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SOME GENERAL CHARACTERISTICS OF THE STRESS–STRAIN RELATION OF POLYCRYSTALLINE METALS

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ABSTRACT

The evolution of the microstructure of polycrystalline metals during plastic deformation is modeled by a stochastic process. By investigating the convergence properties of such a process, a method to determine the steady-state flow stress is developed. When the external load approaches the steady-state flow stress, the overall strain is found to go to infinity by a simple power law with a critical exponent $-3/2$. For large specimens, the size effect of the specimens on the steady-state flow stress can also be expressed by some simple power laws. We believe that the exponents appearing in these expressions should not be sensitive to the material microstructure, and reflect some universal behavior when the external load is near its critical value, in the same way as their counterparts in second-order phase transition problems. Furthermore, some general characteristics of the material microstructure at the steady-state flow state are also predicted. Copyright © 1996 Elsevier Science Ltd

1. INTRODUCTION

For pure ductile polycrystalline metals, a typical stress–strain curve is presented in Fig. 1. When the external load is higher than the yield stress σ_y, overall plastic deformation occurs. Then, considerable strain-hardening is observed even if the behavior of single crystals can be reasonably modeled by elastic–perfectly plastic deformations. The strain-hardening eventually leads to a steady-state flow stress σ^s where no additional hardening is observed upon continued straining. At high homologous temperature ($>0.4T_m$, where T_m is the absolute melting temperature), the steady-state flow stress is achieved at large strain. At low homologous temperature, the steady-state flow stress can also be achieved by compression and torsion testing, which avoids the fracture of materials under extensive deformation (Hockett and Sherby, 1975). Extensive investigations have been performed in order to predict the stress–strain relation of such polycrystalline metals based on single crystal characteristics; see, for example, Taylor (1938), Bishop and Hill (1951), Lin (1957), Hutchinson (1964a,b; 1970), Budiansky (1965), Berveiller and Zaoui (1979), etc.

In this paper, we do not intend to predict the whole plastic deformation behavior

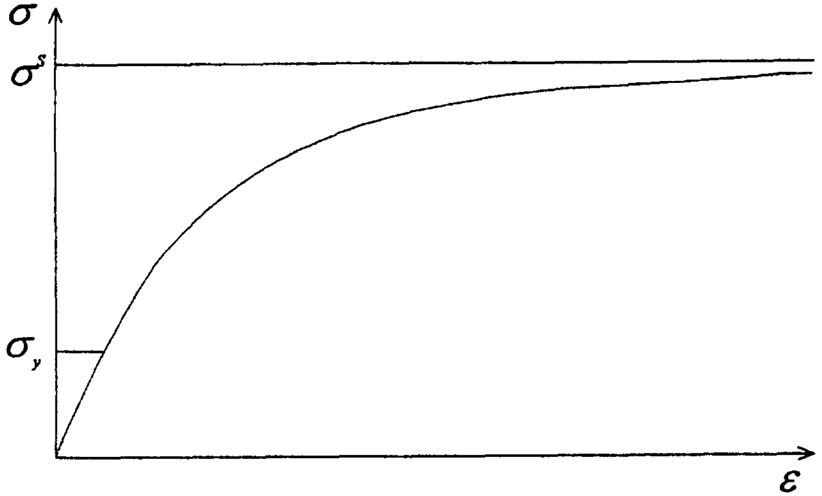

Fig. 1. Schema of a true stress–true strain curve.

of materials; instead, based on a different view of the deformation process, we try to predict the steady-state flow stress and some general characteristics of the stress–strain relation when the external load is approaching the steady-state flow stress.

Consider a polycrystalline metal, of randomly oriented crystals, loaded uniformly. At the initial stage of loading of the aggregate, only the few most favourably oriented crystals slip. When the external load has reached the yield stress, the active crystals make up a non-zero portion of the total crystals. Therefore, the overall plastic deformation which is the volume average of slip displacements of crystals appears. Since each crystal is surrounded by crystals of different orientations, the neighboring crystals will block the slip. On the other hand, the force released from the slip will act on the other crystals and thus it may induce them to slip. So, when the external load is kept at a value that is higher than the yield stress and lower than the steady-state flow stress, if a crystal slips, it may induce its neighbors to slip; then, under the action of the load released from the active crystals, more crystals may become active. This trend should stop after some steps, and these slips will be restricted within some local region. If the external load is approaching the steady-state flow stress, more and more crystals will become active. This process in which one crystal after another becomes active is just as a "domino" process. In this analysis, we treat such a process as a stochastic process, and by establishing the convergence condition of the stochastic process, the steady-state flow stress can be obtained. Furthermore, some general characteristics of the steady-state relation can also be obtained through such an approach.

