A dissipation potential approach to describe flow instability in alloys during hot deformation

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Introduction

Flow instability is the onset of heterogeneous flow intensifying flow localization and leading to further damage in alloys during hot deformation. Some phenomenological approaches in the literature do not account for the microstructure changes of the material. In order to overcome this problem, we introduce a dissipation potential approach as a function of the plastic strain rate, the evolution rate of dislocation density and the heat flux, $D(\dot{\varepsilon}_p, \dot{\rho}, q)$, to describe the flow instability during hot deformation. This approach considers the principle of orthogonality proposed by HANS ZIEGLER and describes large plastic flow with far-fromequilibrium thermodynamics. Moreover, the evolution rate of dislocation density $\dot{\rho}$ is involved and the transient energy dissipation comprises mechanical part due to dislocation movement and thermal part by heat transfer. The necessary condition for stable flow is that the dissipation potential $D(\dot{\varepsilon}_n, \dot{\rho}, q)$ is convex, i.e. the associated Hessian is non-negative. This approach connects the continuum mechanics, non-linear non-equilibrium thermodynamics and microstructure evolution when dealing with hot deformation problems. In this work, the approach was applied to describe the behavior of Ti6Al4V during hot deformation, and using a Kocks-Mecking type model to describe the flow stresses as a function of the dislocation density.

Dissipation potential model

Large plastic deformation of materials is irreversible and in the non-linear non-equilibrium state, especially during hot deformation. And the relative system entropy is increasing presented by dissipation energy. The rate of dissipation energy is introduced as a function of the plastic strain rate $\dot{\varepsilon}_p$, the evolution rate of dislocation density \dot{p} and the heat flux q in the work. A dissipation potential function $D(\dot{\varepsilon}_p, \dot{\rho}, q)$ was developed and which comprised three parts: 1) the plastic work 2) the stored energy and 3) the heat transfer. The three parts are constructed as following equations.

The flow stress described by Kocks-Mecking model

The Kocks-Mecking model was developed to describe the flow stress of a material by considering one hardening term and one recovery term [1, 2]. The flow stress can be expressed as a function of the total dislocation density ρ , and the associated constitutive equations are given by:

$$\sigma = M\alpha G b \sqrt{\rho} = M\alpha_1 G(T) b \frac{h_1}{h_2} \left(1 - \exp\left(-\varepsilon \frac{h_2}{2}\right) \left(1 - \frac{h_2}{h_1} \frac{\sigma_{YS}}{M\alpha G b}\right) \right) \tag{1}$$

$$h_{1} = h_{1,0} \dot{\varepsilon}^{m_{h_{1}}} \exp\left(\frac{m_{h_{1}} Q_{h_{1}}}{RT}\right)$$

$$h_{2} = h_{2,0} \dot{\varepsilon}^{-m_{h_{2}}} \exp\left(-\frac{m_{h_{2}} Q_{h_{2}}}{RT}\right)$$
(3)

$$h_2 = h_{2,0} \dot{\varepsilon}^{-m_{h_2}} \exp\left(-\frac{m_{h_2} Q_{h_2}}{RT}\right) \tag{3}$$

Where: M- Taylor factor; α_1 - Numerical constant; G(T)- Shear modulus; b- Burgers vector; h_1 - Hardening coefficient; h_2 - Recovery coefficient; σ_{YS} - Measured yield stress; $h_{1,0}$ - Ahardening coefficient; $h_{2,0}$ - A constant forrecovery coefficient; m_{h_1} - Strain rate sensitivity for h_1 ; m_{h_2} - Strain rate sensitivity for h_2 ; Q_{h_1} - Activation energy for h_1 (J/mol); Q_{h_2} - Activation energy for $h_2(J/mol)$; $\dot{\varepsilon}$ - Strain rate (1/s); R- Universal gas constant (J/mol·K); T- Temperature (°C).

The stored energy described by Helmholtz free energy

The amount of energy stored as crystal defects inside of material after deformation can be presented by Helmholtz free energy $\Psi(T, \varepsilon^e, \rho)$ as a function of the temperature, elastic stain and dislocation density [3]. For rigid viscoplastic materials, the elastic strain was ignored and the Helmholtz free energy $\Psi(T, \rho)$ is given by

$$\Psi(T,\rho) = E_{\rho}\rho = \alpha_2 G(T)b^2 \rho \tag{4}$$

Where E_{ρ} is the unit length energy of the dislocation.

The heat transfer described by heat flux and temperature gradient

The gradient of temperature ∇T is the driving force for the heat flow [4], and the heat transfer of the system is given by

$$D_T = -\frac{\nabla T}{T}q\tag{5}$$

Where q is the heat flux, and the negative symbol means the heat flow is flowing from higher temperature to lower temperature.

The dissipation potential model

The general dissipation potential function is given by:

$$D(\dot{x}_k) = \sum X_k \cdot \dot{x}_k \tag{6}$$

Where \dot{x}_k is the rate of variables, and X_k are the corresponding thermodynamic forces [5]. According to the coupled interactions among the variables, the dissipation potential can be summarized as two different forms.

