The micro-structure and mechanical performance of Nickel-based single crystal alloy

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Abstract. Because of the increasing temperature in front of turbine in aero-engine field, Ni-base single crystal alloys are of high demand, which achieve high strength at high temperature. Therefore, a variety of methods have been developed to detect or describe nickel-base single crystal alloys. This article will take stock of the alloy valve and the mainstream description of valve methods. This paper will describe the basic micro-mechanism of rafting. Then the channel width method, which is the most widely used method to describe the degree of rafting, is introduced. After that, the updated version of the channel width method, the method to describe the rate of rafting and the effect on its strength, and the related methods of image processing are described. It is hoped that this paper can help readers to have a preliminary understanding of the principle and mathematical description method of nickel-base alloy rafting. There are many branches of mathematical description, but the main ideas are very similar. It is hoped that the researchers concerned will be able to develop some mathematical models that require fewer measurement parameters but not reducing the overall accuracy of the measuremen.

Keywords: nickel-based superalloys,single crystal,rafting,microstructure description.

1. Introduction

In today's aero-engine field, with the higher requirements for engine performance, the mechanical performance requirements for the components used in the manufacture of aircraft turbines, combustors, etc. , in particular, it needs to withstand the huge centrifugal force at high temperature. Therefore, metal materials with higher temperature resistance and better mechanical properties and service life are needed. At present, nickel-based alloys have undergone three generations of development, namely equiaxed crystals, directional crystals and single crystals. These three generations of materials in turn can improve the mechanical properties, creep resistance and fatigue resistance of the alloy. How to correlate rafting microstructure with mechanical properties becomes a frontier of materials science today. particularly important. In today's materials science world, it is important to use mathematical models to describe and calculate this change and become one of the frontiers of metallic materials.

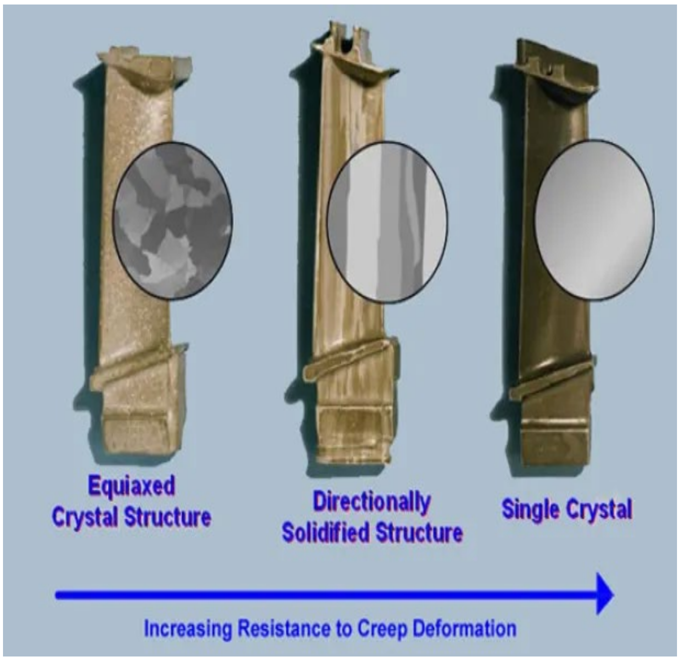

Fig. 1 The evolution of materials for turbine blades with increasing resistance to creep deformation.

Fig. left: The equiaxed crystals of the alloy are irregular in shape and have fine grains

Fig. middle: the directionally crystallized alloy, which allows the crystals to crystallize directionally

Fig. right: The single crystal alloy.