2. A STOCHASTIC MODEL FOR THE SLIPS OF CRYSTALS

Suppose that when the polycrystalline metal is subjected to an external load σ^0, there are Z_0 initial active slip systems. Each active slip system may induce another slip system to become active. The total number of active slip systems induced by the initial Z_0 slip systems is denoted by Z_1. Thus, Z_1 is the number of active slip systems in the first generation. These active slip systems, in their turn, induce further Z_2 slip systems to become active, etc., and $Z_0, Z_1, Z_2, \ldots$ may be treated as random variables. We further assume that active slip systems do not interfere with each other, i.e. for example, every active slip system in Z_i will induce its neighboring slip systems to become active, independently of the other slip systems of Z_i, and also independently of those slip systems which had become active before. Thus, the sequence Z_n $(n = 0, 1, 2, \ldots)$ forms a Markov chain; to be exact, it forms a branching process (Harris, 1963).

The idea for finding the steady-state flow stress is very simple. Consider that the polycrystalline metal is an infinite set of materials. If the external load is quite small, we can imagine that the random sequence Z_n $(n = 0, 1, 2, \ldots)$ will be extinguished for large n, i.e. the slips are restricted within a finite domain. If the external load has reached its critical value, the random sequence Z_n $(n = 0, 1, 2, \ldots)$ will not be extinguished for $n \to \infty$. Thus, we can determine the critical value, which is also the steady-state flow stress, by investigating the convergence properties of the Markov chain Z_n $(n = 0, 1, 2, \ldots)$.

In fact, the independence assumption introduced above is not very reasonable for our problem. But, in order to verify the above idea, as a preliminary study, we still follow the assumption. Since we have reduced the slip process to a branching process, we can use some results obtained from studies about branching processes. For simplicity, we only consider the random sequence Z_n $(n = 0, 1, 2, \ldots)$ created by one slip system, i.e. $Z_0 = 1$. The appropriate adjustments if $Z_0 \neq 1$ are easily made, because we have assumed that the active slip systems develop independently of one another.

According to Harris (1963), we know that if m denotes the average number of active slip systems induced by one slip system in one step, i.e.

$$m = \langle Z_1 \rangle, \tag{1}$$

where the symbol $\langle \cdot \rangle$ means the average, the expected value of Z_n is m^n, i.e.

$$\langle Z_n \rangle = m^n. \tag{2}$$

It can be easily found that if $m < 1$, $\lim_{n\to\infty} \langle Z_n \rangle = 0$, and if $m > 1$, $\lim_{n\to\infty} \langle Z_n \rangle = \infty$. Therefore, $m = 1$ is the critical condition for the extinction of the average value of the random sequence $Z_n (n = 0, 1, 2, \ldots)$. Generally speaking, m is a function of the external load σ^0, so that we can determine the critical load σ^s by using the condition $m = 1$.

Now, we consider the sum

$$Z = Z_0 + Z_1 + Z_2 + \cdots, \tag{3}$$

which means the total number of active slip systems in one cluster. The average value of Z is

$$\begin{aligned} \langle Z \rangle &= 1 + m + m^2 + m^3 + \cdots \\ &= \frac{1}{1-m}. \end{aligned} \tag{4}$$

Since m is a function of the external load, when the external load approaches to its steady-state value, we can expand m around the critical load value in the form

$$\begin{aligned} m &= m(\sigma^s)+m'(\sigma^s)(\sigma-\sigma^s)+\cdots \\ &= 1+m'(\sigma^s)(\sigma-\sigma^s)+\cdots. \end{aligned} \tag{5}$$

Substitution of (5) into (4) yields

$$\langle Z\rangle \sim (\sigma^s-\sigma)^{-1}. \tag{6}$$

In deriving (6), we assume that σ is near σ^s, and neglect the higher order terms in the expansion.

