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A Constitutive Description of the Slip-Twinning Transition in Metals

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ABSTRACT

A constitutive approach is developed that predicts the critical stress for twinning as a function of external (temperature, strain rate) and internal (grain size, stacking- fault energy) parameters. Plastic deformation by slip and twinning being competitive mechanisms (it is, of course, recognized that twinning requires dislocation activity), the twinning constitutive relationship is equated to a slip relationship based on the plastic flow by thermally assisted movement of dislocations over obstacles (the Voehringer and Zerilli-Armstrong equations); this leads to the successful prediction of the slip-twinning transition. The model is applied to cubic and hexagonal metals and alloys: Fe, Cu, brasses, and Ti. As a consequence of the model, the critical twinning stress in shock-wave deformation can be predicted, using the Swegle-Grady equation which relates the shock stress to the strain rate at the shock front . This enables the prediction of the critical shock pressure for twinning.

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1. Introduction

The response of metals and ceramics to mechanical stresses can produce the following structural changes: slip (by dislocation motion),twinning, phase transformations, and fracture. Slip and fracture have received the greatest amount of attention from both theoretical and experimental researchers for the past sixty years. Mechanical twinning and displacive (martensitic) transformations are also a significant response and can dominate under specific deformation conditions. Whereas dislocation motion is highly sensitive to strain rate and temperature(e.g., Becker[1] and Seeger[2-4]),twinning has a much lower sensitivity to the above parameters. Nevertheless, it is well known that dislocation activity is intimately connected with twinning nucleation and growth. Mechanical twinning has been recently reviewed comprehensively by Christian and Mahajan [5] and there are a significant number of overview treatments[6-11].

There has been, in recent years, a considerable effort in the development of constitutive equations to describe plastic deformation of metals based on the fundamental aspects of dislocation motion, impeded by a variety of barriers. Cottrell [12], Seeger [13], and Mott[14] were the early workers, while Ono[14], Voehringer[15], and Kocks et al. [16] varied the barrier shape and configuration to arrive at very satisfactory descriptions of the constitutive response. These ideas were incorporated into equations that are an important component of large-scale computational codes; prominent are the Zerilli-Armstrong[17,18] and the MTS [19] constitutive equations. It is surprising that relatively little effort as been directed toward the incorporation of mechanical twinning into constitutive models. Notable exceptions are the constitutive equation developed by Armstrong and Worthington[20] and the recent computational and experimental efforts by Zerilli and Armstrong [21],showing that twinning can play a significant role. In the shock -wave regime, Meyers et al.[22] obtained results on copper that showed clearly that the threshold pressure for twinning was grain-size dependent. Murr et al. [23] further developed the formalism proposed by Meyers et al. [22] to tantalum and were able to predict a threshold pressure for twinning in Ta. Therefore, the research effort whose results are presented here had two primary objectives:

1. to develop a constitutive description for the onset of twinning,
2. to apply this constitutive description to the shock-wave regime and to obtain a predictive capability of the threshold pressure for twinning that is general and can be applied to all metals.

2. The Twinning Stress

There are excellent overviews, such as the recent work by Christian and Mahajan[5] on the effects of material and external parameters on the twinning stress. Three of these aspects, relevant to the constitutive description implemented here, are discussed below. The critical event in twinning is, for most cases, nucleation. Growth can occur at stresses that are a fraction of the nucleating stress[7,15,16].It has been known for a long time that the local stress , required to nucleate twinning, is considerably higher than the homogeneous stress resulting from the external tractions. The possibility of homogeneous nucleation of twins in near perfect HCP crystals was reported by Bell and Cahn[24] and Price[25]; their results, however, can also be interpreted as twinning being normally initiated by some defect configuration , because of the requirement of much higher stress for the homogeneous nucleation. A number of nucleation and growth mechanisms have been proposed and their description transcends the scope of this paper. Nucleation mechanisms for FCC metals were proposed by Suzuki and Barrett[26], Haasen and King[27], Miura et al. [28], Cohen and Weertman [29], Venables[30], Sleeswik[31], Mahajan and Chin[32], Bolling and Richman[33], among others. For BCC metals , Cottrell and Bilby [34], Sleeswyk[35], Hirth[36], and others proposed or extended mechanisms. An interesting alternative to the above mechanisms, all based on dislocation reactions, is the proposal by Orowan[37]that twins nucleate homogeneously.

Effect of temperature and strain rate. Figure 1 shows a compilation of twinning stresses vs. temperature for a number of metals(both mono and polycrystals).The striking aspect is that there seems to be a critical stress that is temperature insensitive. This issue has been debated in the literature, and there are diverging results. Bell and Cahn [24] observed a large scatter in single crystals. This could, however, be attributed to stress concentration sites other than pile ups(surface notches, internal flaws, etc). Hence , a distribution of twinning stresses, similar to a Weibull distribution for ceramic strength, would be expected. There are also reports of gradual decrease in the twinning stresses with increasing temperature for FCC metals, by Bolling and Richman[33] and Koester and Speidel[38]. Christian and Mahajan [5] discuss this topic in detail. Mahajan and Williams [9] suggested that BCC metals have a negative dependence of twinning stress on temperature, while FCC metals have a slightly positive temperature sensitivity. However, Reed-Hill [8], based on the work on BCC Fe_3Be by Bolling and Richman [31], concluded that whenever the deformation proceeds primarily by twinning, the flow stress tend to have a positive temperature dependence and a negative strain rate dependence. For the purposes of the subsequent calculations, it will be assumed that there is a critical stress for twinning that is temperature independent. For the FCC and HCP structure the strain rate dependence of the twinning stress has not received the same degree of attention, and the only account in which the strain rate is varied over a very broad range is to the authors' knowledge the work of Harding[40,41] on monocrystalline iron, shown in Figure 1. The twinning shear stress at 10^3 s^{-1} is approximately 220 MPa, whereas it is equal to 170 MPa at 10^{-3} s^{-1}. This result is used in a simple constitutive equation for twinning presented in Section 3, but additional experiments are clearly necessary to establish the strain rate dependence.

Effect of grain size. Another highly unique characteristic of twinning, first pointed out by Armstrong and Worthington[20],is the larger grain size dependence of the twinning stress, as compared with the slip stress. For most cases, a Hall Petch relationship is obeyed, but with a slope, k_T, that is higher than the one for slip, k_S:

$$\sigma_T = \sigma_{0T} + k_T d^{-\frac{1}{2}} \tag{1}$$

The Hall-Petch slope for twinning been found by Vöhringer[42] to significantly exceed the one for slip for copper; $k_T = 0.7$ MN/m$^{3/2}$ and $k_S \cong 0.35$ MN/m$^{3/2}$. Recent evidence by Song and Gray[45] suggests that the Hall-Petch slope of zirconium for twinning ($k_T \cong 2.4$ MN/m$^{3/2}$) is ten times the one for slip ($k_S \cong 0.25$ MN/m$^{3/2}$). Table I is a compilation of data for BCC, FCC, and HCP metals from a number of sources. The reason for this difference is not fully understood, but Armstrong and Worthington [20] suggest that twinning is associated with microplasticity, i. e. , dislocation activity occurring before the onset of generalized plastic deformation, whereas the yield stress is associated with generalized plastic deformation.

