Crystallographic Unified Viscoplastic Constitutive Relations of Single-crystal Material

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Abstract. Unified viscoplastic constitutive equations are established in the crystal slip systems on the basis of the theory of crystal slip. Plastic dashpots reflecting the material transient response and Newton dashpots mirroring the material viscosity are introduced in slip systems to establish the viscoplastic flow equations and hardening equations for description viscoplastic properties of material slip systems. The physical mechanism of work hardening is divided into two basic types: plug hardening and tangles hardening. Creep additional hardening is introduced in the hardening functions of single crystal to reflect non equal hardening effect of creep and plasticity. The concept of yield surface is removed from the viscoplastic constitutive equations of the single crystal, resulting not needing to judge the yield condition in the calculation process, not needing to search the moving slip systems and simplified calculation process. The constitutive equations can be used for cyclic plasticity simulations, to describe the creep cyclic interaction.

Introduction

In order to describe the creep, relaxation, viscoplastic mechanical behavior, uniform type of constitutive theory (that did not distinguish between the plastic and creep deformation) have been proposed in the mid-1970s to the early 1980s[1-4].By analyzing potential hardening of the slip systems in the single crystal, macroscopic properties of the material hardening can be calculated, providing the necessary analytic tools for macro analysis[5-9].

The elastic strain energy may be released under certain condition thereby reducing the external energy required for crystal slip. To consider this fact, a single crystal viscoplastic constitutive relations are developed in literature [10].

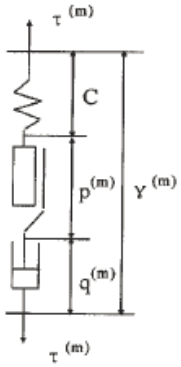

Fig.1 Rate-Dependent Simple Mechanic Model

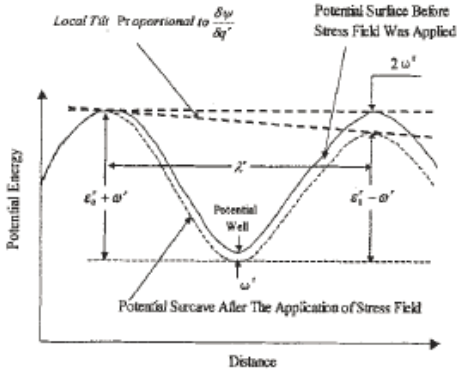

Fig.2 Potential Energy Barriers under Externally Applied Stress Field

In Fig.1,the energy stored in the spring *C* (stiffness *C*)represents the energy stored in the micro-structure of the material and the movement of the plastic slider am (damping coefficient am) represents the movement of irreversible slip systems. We obtained:

$$t_m = c(g_m - p_m) \tag{1}$$

$$t_m = a_m \frac{dr_m}{dV_m} \tag{2}$$

Where ς_m is generalized time measurement for description the m-th slip system.

In crystal plastic deformation process, strengthen slip systems include self-strengthening and potential strengthening. If f_m and H_m describe the two strengthening mechanisms, then:

$$a_m = a_0 f_m H_m \tag{3}$$

Where a0 is the damping coefficient. Link Eq. 1 and Eq. 2, we obtain:

$$dt_m = cdr_m - a t_m dz_m \tag{4}$$

Where Z_m is generalized time for description movement of the m-th slip system, Eq. 4 can be expressed as

$$dt_m = T_m dr_m \quad \text{or} \quad t_m = T_m \dot{r}_m \tag{5}$$

$$T_m = c - a \frac{\Gamma_m}{f_m H_m} t_m \tag{6}$$

Define hardening coefficient:

$$h^{mn} = T_m d^{mn} \tag{7}$$

constitutive relation can be expressed as

$$\dot{\tau}_m = \sum_{n=1}^{N} h^{mn} \dot{\gamma}_n \qquad (m=1,2,3,.....,N) \tag{8}$$

Where N is the number of crystal independent slip systems.

Single Crystal Hardening Function

Depending on the different characteristics, hardening mechanisms can be divided into two basic types: pileup sclerosis and entangled hardening.