(1) The coupled dissipation potential function

$$D(\dot{\varepsilon},\dot{\rho},q;\varepsilon,\rho,T) = \sigma\dot{\varepsilon} - \frac{\partial \Psi(T,\rho)}{\partial \rho}\dot{\rho} - \frac{\nabla T}{T}q + \frac{\partial^2 D}{\partial \dot{\varepsilon}\partial \dot{\rho}}\Big|_{q}F(\dot{\varepsilon},\dot{\rho};\varepsilon,\rho,T) + \frac{\partial^2 D}{\partial \dot{\varepsilon}\partial q}\Big|_{\dot{\rho}}F(\dot{\varepsilon},q;\varepsilon,\rho,T) + \frac{\partial^2 D}{\partial q\partial \dot{\rho}}\Big|_{\dot{\varepsilon}}F(q,\dot{\rho};\varepsilon,\rho,T) \tag{7}$$

Where $F(\dot{\varepsilon}, \dot{\rho}; \varepsilon, \rho, T)$, $F(\dot{\varepsilon}, q; \varepsilon, \rho, T)$ and $F(q, \dot{\rho}; \varepsilon, \rho, T)$ are thermodynamic coupling forces with the associated variables.

(2) The non-coupled dissipation function

$$D(\dot{\varepsilon}, \dot{\rho}, q; \varepsilon, \rho, T) = \sigma \dot{\varepsilon} - \frac{\partial \Psi(T, \rho)}{\partial \rho} \dot{\rho} - \frac{\nabla T}{T} q \approx \sigma \dot{\varepsilon} - \alpha_2 G(T) b^2 \dot{\rho} - \frac{\nabla T}{T} q$$
(8)

Where: $\dot{\rho}$ - Dislocation density rate; ∇T - Temperature gradient; q- Heat flux. The evolution of dissipation potential with regards to dislocation density rate ($\dot{\rho}$), strain (ϵ) and strain rate ($\dot{\epsilon}$) were presented in Figure 1 and Figure 2 respectively.

3. The Hessian matrix of dissipation potential function

The convexity of the dissipation potential assures the stability of the thermodynamic system [5]. This is as saying that its Hessian $H(\dot{\varepsilon}, \dot{\rho}, q; \varepsilon, \rho, T)$ is definite positive.

4. One special case of the non-coupled dissipation potential function: $\nabla T = 0$

When it considers the adiabatic condition, the dissipation potential function is simplified by ignoring the heat transfer effect. The dissipation potential function for Ti64 with single β phase is given by

$$D(\dot{\varepsilon},\dot{\rho};\varepsilon,\rho,T) = \sigma\dot{\varepsilon} - \alpha_2 G(T)b^2\dot{\rho} = M\alpha_1 G(T)b\dot{\varepsilon}\frac{h_1}{h_2} \Big(1 - \exp\Big(-\varepsilon\frac{h_2}{2}\Big)\Big(1 - \frac{h_2}{h_1}\frac{\sigma_{YS}}{M\alpha G(T)b}\Big)\Big) - \alpha_2 G(T)b^2\dot{\rho} \tag{9}$$

The Hessian matrix of the above non-coupled dissipation potential function $D(\dot{\varepsilon}, \dot{\rho}; \varepsilon, \rho, T)$ is given by

$$H(\dot{\varepsilon},\dot{\rho};\varepsilon,\rho,T) = \begin{vmatrix} \frac{\partial^2 D}{\partial \dot{\varepsilon}^2} & \frac{\partial^2 D}{\partial \dot{\rho}\partial \dot{\varepsilon}} \\ \frac{\partial^2 D}{\partial \dot{\varepsilon}\partial \dot{\rho}} & \frac{\partial^2 D}{\partial \dot{\rho}^2} \end{vmatrix} = \begin{vmatrix} \frac{\partial^2 D}{\partial \dot{\varepsilon}^2} & 0 \\ 0 & 0 \end{vmatrix}$$
(10)

For the special case, the Hessian of its dissipation function is always zero, meaning stability of the thermodynamic system.

5. Modelling results

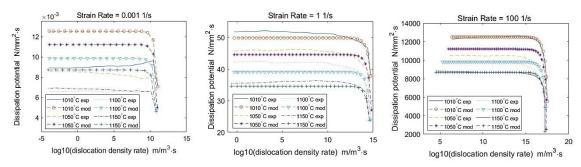


Figure 1. Evolution of dissipation potential with respect to dislocation density rate at different temperatures and strain rates.

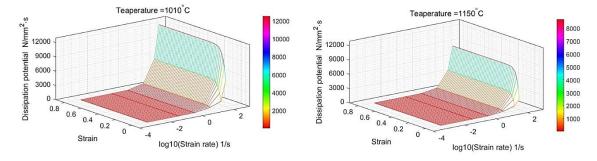


Figure 2. Mesh maps of the dissipation potential with respect to strain and strain rate at different temperatures.

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