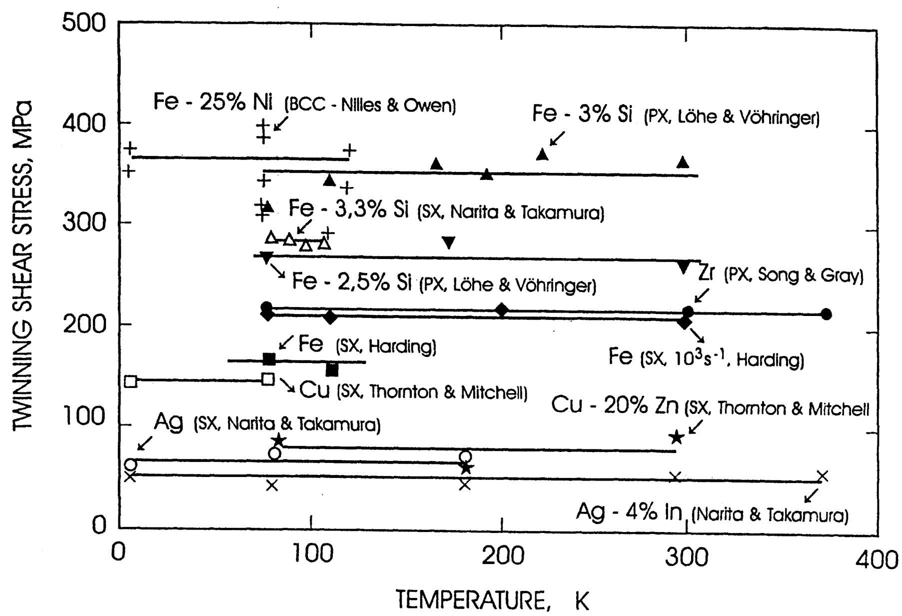


Figure 1. Twinning stress as a function of temperature for a number of metals (both mono and polycrystals).

Effect of stacking-fault energy. It is well known that the twinning stress increases with increasing stacking-fault energy. This is true for mostly for FCC metals, where the classic plot by Venables[30] shows this effect very clearly. However, the strong decrease in the twinning stress when Mo is alloyed with Rh has also been attributed to a stacking-fault decrease[50]. Figure 2 shows a compilation of results by Venables[30] and Voehringer[51].The twinning stress for a number of copper alloys is shown to vary with the square root of the stacking-fault energy, γ_{SF}. There have been a number of analytical predictions of this effect, due to Venables[30], Friedel[51], Suzuki and Barrett[26], and Narita and Takamura[10].This effect is critically discussed in Section 5 and a relationship is proposed.

3. AN ANALYTICAL DESCRIPTION OF THE TWINNING STRESS

In general, the tendency for the occurrence of mechanical twinning in BCC and HCP metals is quite conspicuous at high strain rates and low temperatures, Since the flow stress can be effectively raised up to the level required for twin formation because of their high strain rate sensitivity. In BCC metals, twinning usually occurs prior to macro-yielding, and in many cases it is inhibited by significant plastic deformation. In FCC metals, which have a much lower strain-rate sensitivity, but higher work hardening ability, twinning often occurs after significant plastic deformation. Therefore, the analysis presented in this section does not apply to FCC metals; it is felt that dislocation pile-up formation is restricted after substantial plastic deformation.

TABLE I Comparison of Hall-Petch Slopes for Slip and Twinning

Material	H-P slope slip, k_s MPa*mm1/2	H-P slope twinning, k_T MPa*mm1/2
BCC		
Fe-3wt%Si(Hull)	10.4(RT) 17.64(77K)	38.48
Fe-3%wtSi(Loehe&Voehringer)	12	100
ArmcoFe(Loehe&Voehringer)	20	124
Armco Fe (Moiseev&Trefilov)		90
Steels:1010,1020,1035 (Loehe&Voehringer)	20	124
Fe-25at%Ni (BCC) (Nilles&Owen)	33	100
Cr(Marcinskowski&Lipsitt)	10.08	67.75
Va(Lindley&Smallman)	3.46(20K)	22.37
FCC		
Cu(Voehringer)		21.6(77K)
(Meyers et al.)	5.4(RT)	
(Zerilli&Armstrong)	5.2(RT)	
Cu-6wt%Sn	7.1	11.8(77K)
Cu-9wt%Sn	8.2	7.9(295 K)
Cu-10wt%Zn	7.1	15.7(77K)
Cu-15wt%Zn	8.4	11.8(77 K) 16.7(295 K)
(Voehringer ; Koester&Speidel)		
HCP		
Zr(Song&Gray)	8.25	79.2
Ti (Okazaki&Conrad)	6(78 K)	18(4 K)

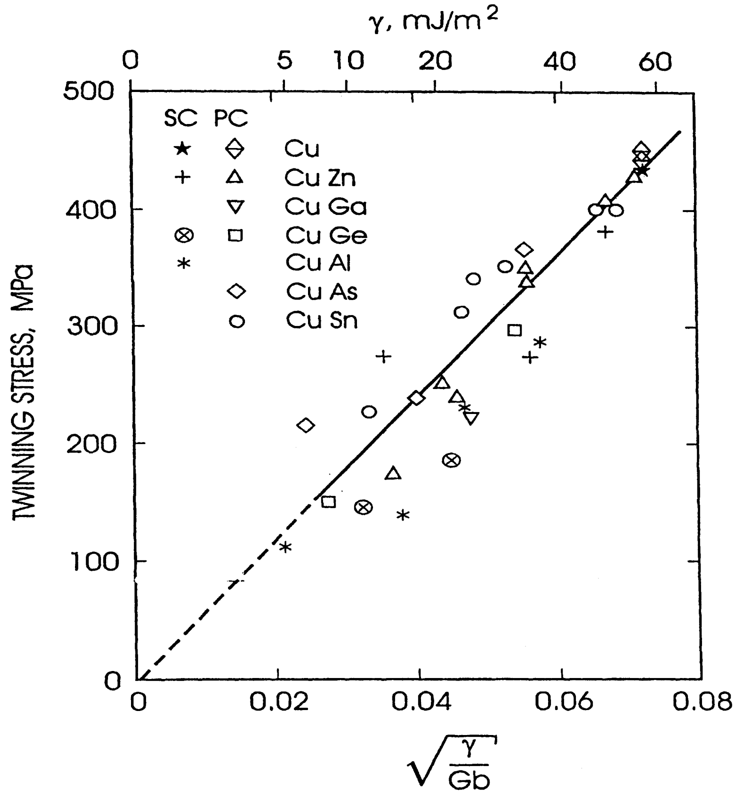
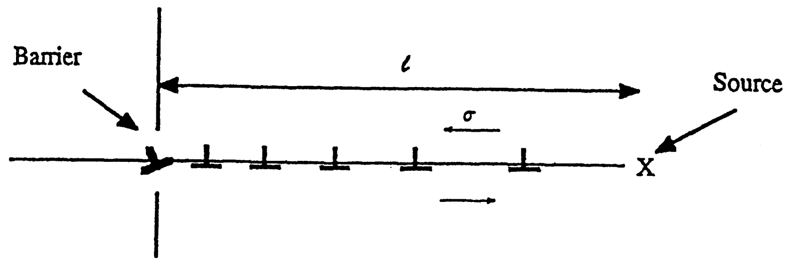