The basic microstructure of single crystal alloy is composed of two phases: matrix phase (γ phase) and precipitation phase (γ' phase) . γ phase is a face-centered cubic structure composed of nickel, chromium, molybdenum, etc., γ' phase is an ordered face-centered cubic structure composed of nickel, aluminum, titanium, etc. Under the action of high temperature and stress, a kind of microstructure evolution phenomenon called rafting occurs in single crystal alloys. Rafting refers to the transverse or longitudinal growth of γ' phase along the direction of stress, forming rod-like or plate-like structures, while γ-phase forms channels similar to water flow. Rafting phenomenon can affect the mechanical properties and life of single crystal alloy, which depends on the type, degree and direction of rafting. Generally speaking, lateral rafting will decrease the yield strength and creep properties of single crystal alloys, while the directionally crystallized alloy improves its performance mainly by applying the direction of greatest resistance to creep and valving to the direction of greatest stress in an aeroengine. The longitudinal rafting will improve the yield strength and creep properties of single crystal alloys since the grain boundaries in the alloy are completely eliminated. However, rafting also affects the fatigue behavior and crack growth mechanism of single crystal alloys.

How to correlate rafting microstructure with mechanical properties becomes particularly important. To achieve this correlation, a mathematical description (modeling) of the microstructure, or the formation of a variable, this paper mainly discusses the existing methods of microstructure description, summarizes them, points out the advantages and disadvantages of the existing methods, and gives the prospect.

2. Alloy Rafting

The rafting phenomenon of single crystal alloy is mainly caused by thermo-mechanical coupling effect and dislocation movement. The thermo-mechanical coupling effect is that the γ' phase will expand or contract when it is elastic deformation under the action of stress, which results in the interfacial stress between γ' phase and γ phase. When the dislocation passes through the γ' phase, it will leave a shear step or a mismatched dislocation loop at the γ/γ' interface, which will lead to the generation of strain energy at the interface. [1] These strain energies drive γ' phase to grow along the direction of dislocation motion, forming rafting structure. Rafting of single crystal alloys is a complex non-equilibrium process, which is affected by many factors, such as temperature, stress, time, alloy composition, initial microstructure and so on.

2.1 the types of alloy rafting

In the process of tensile deformation, due to the action of stress, some grains in the alloy undergo directional oxidation reaction, forming oxide film with certain orientation, therefore, the oxidation resistance and mechanical properties of the alloy are improved. The grain valve direction is related to the composition, structure, temperature and stress state of the alloy. Generally speaking, the grain valve direction is perpendicular or parallel to the tensile stress axis.

For example, figure A is the original crystalline phase of the alloy, which is a regular cubic shape, while figure B and figure C are the valve state after compression and tensile stresses are applied in the vertical direction, respectively, the plane in which the alloy is valved is perpendicular to the direction in which the stress is applied.

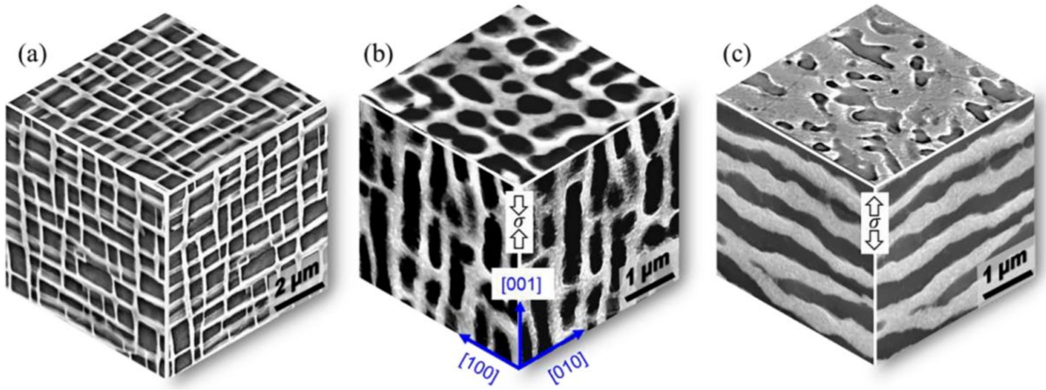

Fig. 2 (a) the original crystalline phase of the alloy, which is a regular cubic shape; (b) is the valve state after compression with the crystalline phase extruded into rings perpendicular to the compressive stress. (c) is when tensile stresses are applied in the vertical direction, the phase is in annular strips drawn perpendicular to the compressive stress [2].