Weng[11] gave the following single crystal hardening law based on analysis of Orowan precipitation hardening mechanism :

$$h^0 = b^i b^j h^j \tag{9}$$

Where $\beta^i = n^i \otimes s^i$, n^i & s^i were the unit vector of slip surface normal and slip direction respectively, h^j is work hardening rate in the slip system caused by of the pileup stress field of j-th slip system.

The first feature of entangled hardening is: entangled hardening on slip systems has isotropic characteristics. The second: its corresponding mathematical description is complicated. Single crystal hardening law shall not only reflect the entangled hardening historical correlation, but also reflect the characteristic differences of entangled hardening between different slip systems.

Bassani[12] presented below single crystal hardening law based on his reinterpretation of the potential hardening :

$$h^{ij} = H^i d^{ij} \tag{10a}$$

$$H^i = \left\{ (h_0 - h_s) \sec h^2 \frac{h_0 - h_s}{t_1 - t_0} g^j + h^s \right\} \times \left\{ 1 + \sum_{k=j} f_{jk} \tanh \frac{g^k}{g_0} \right\} \tag{10b}$$

Where h_0, h_s,τ_0, τ_1, f_{jk} and γ_0 are material parameters. The parameter f_{jk} is related to j-th and k-th slip systems.

In the case of potential hardening in this paper, the hardening function H_m is introduced in Eq. 3 to express:

$$H_m = 1 + \sum_{k \neq m} f_{km} \tanh(2 b_s g^k) \qquad (m=1,2,3,.....,N) \tag{11}$$

Where β_s, f_{km} are material parameters.γk integration includes the positive and reverse slip process of slip systems, namely γ_k is the sum of the cumulative slip rate of the k-th positive and its reverse. This parameter reflects the entangled hardening history and the difference of dislocation entangled hardening between slip systems is reflected by the parameter f_{km}.

Physical meaning of f_{ij} is a measure on the mutual influence of slip system hardening effect. Here we give a specific form of f_{ij} according to the discussion in literature [12].

In the single crystal, under decomposition shear stress $\tau^{(m)}$, the m-th crystal slip system may appears the following three aspects deformation. The generalized displacement of damper $b^{(m)}$ is represented by $q^{(m)}$. The above deformation mechanism can be visualized graphically by the mechanical model in figure 1. In fig.1, $\gamma^{(m)}$ represents the total deformation of m-th slip systems. We get:

$$t^{(m)} = c(g^{(m)} - p^{(m)} - q^{(m)}) \tag{12}$$

The relevant results of Bassani are directly cited as a potential hardening function, namely:

$$H_m = 1 + \sum_{k \neq m} f_{mk} \tanh(2 b_s z_k) \quad (m=1,2,.....,N) \tag{13}$$

Where ζ_k is the cumulative slip of k-th slip system. β_s and f_{mk} are the material parameters.β_s represents the speed of H_m tending to saturation. f_{mk} is the coupling hardening coefficient between the k-th and the m-th slip system. It is determined by the relative orientation between slip systems, reflecting the effect of cumulative slip in the k-th slip system on hardening in the m-th slip system.

For generalized time-dependent displacement $q^{(m)}$,it may be assumed as average displacement of atom group across associated energy barrier of the m-th slip systems, as shown in fig.2. The average velocity across the energy barrier with height $\varepsilon_0^{(r)}$ is determined by the skew $w^{(r)}$ of energy barrier under the applied stress.

If take the average energy barrier height and skew amount as $\bar{e}_0^{(r)}$, $\bar{w}^{(r)}$, we can approximate:

$$\frac{dq^{(m)}}{dt} = K e^{-b\bar{e}_0^{(r)}} \sinh(b\bar{w}^{(r)}) \tag{14}$$

Where K and $\bar{e}_0^{(r)}$ are material parameters, $b = \frac{1}{KT}$,where T is the absolute temperature and K is Bltzmann constant.

Numerical simulation of DD3

Numerical simulation is carried out by using constitutive equations on different orientations, and strain rate of DD3 single crystal material.The tensile and Creep experiment data were extracted from literature[13] under 950□ and in [001], [011],[111]three crystal orientations. The tensile experiment data and calculation results are shown in fig.3,with the Tensile strain rate 2×10^{-4},1×10^{-3},3.2×10^{-3}.