Figure 2. Twinning stress as a function of stacking fault energy for copper and copper solid solutions .

A simple constitutive twinning model is developed below. It is based on the stress concentration generated by a pileup due to the activation of a Frank Read or Koehler [53] source. A dislocation pile-up is created by a dislocation source, such as a Frank-Read source or a Koehler source, as shown in Figure 3(a).The number of dislocations piled up is determined by the distance, l, between the source and barrier and the applied stress. The local stress in front of the barrier is equal to the product of the applied stress and the number of piled-up dislocations. If a unique threshold twinning stress exists, the macroscopically measured twinning stress, or applied stress, will strongly depend on the microstructure of the sample because the distance, l, is microstructure-dependent. The initiation and propagation of the twin in a neighboring grain are shown. The velocity of dislocations traveling from the source to the barrier is given by Johnston-Gilman equation [52]:

$$v = A\tau^{m}e^{-Q/RT} \qquad (2)$$

where τ is the stress acting on the dislocation, Q is the activation energy, and A and m are constants. This equation applies to the low-velocity regime, before viscous drag and relativistic effects come into play. The time for an individual dislocation to travel from source to barrier is:



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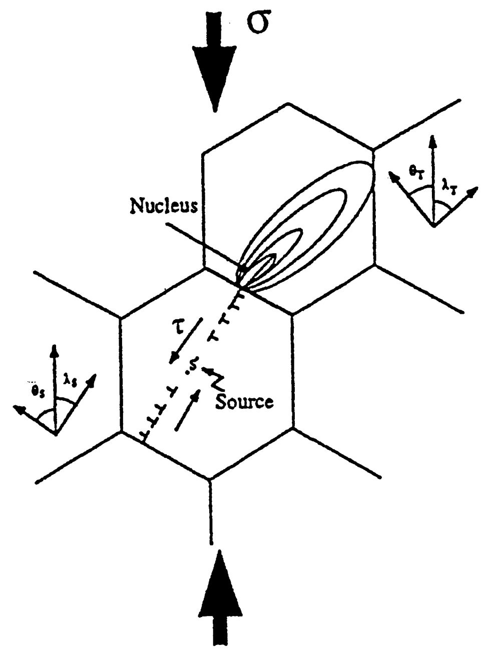


(b)

Figure 3(a) Schematic of edge dislocations piled up at a barrier [3].
(b) Frank-Reed or Koehler source creating pile-up at grain boundary and twinning in neighboring grain

$$t_l = \frac{l}{\upsilon} \quad (3)$$

If the number of dislocations at a pile-up required for twinning is n^*, the local stress in front o the pile-up, τ_i, is

$$\tau_i = n^* \tau_{AP} \quad (4)$$

where τ_{AP} is the externally applied stress. Assuming, to a first approximation, that the time fo all the dislocations arriving at the pile-up traveling from source is the same and equal to t_l, th total time required to build up the dislocation pile-up is then equal to:

$$t = n^* t_l \quad (5)$$

This assumes that no two dislocations are simultaneously traveling to the barrier. Insertin Eqns. 2 and 3 into Eqn. 5, one obtains:

$$t = \frac{n^* l}{A \tau^m} e^{Q/RT} \quad (6)$$

Because microslip occurs in the elastic stage, the relationship between stress and strain in a uniaxial loading configuration is:

$$E = \frac{\sigma}{\varepsilon} \quad (7)$$

or $$E = \frac{\sigma}{\dot{\varepsilon} t} \quad (8)$$

Substituting Eqn. 6 into Eqn. 8 and using

$$\sigma = M\tau$$

$$\sigma_{0T} = M\left(\frac{n^* l E}{A}\right)^{\frac{1}{m+1}} \dot{\varepsilon}^{\frac{1}{m+1}} e^{\frac{Q}{(m+1)RT}} = K \dot{\varepsilon}^{\frac{1}{m+1}} e^{\frac{Q}{(m+1)RT}} \quad (9)$$

This equation is applied to iron in order to establish the strain rate and temperature dependenc of twinning. The experimental results of Stein and Low [57] for Fe-3wtSi are used for m (=36 and Q(=51.66kJ/mole). The activation energy was obtained by plotting the dislocation velocit (at a constant stress) as a function of 1/T. The term $K=2(n^* lE/A)$ is obtained by fittin Equation 9 to the experimental results reported by Harding[40,41]for the twinning stress. Th following equation is obtained:

$$\sigma(in \ \ MPa) = 380 \dot{\varepsilon}^{1/37} e^{0.17/T} \quad (10)$$

The results are shown in Figure 4 for slip. The Zerilli-Armstrong equation for BCC metals, with parameters given by Zerilli and Armstrong [18], was used

$$\sigma = \sigma_G + C_1 \exp(-C_3 T + C_4 T \ln \dot{\varepsilon}) \qquad (11)$$

The parameters are given in Table II. It can be seen that the slip and twinning response differ drastically. Twinning exhibits a very low temperature dependence; below 20K, the Gilman equation breaks down, because the stress goes to infinity. It is known that this is physically incorrect and an equation of the Seeger's form, incorporating barriers of specific height and shape, would be preferable. An important conclusion that can be drawn from Figure 4 is that the slip-twinning intersection is strongly dependent on strain rate. So it increases from 120K, at 10^{-3} s^{-1} to 200K, t 10^{3} s^{-1}.