Therefore, the components of the planes in which the alloy is valved can be installed perpendicularly to the direction in which the stress is applied.

2.2 the influences of alloy rafting

As M. Cottura mentioned in the article “Microstructure evolution under creep in Ni-base superalloys” [3] The microstructure formation and evolution of Ni-base superalloy during creep under near tensile loading were simulated in three dimensions. Starting from the cubic structure, the microstructure of rod-shaped precipitates was obtained under constant stress. These rod-shaped precipitates are γ' phases composed of intermetallic compounds such as Ni3Al or Ni3Ti, which have high antioxidant activity and strength.

In view of the effect of fatigue resistance of single crystal alloys after rafting, Zeng [4] proposes that based on the low cycle fatigue tests of DD3 ni-base single crystal superalloy under uniaxial tension/compression and multi-axial tension/torsion unsymmetrical cyclic loading, the data obtained from the tests are analyzed, it is found that obvious stress relaxation behavior occurs under high temperature asymmetric cyclic loading, which results in stress weakening damage and influence on fatigue life.

In order to offset the influence of rafting, Yang has made the analysis of via experiments and phase-field simulations[5], the results are shown in the figure below.

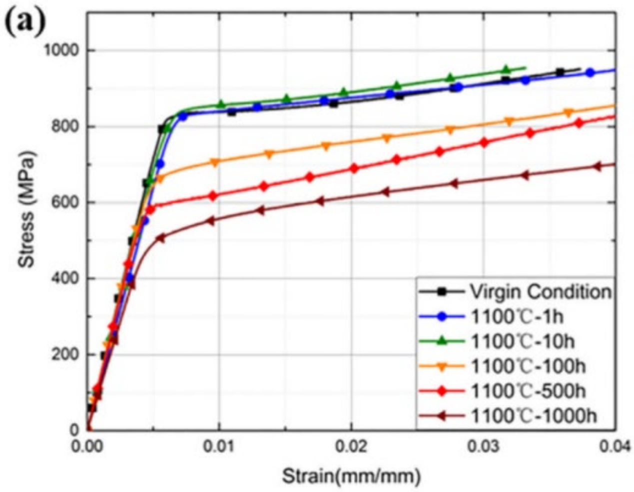

Fig. 3 Comparison of stress-strain curves after rafting with different periods [6].

It can be seen from the figure that with the increase of strain, the stress tolerance of the alloy increases, but the increasing range gradually slows down, and the mechanical strength of the alloy gradually decreases with the increase of high temperature treatment time, this is the result of internal phase creep.

In the actual service of aviation engines, many stresses and strains are concentrated at geometric singularities, such as film cooling holes and turbine blade slits, which affect the spatial uniformity of the microstructure rafting. [7]

3. Mathematical description of rafting microstructure morphology

Because the alloy rafting has a great impact on its performance, so in the design of an aero-engine component when it needs to carry out accurate quantitative calculation of its performance, this requires a mathematical description of the method to achieve this goal.

More often, channel width is utilized to measure the extent of alloy rafting. In the basic version of channel width method, an image processing program is developed to investigate the probability characteristic of γ channel width, and a channel width evolution model considering non-quasi-static modifcation which obeys lognormal distribution is put forward, also, the mean values follow linear relationship with standard deviations.[8] In this method, the alloy's degree of valve is considered to be proportional to its channel width between its γ ′ phases.