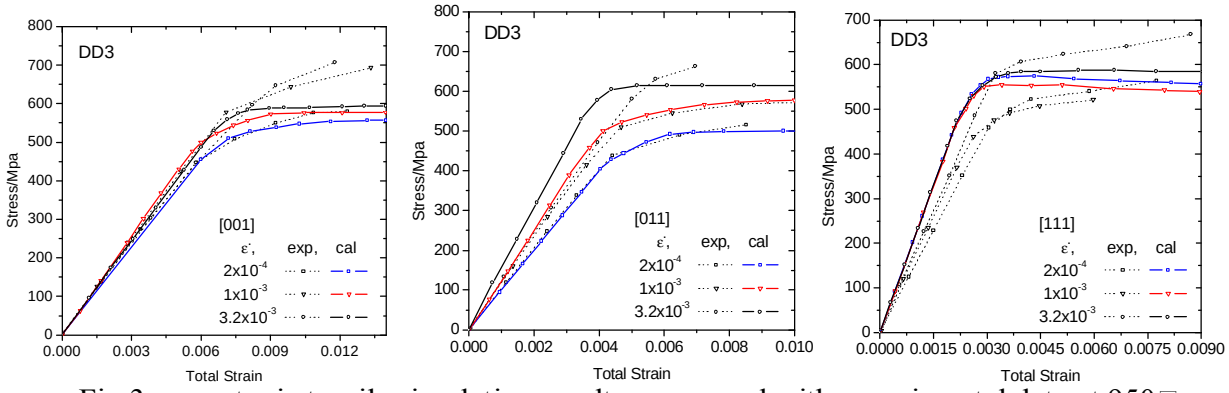

Fig.3 monotonic tensile simulation results, compared with experimental data,at 950□,

The creep experiment data and calculation results are shown in fig.4 with different stress levels.

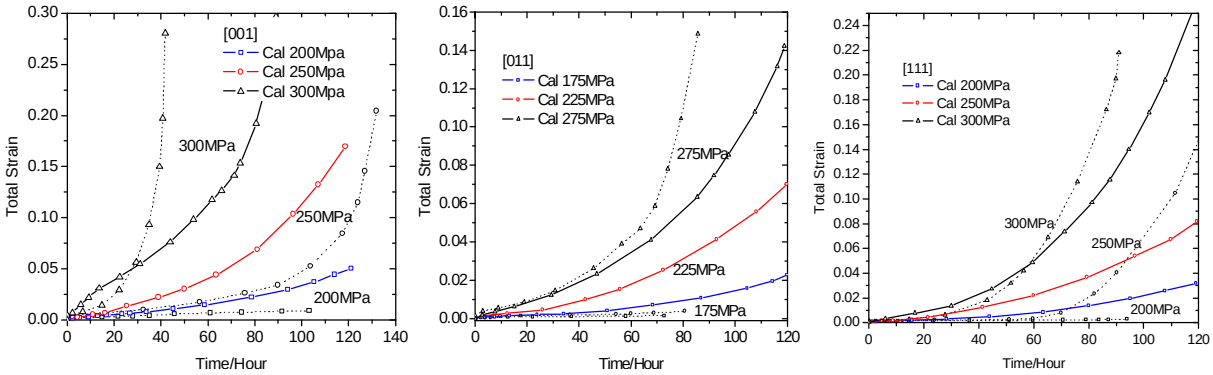

Fig.4 creep simulation results,compared with experimental data,at 950□

The constitutive equation can be used to simulate the monotonic tension and creep, and it can be used to simulate the cyclic plasticity.

Conclusions

In the process of establishing hardening rate law of single crystal, the physical mechanism of work hardening is based on the experimental data of single crystal hardening. The establishment of the single crystal viscoplastic constitutive equations without introducing the concept of yield surface, resulting in the calculation process without judgment yield condition, and not needing to slip systems to search, and the calculation is greatly simplified, easy to use.The monotonic tension and creep of the single crystal alloy DD3 under high temperature environment are simulated, and compared with the experimental data, with high accuracy. Monotonic tension simulation is carried out with different strain rate, and the simulation results are in good agreement with the experimental data in three directions.In different crystal orientations and under different stress levers, cyclic plasticity simulations can be simulated also with the constitutive equations.

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