4. CONSTITUTIVE DESCRIPTION OF THE SLIP-TWINNING TRANSITION

The rationale to be used in this section is: the onset of twinning occurs when the slip stress,, σ_S, becomes equal to the twinning stress, σ_T:

$$\sigma_T = \sigma_Y \qquad (12)$$

This rationale will be applied to typical metals representative of the three crystalline systems of greatest importance for metals: Fe(BCC), Cu(FCC), Ti (HCP). It should be noted that no attempt was made, at the present stage, to compare the calculated slip-twinning transitions with experimental results on the initiation.

a) *Iron (BCC).* The constitutive equations given in Section 3(Eqns. 9 and 11) are applied to Eqn. 12, with the addition of the Hall-Petch terms for slip and twinning, k_S and k_T, respectively. This leads to

$$\sigma_G + K e^{\frac{1}{m+1}} e^{\frac{Q}{(m+1)RT}} - C_1 e^{-(C_3 - C_4 \ln \dot{\varepsilon})T} + (k_T - k_S) d^{-\frac{1}{2}} = 0 \qquad (13)$$

Figure 5(a) shows the slip and twinning curves for strain rates of 10^{-6}, 10^{-3}, 10^{0}, 10^{3}, and 10^{6} s^{-1} for iron with 100 μm grain size. The intersections of these curves are given by the solution of Eqn. 13. Figure 5(b) shows the slip-twinning transition for different grain sizes. The effect of grain size is clearly seen and is due to the fact that $k_T > k_S$. The values for k_T and k_S are given in Table I. The twinning domain for monocrystalline iron is much larger than for polycrystalline iron.

b)*Copper (FCC).* It was not possible to apply the constitutive equation for twinning given in Section 3 to copper. Attempts were made at obtaining the activation energy and dislocation velocity exponent m from Jassby and Vreeland [59] ,Greenman et al.[60] Kleintges and Haasen [61] , and Suzuki and Ishi[62]. Jassby and Vreeland [59] only report dislocation velocities of 10 cm/s and higher; this results in low value for m and unacceptably high temperature and strain rate sensitivity for the twinning stress. Therefore, it was decided to simply use the twinning stress determined experimentally. Thornton and Mitchell[46] report a shear twinning stress for monocrystalline copper of 150 MPa and this value is taken. The Hall-Petch slope for twinning is given in Table I and was obtained by Voehringer[42]; it is equal to

Table II Parameters for Zerilli-Armstrong[17,18] and twinning equation for iron

Zerilli-Armstrong Parameters	
σ_{0G} (MPa)	0
C_1(MPa)	1033
C_3(K^{-1})	0.00698
X_4 (K^{-1})	0.000415
Twinning Eqn. Parameters	
K (MPa)	380
m	36
Q (kJ)	51.66

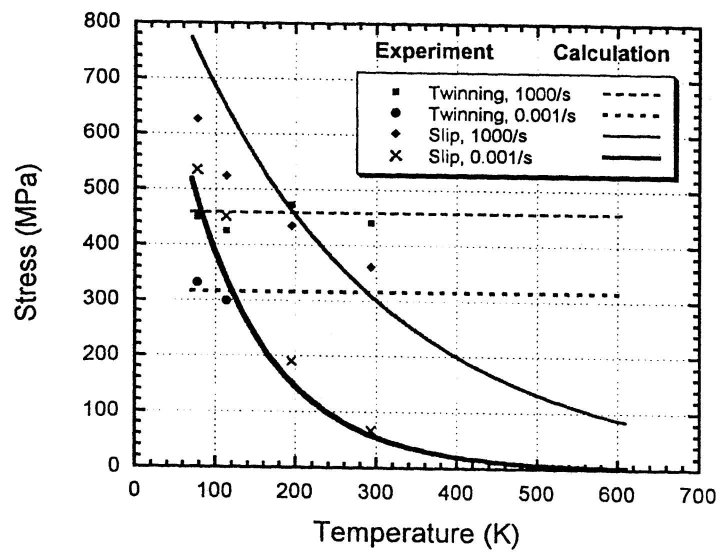


Figure 4 Comparison between the computed and the experimental stresses for slip and twinning in single crystal iron (data from Harding [41,42])

21.6 MPa*mm$^{1/2}$ .The slip response was modeled by the Zerilli-Armstrong equation for FCC metals, with parameters given in Table III. The equation is:

$$\sigma = \sigma_G + C_2\varepsilon^n \exp(-C_3T + C_4 \ln \dot{\varepsilon}) + k_s d^{-1/2} \quad (14)$$

The constitutive responses are shown in Figure 6 , at two levels of plastic strain; 0.2 and 0.8.It is seen that no twinning is obtained at 0.2 ,but that at 0.8 twinning occurs for all strain rates, for the grain size of 10 μm.

The slip-twinning transition as a function of grain size is shown in Figure 7(a). This is done for a plastic strain of 0.2. The effect of grain size is dramatic and influences the occurrence of twinning in a significant way. The effect of plastic strain is more clearly seen in the slip-twinning transition plot of Fig. 7(b).These calculations were done for a constant grain size of 10 μm . A plastic strain of 0.3 is necessary to initiate twinning . At ambient temperature, a strain rate of $5*10^3$ s^{-1} and strain of 0.8 are required to produce twinning.

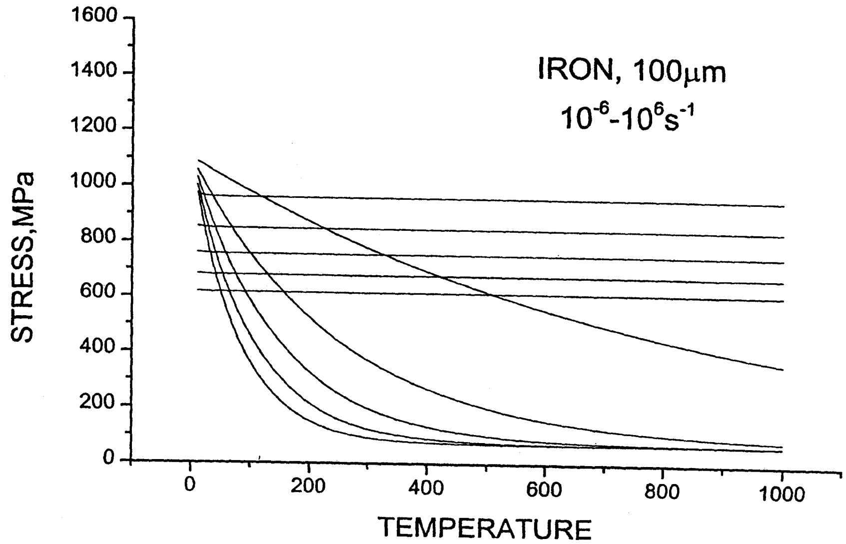
c) Titanium (HCP). Zerilli and Armstrong [3, 64] have demonstrated that the constitutive response of BCC metals can represent the behavior of titanium, with a few modifications to incorporate the decrease in work hardening rate as the temperature is increased. The equation is:

$$\sigma = \sigma_G + C_1\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)^{-C_3T} + \frac{C_2}{e^{-C_4T}}\varepsilon^n + k_s d^{-1/2} \quad (15)$$