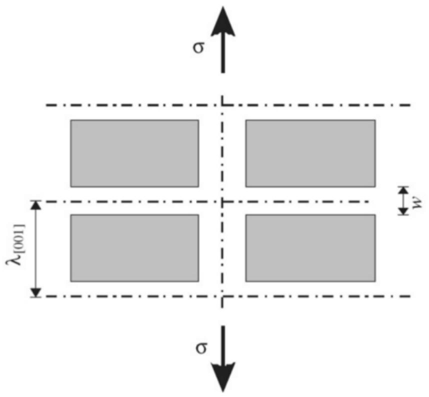

Fig. 4 Sketch map of channel width method [14].

Because the grains are not completely split, the adhesion between them matters. Thus, an optimized version of channel width is proposed. R. Desmorat et al. developed a model to analyse the effect of microstructural degradation [9](i.e. precipitate-directional-coarsening) on the viscoplastic behavior of single crystal superalloys under high temperature. Modeled by a tensorial description of g channel width evolution and coupled to the Kelvin modes based viscoplasticity. The model has been calibrated at the temperatures of 950°C and 1050°C. Several validation tests have been simulated, to further enhance its accuracy.

However, there were still some space of accuracy using the traditional channel width method, thus Caccuri et al. [11] based on the channel width and considering the average width in each direction, he proposed a fabric tensor to describe it with greater accuracy than before. Weng et al. [12,13] applied the fabric tensor to represent microstructures of single-crystal alloys with neural networks. The model has been calibrated for a couple of temperatures,[14] Several validation tests have been simulated, to further enhance its accuracy. Also, MARTIN Y.M. et al. [15]developed a new method called intercept segment deviation (ISD) and characterize the structural anisotropy of a highly porous structure based on the channel width method [15](using the mean intercept length (MIL) method) with extensive pore interconnectivity and surface area, such as scaffolds in tissue engineering.

Wu et al. calculated the distribution of elastic strain energy density of γ and γ ′ precipitation phase in Ni-base single crystal alloy with orientation by using finite element method, the directional coarsening process is analyzed according to the diffusion property of elements. The results show that external stress changes the distribution of strain energy density in matrix channels, and the directional coarsening of γ ′ precipitates is closely related to the distribution of strain energy density in matrix channels.[15]

Fan et al. [17] utilized an image processing method named chord length distribution combined with principal component analysis (PCA) to obtain the core statistical information of morphology and size features of microstructures.

While the channel width method is the most common method, there are other mathematical description models. Here are a method related to image processing and measuring the extent of rafting. Three-point correlation functions were used by Cheng et al. [18] to represent microstructures of single crystal materials. Subsequently, Bayesian optimization was employed to reduce the full sets to a 100-fold smaller subset, which is concise, nearly-complete, and explainable.

Although the target material is not the single crystal, area tensor presented by Wetzel and Tucker can also be a reference method to describe the local morphology of two-phase materials.

And[19] Microstructure assessment can be generated by Scanning electron microscope (SEM) using a secondary electron mode on the gauge cross section which parallel to the stress axis of the creep specimen and on the cross section of the aged specimen cut perpendicular to the growth axis of the single crystal rod. Using Fredholm's previously established method, the microstructure changes occurring during creep and long-term aging treatments were quantified by measuring the change in the number of specific junctions of NA (γ ') in the γ ' phase over time.

4. Conclusion

The main contributions of this paper are as follows: the rafting phenomenon of single crystals is described, and the mathematical description method of rafting microstructure is summarized.

Some viewpoints and conclusions of rafting micro-structure mathematical description method:

Channel width is one of the most popular methods, which can be used under creep or aging, with the development of computer technology, mathematical description began to adopt some image analysis methods, such as autocorrelation and cross-correlation, three-point correlation functions and other methods outlook: while current methods are mature, the next step for researchers should be to explore whether the number of descriptive variables can be reduced while maintaining mathematical models of computational accuracy.

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Outlook: while current methods are mature, the next step for researchers should be to explore whether the number of descriptive variables can be reduced while maintaining mathematical models of computational accuracy.

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