In practice, there are many initial active slip systems, i.e. $Z_0 > 1$. Therefore, they will develop many separate clusters, each of which contains a different number of active slip systems. We can determine the distribution of the number of active slip systems in the clusters when the external load is approaching its steady-state value. In fact, this distribution is the main characteristic of the microstructure at that stage. According to the theorem obtained by Otter (1949) for the multiplicative process, we can derive that when the external load is equal to its steady-state value, the occurrence probability $P(Z = S,\ \sigma = \sigma^s)$ of a large cluster with S active slip can be expressed in the form

$$P(Z = S, \sigma = \sigma^s) \sim S^{-3/2}, \quad S \to \infty. \tag{7}$$

Equations (6) and (7) are power laws, which suggest treating the steady-state flow point in metal plasticity like the second-order critical point as in phase-transition physics (Ma, 1976). When the load is near its critical value, the occurrence probability that a cluster contains S active slip systems can be expressed by the following scaling law

$$P(Z = S) = S^{-\tau}\Phi[(\sigma^s-\sigma)S^{\gamma}], \quad \sigma \to \sigma^s, \quad S \to \infty, \tag{8}$$

where $\Phi[(\sigma^s-\sigma)S^{\gamma}]$ is called the scaling function, which only depends on the combination $(\sigma^s-\sigma)S^{\gamma}$. The exponents appearing in (8) can be determined by using the exponents appearing in (6) and (7) as follows.

By letting $\sigma = \sigma^s$ in (8) and comparing with (7), we know that $\tau = 3/2$. The average value of Z can be determined by using (8) as follows

$$\begin{aligned} \langle Z\rangle &= \Sigma SP(Z = S) \\ &= \int S^{-\tau+1}\Phi[(\sigma^s-\sigma)S^{\gamma}]\,\mathrm{d}S \\ &= (\sigma^s-\sigma)^{(\tau-2)/\gamma}\int \frac{1}{\gamma}x^{(2-\tau-\gamma)/\gamma}\,\Phi(x)\,\mathrm{d}x \\ &\sim (\sigma^s-\sigma)^{(\tau-2)/\gamma}. \end{aligned} \tag{9}$$

In deriving (9), we have replaced the sum by an integral, and used $x = (\sigma^s-\sigma)S^{\gamma}$, which are common tricks in the scaling theory of percolation clusters.

By comparing (6) with (9), one obtains

$$\gamma = 0.5. \tag{10}$$

If one is familiar with the percolation theory (Stauffer, 1985), it can be found that the critical exponents obtained by our analysis are the same as those for the Bethe lattice. In fact, the branching process that is introduced in this paper to model the active slip systems should form a Bethe lattice. By using the results for the Bethe lattice, one can determine the correlation length ξ of a cluster, which is also equivalent to the average size of the region occupied by those slip systems that are created by a parent slip, i.e.

$$\xi \sim (\sigma^s - \sigma)^{-\nu}, \tag{11}$$

where $\nu = 0.5$.

Now, consider the following problem: in the polycrystalline metal, each cluster of active slip systems is assumed to develop on a favorite plane, so that we can treat each cluster as a big active slip system which has an average radius ξ. We further assume that the slip systems display perfect plasticity, i.e. once it becomes active, the resistance shear stress along the slip direction keeps constant; thus, in the same way as deriving the effective constants of a solid with a random distribution of cracks [see, for example, Horri and Nemat Nasser (1983)], the overall strain can be derived in the form

$$\begin{aligned} \varepsilon &\sim \xi^3 \\ &\sim (\sigma^s - \sigma)^{-3/2}. \end{aligned} \tag{12}$$

One should bear in mind that we do not even focus our attention on any specific polycrystalline metal in deriving the macroscopic stress–strain relation (12). Thus, we believe that for any polycrystalline metal composed of elastic–perfectly plastic crystals, the exponents appearing in (12) and the other equations should be universal in the sense that they do not depend on the details of the material microstructure.

3. DETERMINATION OF THE STEADY-STATE FLOW STRESS

In contrast with the universal exponents, the critical load depends on the details of the material microstructure. For simplicity, we consider a polycrystalline metal which is composed of non-hardening FCC crystals as an example to determine its steady-state flow stress. According to the discussion in Section 2, we know that the condition for determining the steady-state flow stress is that the average number of active slip systems created by a slipping crystal is equal to one. So, we should first determine the change in the stress field produced by a slipping crystal.

For elastic–perfectly plastic crystals, when a crystal becomes active, it can be treated as in a homogeneous inclusion with a negligible shear modulus along the slip direction. Thus, the slip quantity of the slip system can be determined as a function of the external load by inclusion theory (Mura, 1987), and then the stress field around the active crystal can be calculated.