The term e^{-C_4T} decreases the work hardening as T increases. The twinning stress is simply represented by:

$$\sigma_T = \sigma_{To} + k_T d^{-1/2}$$

Gray [65] reported a greater propensity for mechanical twinning of large grain sized(240 μm) than smaller grain sized(20 μm) Ti in dynamic testing , in accordance with the assumption that $k_T > k_S$ .Conrad et al. [66] report similar effects. The critical twinning stress is reported by Zerilli and Armstrong[64]. It is known that interstitials have a major effect on the mechanical response of Ti[67]. For instance, the yield stress of Ti at RT increases from 150 to 600 MPa, when the oxygen equivalent (O+N+C) percentage is increased from 0.1 to 1.0 %. This effect is more important than the grain size, where the yield stress increases from 450 to 600 MPa when the grain size is decreased from 1.5mm to 1.5 μm(for 1%Oeq.). The Hall Petch slope for slip was obtained by Okazaki and Conrad[67] and was found to be relatively insensitive to interstitial content. Conrad et al. [66] report twinning shear stresses in monocrystalline Ti, for ($(10\bar{1}2)$ and $(11\bar{2}1)$ planes, between 420 and 380 MPa, respectively. These twinning stresses decrease with decreasing temperature. Taking a value of 800 MPa for the normal stresses, the slip-twinning transition was estimated for grain sizes of 3, 10, and 100 μm . These values are given in Figure 8. It should be noted that the calculations were carried out for Marz titanium, with 0.1 Oeq. and not with the material given by Zerilli and Armstrong[63], which has Oeq. ~1% and a yield stress at ambient temperature and 10^{-3} s^{-1} of 400MPa.The interstitial content has a significant effect on the twinning stress, as discussed by Conrad et al. [66]. The rise in the twinning stress with interstitial content is more significant than the slip stress; this explains why the tendency for twinning decreases with interstitial increase. The effect of interstitials manifests itself in both the thermal and athermal components of the stress, and Conrad et al.



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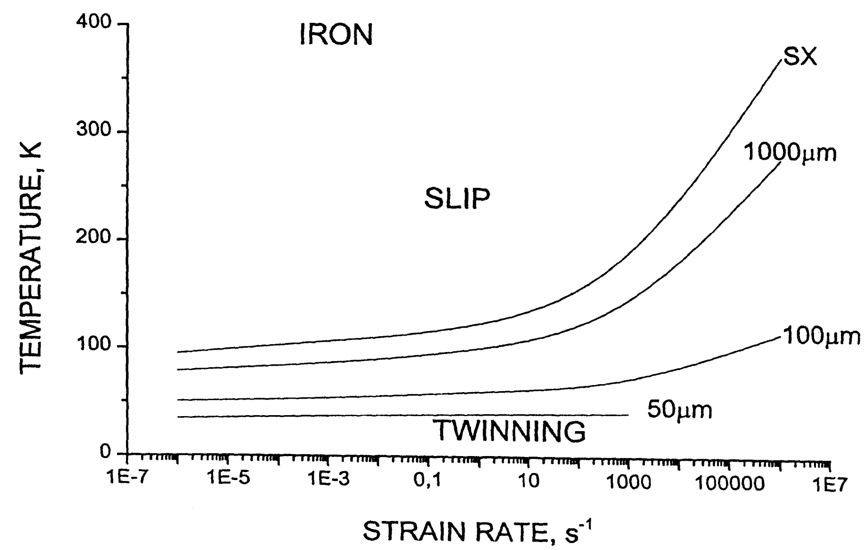


(b)

Figure 5 (a) Calculated slip and twinning stresses for monocrystalline iron (G. S. 0.1mm) as a function of strain rate
(b) Calculated slip- twinning transition for iron of different grain sizes.

Table III. Zerilli-Armstrong parameters for Cu and Ti

	Cu	Ti
σ_G	46.5 MPa	0
C_1	—	990
C_2	890 MPa	700
C_3	0.28×10^{-3} K^{-1}	1.06×10^{-3}
C_4	1.15×10^{-4} K^{-1}	6.8×10^{-4}
C_5	—	—
n	0.5	0.5
k_s	5 MPa $mm^{1/2}$	6 MPa $mm^{1/2}$

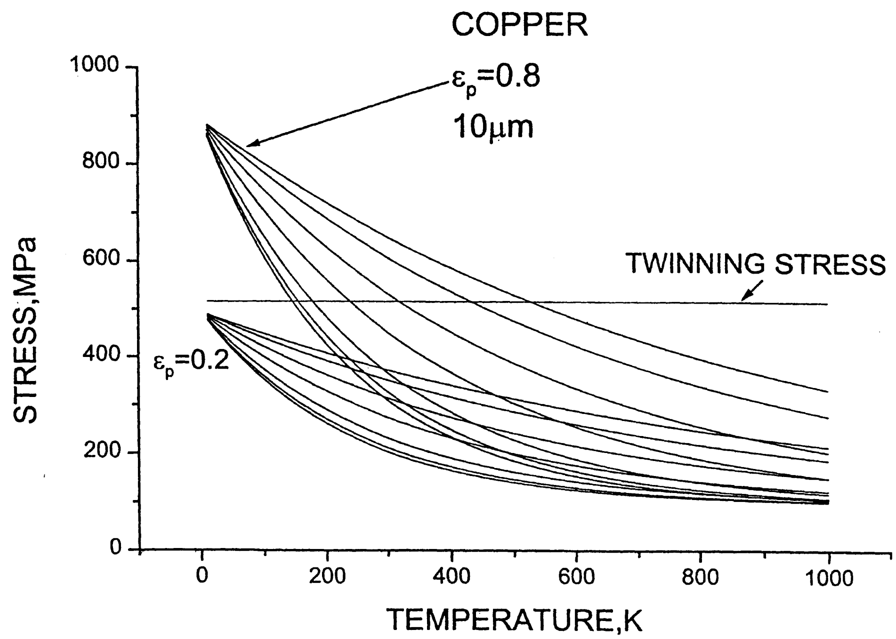
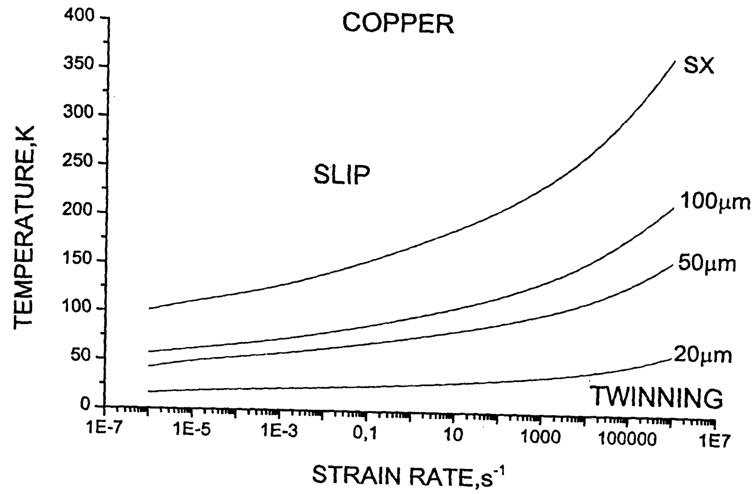


Figure 6 Twinning and calculated slip stresses (at two levels of plastic strain) for 10 μm grain size copper.



