propagation process of preset micro cracks in alloys is simulated by molecular dynamics method, and the fatigue crack growth behavior of different synthetic materials is studied. According to the basic principle of molecular dynamics, the expression of interaction force between atoms is deduced, and the process of tension, shear and bending of single crystal copper is simulated by establishing molecular dynamics model. The experimental results show that the cracks affect the mechanical behavior of the strength and modulus of elasticity of single crystal copper plate.

4. Reference

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