Consider an infinite matrix containing an active crystal; the elastic moduli of this crystal are different from that of the matrix since one of its shear moduli is zero due to the slip. According to the eigenstrain method in inclusion theory (Eshelby, 1957), the eigenstrain ε^*_{kl} caused by the slip in the crystal can be obtained through the following equation

$$C^{s}_{ijkl}(\varepsilon^0_{kl}+S_{klmn}\varepsilon^*_{mn}) = C^0_{ijkl}(\varepsilon^0_{kl}+S_{klmn}\varepsilon^*_{mn}-\varepsilon^*_{kl}), \tag{13}$$

where C^0_{ijkl}, C^s_{ijkl} are the elastic moduli tensors of, respectively, the matrix and the active crystal, S_{klmn} is the Eshelby's tensor, and ε^0_{kl} is the external strain field.

If we further assume that the non-active crystals are isotropic and that the crystals are of spherical shape, the eigenstrain ε^*_{ij} can be obtained in a crystal local coordinate system as

$$\varepsilon^{*L}_{ij} = \begin{cases} \dfrac{15(1-\gamma)}{2\mu(5\gamma-7)}(\sigma^L_{23}-\tau^C)(\delta_{i2}\delta_{j3}+\delta_{i3}\delta_{j2}) & |\sigma^L_{23}| > \tau^C \\ 0 & |\sigma^L_{23}| \leqslant \tau^C \end{cases}, \tag{14}$$

where μ and γ are, respectively, the shear modulus and the Poissson ratio of the material and τ^C is the critical shear stress of the crystals. From (14), one can find that ε^{*L}_{23} is the only non-zero component of the eigenstrain due to the slip in the local coordinate system.

If the active crystal is positioned at the origin, the stress field at $\vec{r}$ produced by the slip of the crystal under the external field σ^0_{ij} is given by (Mura, 1987)

$$\sigma_{ij}(r = \sigma^0_{ij}+C^0_{ijkl}\,D_{klmn}(\vec{r})\varepsilon^*_{mn}, \tag{15}$$

where $D_{ijkl}(\vec{r})$ is given by

$$\begin{aligned} 8\pi(1-\gamma)D_{ijkl}(\vec{r}) = \frac{4\pi a^3}{r^3}\Bigg[& \frac{1-2\gamma}{3}(\delta_{ik}\delta_{jl}+\delta_{jk}\delta_{il}-\delta_{ij}\delta_{kl}) \\ & + \frac{a^2}{5r^2}(\delta_{ij}\delta_{kl}+\delta_{jk}\delta_{jl}+\delta_{jk}\delta_{il})-2\gamma n_i n_j \delta_{kl} \\ & -(1-\gamma)(n_k n_j \delta_{il}+n_i n_k \delta_{jl}+n_l n_j \delta_{ik}+n_i n_l \delta_{jk}) \\ & -\left(\frac{a^2}{r^2}-1\right)(n_l n_k \delta_{ij}+n_j n_l \delta_{ik}+n_i n_l \delta_{jk}+n_j n_k \delta_{il} \\ & +n_i n_k \delta_{jl}+n_i n_j \delta_{kl}\Bigg]+\left(\frac{7a^2}{r^2}-5\right)n_i n_j n_k n_l, \end{aligned} \tag{16}$$

where a is the radius of the crystal, $r = |\vec{r}|$, and $n_i = r_i/r$.

Due to the symmetry of the FCC crystals, it is sufficient to consider one of the 24 crystallographically identical slip systems whose normal m_i and slip direction n_i are defined with respect to the grain axes by

$$m_i = \frac{1}{\sqrt{3}}[1,1,1], \quad n_i = \frac{1}{\sqrt{2}}[-1,1,0]. \tag{17}$$

The resolved shear stress τ on this system is (Hutchinson, 1970)

$$\tau = \frac{1}{\sqrt{6}}(-l_{1i}l_{1j}+l_{2i}l_{2j}-l_{1i}l_{3j}+l_{2i}l_{3j})\sigma_{ij}, \tag{18}$$

where l_{ij} are the direction cosines relating the grain axes (i) to the axes (j) of the components of the overall applied stress. Thus, the average number of active slip systems created by one slipping crystal is given by

$$m = N\int_{\infty-\Omega_0}\left(\frac{Pr(\hat{\tau}\geqslant\tau^c\,|\,\vec{r})-Pr(\tau\geqslant\tau^c\,|\,\vec{r})}{Pr(\tau\leqslant\tau^c\,|\,\vec{r})}\right)\mathrm{d}v(\vec{r}),$$
$$= 1, \tag{19}$$

where N is the average number of crystals by unit volume, Ω_0 is the region occupied by the parent slipping crystal, and

$$\tau = \frac{1}{\sqrt{6}}(-l_{1i}l_{1j}+l_{2i}l_{2j}-l_{1i}l_{3j}+l_{2i}l_{3j})\sigma^0_{ij}, \tag{20}$$

$$\hat{\tau} = \frac{1}{\sqrt{6}}(-l_{1i}l_{1j}+l_{2i}l_{2j}-l_{1i}l_{3j}+l_{2i}l_{3j})[\sigma^0_{ij}+C^0_{ijkl}\,D_{klmn}(\vec{r})\varepsilon^*_{mn}]. \tag{21}$$