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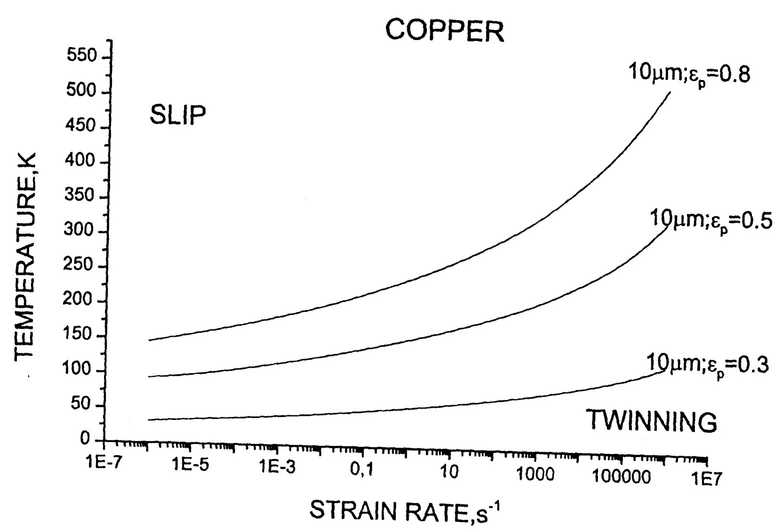


(b)

Figure 7 (a)Calculated slip-twinning transition for copper of different grain sizes.
(b)Calculated slip-twinning transition for 10 μm copper, for different plastic strain levels.0.3, 0.5, 0.8.

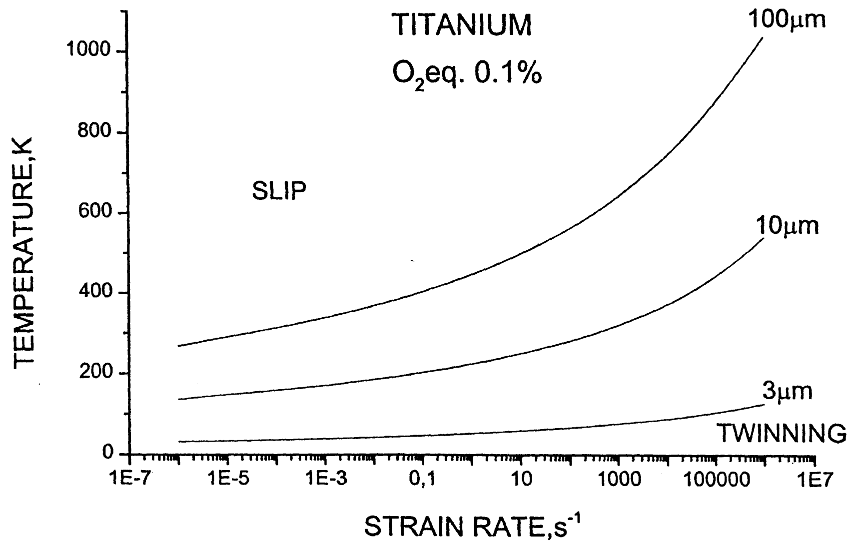


Figure 8. Calculated slip-twinning transition for titanium of different grain sizes

[66] give a value of $\Delta\tau = 0.02\ C_i^{1/2}$ at 300 K, where C_i is the atomic concentration of interstitials. This value can be used to modify the Zerilli-Armstrong equation for HCP metals (Eqn. 15):

$$\sigma = \sigma_G + C_1\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)^{-C_3T} + \frac{C_2}{e^{-C_4T}}\varepsilon^m + 0.02GC_i^{1/2} + k_s d^{-1/2} \qquad (16)$$

5. EFFECT OF STACKING -FAULT ENERGY

Figure 2 shows the significant effect of the stacking-fault energy, γ, on the twinning stress for FCC metals. As an illustration of the effect of SFE on the incidence of twinning , the Cu-Zn system is analyzed. Gallagher[68] and Voehringer[69] correlated the SFE to the e/a ratio in copper alloys and arrived at the following expression:

$$\ln\gamma = \ln\gamma_{Cu} + K_1\left(\frac{C/C_{max}}{1 + C/C_{max}}\right)^2 \qquad (17)$$

γ_{Cu} is the stacking fault energy for copper and C is the concentration of solute atoms. C_{max} is the maximum concentration of the solute. The best fit was obtained with K_1=12.5; γ_{Cu} =57±8 mJ/m^2. Eqn. 17 can be combined with the mathematical representation of Figure 2:

$$\sigma_T = K_2\left(\frac{\gamma}{Gb}\right)^{1/2} \qquad (18)$$

A good fit is obtained with K_2=6 GPa. Substitution of Eqn17 into Eqn18 yields:

$$\sigma_T = \frac{K_2}{(Gb)^{1/2}} \exp\left[\ln \gamma_{Cu} + K_1 \left(\frac{C^*}{1+C^*} \right)^2 \right]^{1/2} \tag{19}$$

The effect of solid solution (Zn, Ag, Al, Sn, Ge) atoms on the mechanical response of Cu has been established quite carefully; the effects of these solutes on the Hall Petch equation has also been established. Voehringer[69] proposed the following expression, which is used for the yield stress:

$$\sigma_s = \sigma_G + \sigma^* + k_s d^{1/2}$$

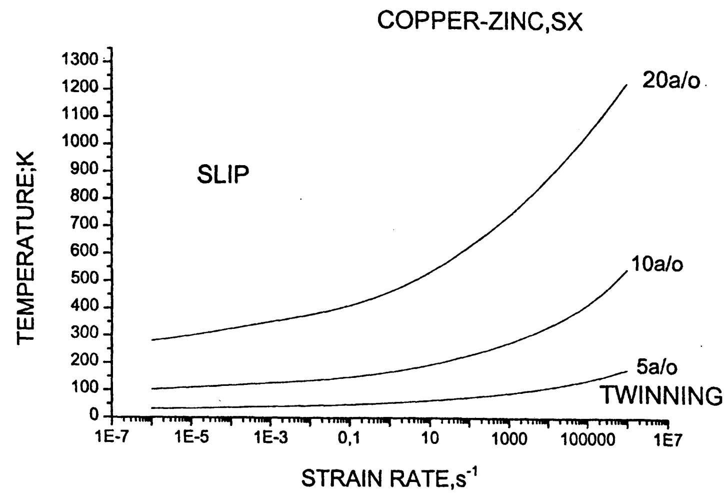
$$= \sigma_0 + K_3 \varepsilon_L{}^{4/3} C^{2/3} + \left[\left(\sigma^* + K_4 \varepsilon_L C^{2/3} \right) \left(1 - \frac{k \ln \dot{\varepsilon}_0 / \dot{\varepsilon}}{\Delta G_0} \right)^{1/p} T^{1/p} \right]^{1/q} + k_s d^{-1/2} \tag{20}$$

