Computational Materials Science 129 (2017) 147–155

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

A novel temperature dependent yield strength model for metals considering precipitation strengthening and strain rate

Xianhe Zhang [a], Weiguo Li [a,*], Jianzuo Ma [a], Peiji Geng [a], Jiaxing Shao [a], Xiaozhi Wu [b]

[a] State Key Laboratory of Coal Mine Disaster Dynamics and Control, College of Aerospace Engineering, Chongqing University, Chongqing 400030, China
[b] College of Physics, Chongqing University, Chongqing 400030, China

A R T I C L E I N F O

Article history:
Received 30 October 2016
Received in revised form 29 November 2016
Accepted 2 December 2016

Keywords:
Yield strength
Temperature dependent model
Metallic materials
Precipitation strengthening
Strain rate

A B S T R A C T

In this work, we proposed a novel temperature dependent yield strength model for metallic materials which has no fitting parameters. The temperature dependent yield strength at arbitrary temperatures can be predicted. And a critical yield energy density with material yield is introduced, which comprises the distortional strain energy, potential energy and kinetic energy of atomic motion. A kind of quantitative relationship between the yield strength, temperature, elastic modulus and Poisson's ratio is presented. The agreement between theory and experiment is of good satisfaction. Moreover, a temperature dependent yield strength model considering the precipitation strengthening is introduced to predict the yield stress of precipitation strengthened superalloy. Based on the proposed temperature dependent model, a new temperature and strain rate dependent yield strength is established. The good agreement between theory and experiment is found at the temperatures and strain rates considered.

1. Introduction

Some metallic structural materials, e.g. the holder of combustors, the hot end of engines and turbines, and fire prevention structures, need to withstand the high temperature environment and can still work for a long time. And as is known to all, the yield strength of metals and alloys is sensitive to temperature. This has resulted in a high demand to better know the yield behavior of metals at different temperatures. Many researchers have done a large number of studies in characterizing yield behavior through both phenomenological and physical based models. The Johnson-Cook (JC) model [1] is a classical phenomenological model that is widely used for prediction of the material plastic behavior at different strain rates and temperatures. And many modified models were established through the introduction of internal state variables, which are very necessary to describe behavior of materials [2–5]. But these models are semi-empirical formulas that lack detailed physical mechanism and introduce more parameters which make the application of these models inconvenient. On the other hand, the Zerilli-Armstrong (ZA) [7], Mechanical Threshold Stress (MTS) [8] models are developed based on the thermal activation analysis for dislocation motion overcoming local obstacles. However, these models are usually parameterized using microcosmic data of polycrystals and therefore are not suitable for the descriptions of macroscopic deformation. The crystal plasticity finite element models [9–12] and molecular dynamics (MD) simulations [13–15] have been used to predict the yield strength and texture evolution of metallic materials. The finite element models are not appropriate for describing the temperature and strain rate dependence of the flow stress of metals [6]. MD simulations can indeed do some qualitative analysis of materials properties, but their computing objects are nano-sized owing to the limit of calculation scale. To obtain the mechanical properties required for operational conditions up to very high temperatures in service, precipitation strengthening is commonly used as one of the major strengthening mechanisms for superalloys. Recently, a large amount of research on the effect of precipitate particles on the properties of superalloy at different temperatures was done [17–20]. However, the effect of precipitation strengthening mechanism on temperature dependent yield strength (TDYS) was not investigated clearly.

Plastic slip in crystalline materials is due to motion of dislocations [21]. The resistance of the lattice atoms to hinder the dislocation slip will decrease with increasing temperature; under applied stress, grain boundary premelting will appear at a temperature

Abbreviations: JC, Johnson-Cook; ZA, Zerilli-Armstrong; MTS, Mechanical Threshold Stress; TDYS, temperature dependent yield strength; CYED, critical yield energy density; MD, molecular dynamics.

* Corresponding author.
E-mail address: wgli@cqu.edu.cn (W. Li).

http://dx.doi.org/10.1016/j.commatsci.2016.12.005
0927-0256/

much lower than melting point [22]. And it is proposed that thermal fluctuations will cause the dislocation system to cross the barrier, and trigger the yield of the material [23]. It is clearly that there are some similarities between yielding and melting process of metallic materials [24]. Both phenomena occur accompanied by collective atomic motions, which need enough energy to overcome the bonding force between atoms [25,26]. From micro perspective, it is also found that yielding of material is related to the potential energy between atoms and kinetic energy of atomic motion [27]. In view of the equivalence between a thermal energy and distortion energy, Li has proposed a new model to consider the influence of temperature on the yield strength of materials [28]. Li's model can be expressed as follow:

$$\sigma_y(T) = \left[\frac{(1+\nu_{T_0})E_T}{(1+\nu_T)E_{T_0}}\left(1-\frac{\int_{T_0}^{T} C_p(T)dT}{\int_{T_0}^{T_m} C_p(T)dT}\right)\right]^{0.5}\sigma_y(T_0) \tag{1}$$

where $\sigma_y(T)$ is the yield strength, T is the temperature (in Kelvin), T_0 is a reference temperature, ν_T and ν_{T_0} are corresponding Poisson's ratio at temperature T and T_0, E_T and E_{T_0} are elastic modulus, T_m is the melting point, $C_p(T)$ is the specific heat capacity at constant pressure, $\sigma_y(T_0)$ is the yield strength at reference temperature.