$Pr(\tau\geqslant\tau^c\,|\,\vec{r})$ is the probability that the resolved stress τ is larger than the critical shear stress at $\vec{r}$. The terms in the bracket in (19) show the increment in the probability that the crystal at $\vec{r}$ becomes active due to the slip of the crystal Ω_0 under the condition that the crystal at $\vec{r}$ is not active when it is subjected to the external load σ^0_{ij}.

As an example, consider polycrystalline Cu with grain size $a = 0.03$ mm subjected to a uniaxial stress σ^0, through numerical calculation of (19), the steady-state flow stress can be obtained as

$$\frac{\sigma^s}{\tau^c} \approx 21.36. \tag{22}$$

4. THE SIZE EFFECT OF THE SPECIMEN ON THE STEADY-STATE FLOW STRESS

From the above analysis, we know that the steady-state flow stress for an infinite material corresponds to the formation of an infinitely large cluster of slip systems. For a specimen with finite size, the steady-state flow stress, which is a random variable, corresponds to the formation of a percolating cluster which connects the bounds of the specimen. For a given specimen and an external load, if we denote by R the probability of the formation of such a percolating cluster in the specimen, i.e. the probability that the load has reached its steady-state flow stress, it should depend on the external load and the size L of the specimen. According to the scaling law in percolation theory (Stauffer, 1985), when the size L is large, and the external load is near the steady-state flow stress of an infinite specimen, we can express R in the following form

$$R = \Psi[(\sigma^{s} - \sigma)L^{1/\nu}]. \tag{23}$$

The derivative of R gives the probability density function of the steady-state flow stress for a finite-size specimen

$$\frac{dR}{d\sigma} = -L^{1/\nu}\Psi'[(\sigma^{s} - \sigma)L^{1/\nu}]. \tag{24}$$

The average steady-state flow stress $\langle\sigma\rangle_s$ for a finite-size specimen is given by

$$\begin{aligned}
\langle\sigma^{s} - \sigma\rangle &= \sigma^{s} - \langle\sigma\rangle_s \\
&= \int(\sigma^{s} - \sigma)\frac{dR}{d\sigma}\,d\sigma \\
&= \int(\sigma^{s} - \sigma)L^{1/\nu}\Psi'[(\sigma^{s} - \sigma)L^{1/\nu}]\,d\sigma \\
&= \int Z\Psi'(Z)L^{-1/\nu}\,dZ \\
&\sim L^{-1/\nu},
\end{aligned} \tag{25}$$

where $\nu(=0.5)$ is determined by (11).

The mean square deviation of the steady-state flow stress can also be determined by the following equation

$$\Delta^2 = \int(\sigma - \langle\sigma\rangle_s)^2\frac{dR}{d\sigma}\,d\sigma. \tag{26}$$

One obtains

$$\Delta \sim L^{-1/\nu}. \tag{27}$$

5. CONCLUSIONS

The evolution of the microstructure of polycrystalline metals during the plastic deformation was modeled by a stochastic process. By investigating the convergence properties of such a process, we developed a method to determine the steady-state flow stress. When the external load approached its steady-state flow stress, the overall strain was found to go to infinity by a simple power law with a critical exponent $-3/2$. For large specimens, the size effect of the specimens on the steady-state flow stress can be expressed in the form

$$\langle \sigma^s - \sigma \rangle = \sigma^s - \langle \sigma \rangle_s \sim L^{-2}, \quad L \to \infty, \tag{28}$$

where σ^s is the steady-state flow stress for infinite specimens, and $\langle \sigma \rangle_s$ is the average steady-state flow stress for the specimens with size L. We believe that the exponents predicted by the model should not be sensitive to the material microstructure, and reflect some universal behavior when the external load is near its critical value in the same way as their counterparts in the second-order phase transition problems. Furthermore, some general characteristics of the material microstructure at the steady flow state were also predicted.

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