Eqn.20 is based on the overcoming of short-range obstacles , that have the shape dictated by the parameters p and q. The effect of the solid solution atoms is manifested (both in the thermal and athermal components of stress) through the $C^{2/3}$ relationship and Labusch parameter ε_L, which has different values for different solid solution atoms. K_3 and K^*_4, are parameters, and ε_0 is a reference strain rate, that was taken by Voehringer[69] as $10^{20}s^{-1}$.
The effect of work hardening can be incorporated into Eqn. 20 by adding the term $C_2\varepsilon^n$ to the thermal component of stress, since work hardening increases, in FCC metals, the density of forest dislocations, which constitute short-term barriers. The parameters that were used for the Cu-Zn are given in Table IV.

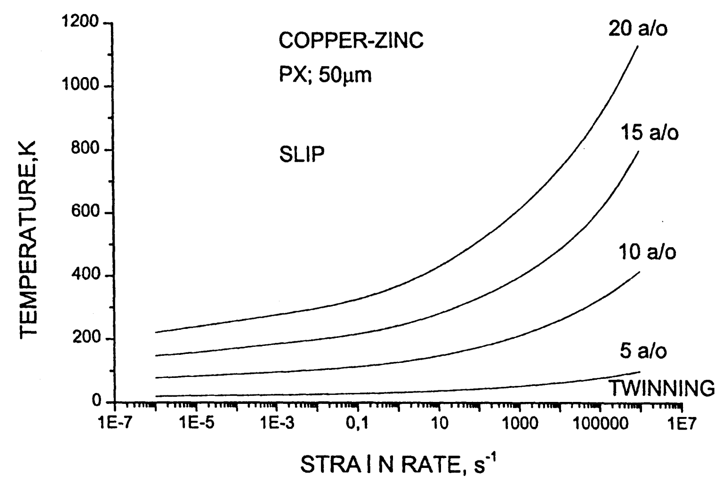
Table IV. Slip and Twinning Parameters for Cu-Zn Alloys (from Vöhringer [15, 42])

Slip		**Twinning**	
K_3(MPa)	96	K_1 (MPa)	12.5
K_4(MPa)	300	K_2 (MPa)	6000
$\ln \dot{\varepsilon}_0$	20	γ_{Cu} (mJ/m^2)	57±8
ε_L	0.98	G (GPa)	43
p	3/2	B (nm)	0.3
q	1/2	k_T (MPamm$^{1/2}$)	16
k_s (MPamm$^{1/2}$)	8.2		
ΔG_0(J)	$1.6\text{x}10^{-7}$		

The results of the calculations are represented in the slip-twinning transition plots of Figure 9, in which Eqns. 19 and 20 were used. These calculations were carried out for different Cu-Zn alloys: 5, 10, 15, and 20% at Zn. Figure 9(a) shows the results for monocrystalline brass, while Figure 9 (b) shows the results for a grain size of 50μm. It is clear that the addition of Zn increases the propensity for twinning, displacing the slip-twinning transition upwards. By using Eqn.20 with the addition of the term $C_2\varepsilon^n$ it is possible to establish the onset of twinning after



(a)



(b)

Figure 9. Calculated slip-twinning transition for Cu-Zn brasses, (a) moncrystal; (b)polycrystal grain size 50μm.

different amounts of plastic deformation. Since Cu-Zn is FCC, the occurrence of twinning can occur after significant plastic deformation.

6. IMPLEMENTATION IN THE SHOCK REGIME

It has been demonstrated that the threshold stress for twinning is orientation dependent by De Angelis and Cohen[71]. This response is analogous to the quasi-static one, in which we assume a threshold stress for twinning. These threshold pressures were experimentally determined by Murr [72] and correlated to the stacking-fault energy in FCC metals.

It is possible to extend the prediction of the slip-twinning transition to the shock compression regime; this enables the calculation of the threshold shock stress for twinning. Up to this time, only empirical relationships have existed, and the most noteworthy correlation is the plot developed by Murr [12]. Under shock compression, the strain rates can be calculated through the phenomenological relationship obtained by Swegle and Grady [73,74], by measuring the shock-wave profiles for a number of materials. Swegle and Grady [73,74] determined the strain rate at the shock front as shown schematically in Figure 10. The rise of the shock front was estimated to be linear and the two positions (up and down) were used to calculate the total rise time. The strain rate was calculated by using the shock strain, ε and dividing it by the rise time, (x_0-x_1) / v. These profiles enabled the determination of strain rates which are plotted together with the data from Swegle and Grady [73,74] in Figure 11. The following relationship was experimentally observed:

$$\dot{\varepsilon} = K_5 \sigma_{sh}^{\ 4} \tag{21}$$

where k is material dependent and σ_{sh} is shock stress. The unique significance of Swegle and Grady's [73,74] relationship is the universality of the exponent 4, which still not completely understood. However, Swegle and Grady did not characterize tantalum. Furnish et al. [75] and Steinberg [76] obtained shock-wave profiles for tantalum at pressures of 8 and 12 GPa. The Swegle - Grady relationship is obeyed (Eqn 21) and k = 27.34 s^{-1} $(GPa)^{-4}$ is obtained. The application of Eqn. 21 enables the prediction of the critical shock pressure of the slip-twinning transition from the critical strain rates obtained by solving any of the equations presented in the previous sections. As an illustration, a BCC metal is chosen , and Eqn. 21 is applied to Eqn. 13.

$$K\left(K_5 \sigma_{sh}^{\ 4}\right)^{\frac{1}{1+m}} e^{\frac{1}{T}} - C_1 e^{-\left(C_3 - C_4 \ln K \sigma_{sh}^{\ 4}\right)T} + \left(k_T - k_S\right) d^{-\frac{1}{2}} = 0 \tag{22}$$

Eqn. 22 gives the shock stress for the onset of twinning as a function of temperature and grain size. A graphical representation of Eqn. 22 for five temperatures (77, 200, 300, 450, and 600 K) for tantalum is shown in Figure13 . The grain size is decreased , the threshold stress, σ_{sh}, increases. A similar grain size dependence of the shock stress for twinning in copper was observed by Meyers et al.[22].