In this work, the relations between temperature and yield strength were analyzed in a novel way. A new idea is proposed: assuming there is an equivalence relation between potential energy and atomic kinetic energy. A quantitative TDYS model is established. The relationship between the yield strength, temperature, elastic modulus and Poisson's ratio is built. In addition, a new TDYS model of precipitation strengthened superalloys is developed based on the Orowan model [29]. To consider the coupling effect of strain rate and temperature, a new temperature and strain rate dependent yielding model for metallic materials is developed on the basis of TDYS model.

2. A new temperature dependent yield strength model

2.1. Analysis and assumptions

In thermodynamics, the internal energy of a system is the energy contained within the system, excluding the kinetic energy of motion of the system as a whole and the potential energy of the system as a whole due to external force fields. The microscopic kinetic energy of a system arises as the sum of the motions of all the system's particles with respect to the center-of-mass frame. The microscopic potential energy algebraic summative components are those of the chemical and nuclear particle bonds, and the physical force fields within the system, such as due to internal induced electric or magnetic dipole moment, as well as the energy of deformation of solids (stress-strain). Learning from Li's previous work [28], a new idea is proposed to consider the influence of temperature on the yield strength of metals. We assume that the potential energy between atoms and kinetic energy of atomic motion have an equivalent relations during the yielding of material; in an isothermal process, the strain energy is equal to the variation of the potential energy. The material will yield when the distortion energy can reach a critical value, which is related to the crystal bonding force [30,31]. Huber attributed the physical meaning to the yield criterion: as long as the distortion energy cannot reach the critical value, the material will remain elastic [32]. The energy of distortion, which can be separated from the total strain energy, is responsible for reaching a limit state. So it is supposed that in unit volume there is a maximum storage of energy which is corresponding to the onset of yield of material and temperature independent. The maximum stored energy in unit volume can be defined as critical yield energy density (CYED) that consists of the distortional strain energy, the corresponding equivalent kinetic energy and potential energy of atoms.

2.2. Theoretical derivation

As discussed above, the CYED has the form:

$$\mathrm{W}_{\mathrm{total}} = W_d(T) + \alpha * E_k(T) + \beta * E_P(T), \tag{2}$$

where the $\mathrm{W}_{\mathrm{total}}$ is the CYED corresponding to the beginning of the material yield, which depends on the type of material and its microstructure. $W_d(T)$ is the critical distortional strain energy density corresponding to the beginning of the material yield at temperature T. α, a hypothetical constant, is the effective coefficient of the atoms' kinetic energy. $E_k(T)$ is the kinetic energy of atomic motion in per unit volume at temperature T, which has the following expressions when the temperature is beyond room temperature:

$$E_k(T) = \frac{3}{2}kNT, \tag{3}$$

k is the Boltzmann constant, N is the amount of atoms in unit volume, T is the temperature (in Kelvin). β, a hypothetical constant, is the effective coefficient of the potential energy. $E_P(T)$ is the potential energy of atoms in per unit volume which is a value of change caused by temperature. Here, the potential energy is assumed to be zero at 0 K when the interaction force between atoms is equal to zero. The kinetic energy and potential energy of the vibrating atoms change periodically in the solid, and the average kinetic energy and the average potential energy are equal. So $E_P(T)$ can also be calculated by using the following formula:

$$E_p(T) = \frac{3}{2}kNT, \tag{4}$$

When the temperature T is taken as the melting point T_{m}, the material can no longer bear any stress. Therefore, there is no external work: $W_d(T_{\mathrm{m}}) = 0$.

Plugging $T = T_{\mathrm{m}}$ into Eq. (2), we can get that:

$$\mathrm{W}_{\mathrm{total}} = \frac{3}{2}(\alpha+\beta)kNT_m. \tag{5}$$

Putting $T = T_0$ into Eq. (2), where T_0 is a reference temperature which can be chosen arbitrarily, we can obtain that:

$$\mathrm{W}_{\mathrm{total}} = W_d(T_0) + \frac{3}{2}(\alpha+\beta)kNT_0. \tag{6}$$

To solve simultaneous equation of Eqs. (5) and (6) yields:

$$\alpha+\beta = \mathrm{W_d}(T_0) \Big/ \frac{3}{2}kN(T_m - T_0). \tag{7}$$

Substituting $\alpha+\beta$ (Eq. (7)) into Eq. (2), we can get that

$$\mathrm{W}_{\mathrm{total}} = W_d(T) + \frac{\mathrm{W_d}(T_0) * T}{T_m - T_0}. \tag{8}$$

To solve simultaneous equation of Eqs. (5) and (8), $W_d(T)$ can be worked out:

$$W_d(T) = W_d(T_0) * \frac{T_m - T}{T_m - T_0}. \tag{9}$$

Under uniaxial tension, the distortional strain energy density of linear elastic solids can be written as:

$$W_d(T) = \frac{1+\nu_T}{3E_T}(\sigma_y(T))^2. \tag{10}$$

where ν_T, E_T and $\sigma_y(T)$ are the Poisson's ratio, elastic modulus and yield strength respectively at temperature T.