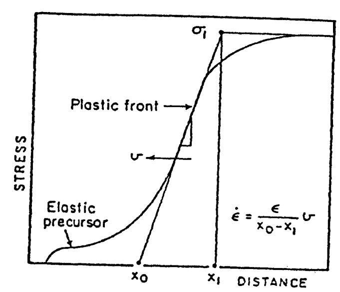


Figure 10 Schematic of the determination of the strain rate at shock front from the measured shock profile.

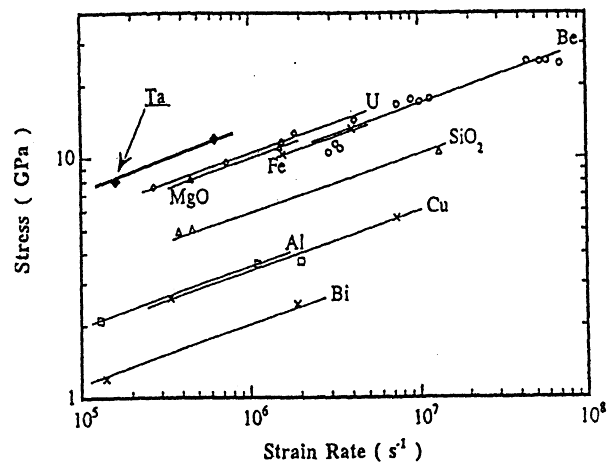


Figure 11 Swegle - Grady plot [73, 74] relating peak stress and strain rate at the shock front; tantalum data by Steinberg and co-workers [76].

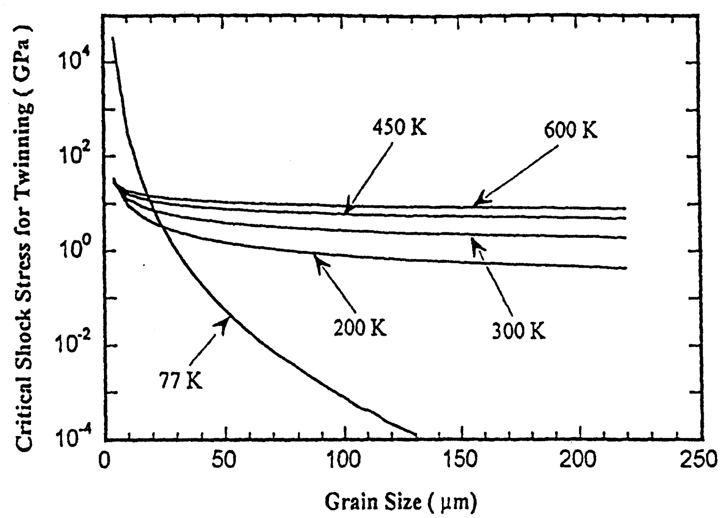


Figure 12 Calculated shock threshold pressure in tantalum vs. grain size for different temperatures.

It should be noticed that this simple constitutive description does not incorporate a temperature correction for shock heating. This behavior is consistent with the overall shock response of BCC and FCC metals and alloys, and therefore it is proposed that the constitutive description presented herein is not restricted to tantalum. The predictions of Figure12 are only in qualitative agreement with the experimental results. The predicted pressure for the onset of twinning, for a grain size of 100 μm and initial temperature of 300K, is ~6GPa, whereas the onset of twinning experimentally established is of ~20 GPa. However, considering all the uncertainties in the data and constitutive description, the prediction is satisfactory. Figure 13 shows the shock temperature rise for tantalum; the temperature before shock is 293 K [77]. At the pressure of 45 GPa, the temperature rise of tantalum upon the passage of shock wave is equal to 289 K at shock front and 156 K after shock wave passage. To a first approximation, this temperature rise due to shock wave should be added to the initial temperature. The calculated threshold stress decreases with decreasing temperature and increasing grain size. An effect of grain size on the threshold twinning pressure was also observed in Mo[78].

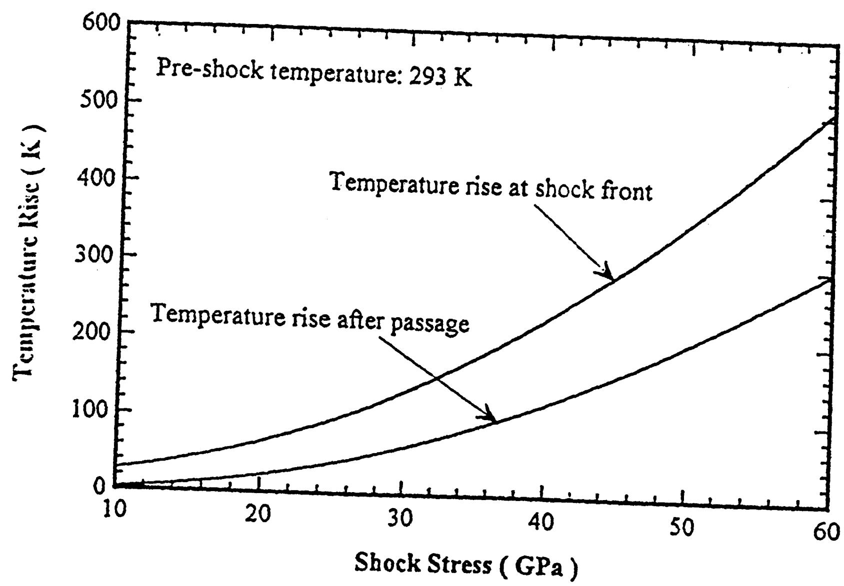


Figure 13 Shock temperature rise of tantalum as a function of shock pressure[77].

7. CONCLUSIONS

An analytical treatment that describes the initiation of mechanical twinning is developed and presented in graphical form as strain rate-temperature plots. This constitutive description is applied to metals representative of these principal crystal system: BCC (iron); FCC (copper and Ca-Zn brass); HCP (titanium). For BCC metals, an equation for the twinning stress is derived from the activation of Frank-Read sources. This provides a temperature and strain rate dependence that are compared with experimental results on iron by Harding[40, 41]. For FCC and HCP metals, the authors are not aware on any experimental results on the effect and it is therefore assumed constant. For brasses, the stacking-fault energy dependence of the twinning stress is incorporated into the twinning equation. An important phenomenon is that the Hall-Petch slope for twinning is consistently larger than the one for slip. This manifests itself in a considerable enhancement of the predisposition to twinning as the grain size is increased. The difference between the two slopes not well understood.

The slip-twinning constitutive equation is applied to the shock compression regime; the use of the Swegle-Grady [73,74] equation enables the prediction of the threshold pressure for twinning as a function of grain size and temperature. This is applied to tantalum, as an illustration.

It should be emphasized that the calculation results presented herein are not compared with experimental results , since the emphases of this communication is on the methodology.

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