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J. Phys. III 1 (1991) 989-996 JUIN 1991, PAGE 989

Classification
Physics Abstracts
81.40L

Report of the discussion at the « Round Table on the Yield Stress Anomaly »

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(*Received June 19, 1990 ; accepted October 4, 1990*)

Résumé. — Les organisateurs de la conférence ont prévu une séance de discussion sur les anomalies de limite élastique dans les métaux et les alliages ordonnés, « animée » par le Professeur Sir Peter Hirsch, et par le Docteur Denis Dimiduk. Les modèles existants se sont révélés incompatibles avec la faible valeur mesurée de la dépendance de la contrainte en vitesse de déformation. D'autres modèles ont été discutés, et les difficultés et les principaux problèmes correspondants ont été identifiés.

Abstract. — The conference organisers included a discussion period on the yield stress anomaly in metals and ordered alloys, « animated » by Professor Sir Peter Hirsch and Dr. D. Dimiduk. The existing models were shown to be incompatible with the observed small strain-rate dependence of the yield stress. Alternative models were discussed, and difficulties and outstanding problems identified.

Professor Hirsch introduced the discussion by highlighting some difficulties with existing theories or proposed mechanisms, and by raising questions concerning the interpretations of electron microscope observations. In particular he drew attention to the inconsistency between the Paidar, Pope and Vitek (PPV) [1] model on the yield stress anomaly in $Ni_3(Al, X)$, with the known very small strain-rate dependence of the yield stress on temperature. The classical results are due to Thornton *et al.* [2] who carried out instantaneous change in strain-rate ($\dot{\varepsilon}$) experiments on Ni_3Al and $Ni_3(Al, Cr)$. The change in flow stress for a change in $\dot{\varepsilon}$ by a factor of 100, was found typically to be about 1 % below 600 °C. Figure 1 reproduces their results of the strain-rate sensitivity parameter S with temperature (T).

$$S \equiv \frac{1}{T}\left(\frac{\delta \log \tau}{\delta \log \dot{\varepsilon}}\right)_T = K/\tau v \tag{1}$$

where K is the Boltzmann factor, τ the stress and v the activation volume ;

$$v = -\left(\frac{\delta H}{\delta \tau}\right)_T \tag{2}$$

where H is the activation enthalpy. Comparison of the variation of S and τ with temperature

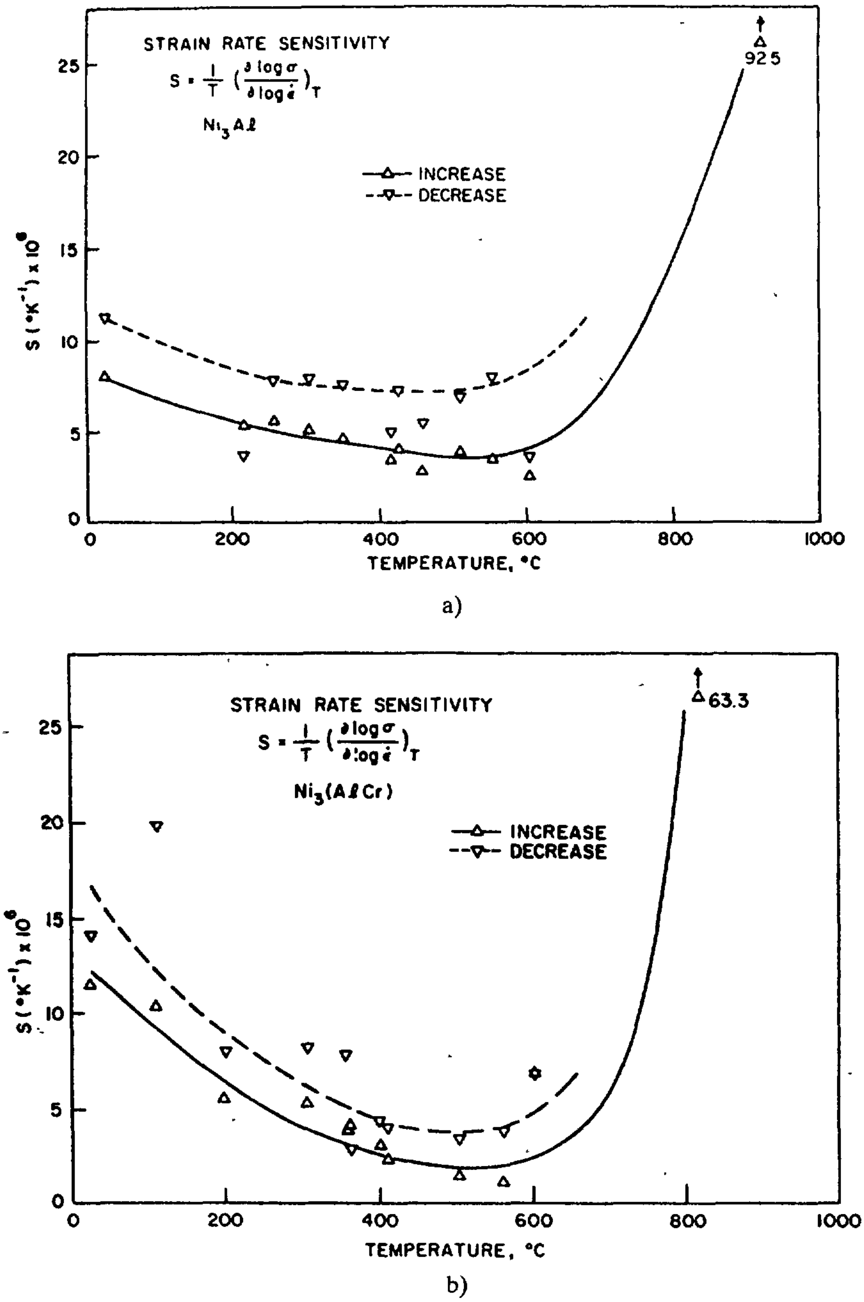

Fig. 1. — Temperature dependence of the strain rate sensitivity. (a) Ni_3Al ; (b) $Ni_3(AlCr)$. (From Thornton, Davies and Johnston, 1970.)

for Ni_3Al shows that above about 200 °C, v decreases with increasing temperature towards the peak ; at 500 °C, $v \sim 700\, b^3$. The PPV model however implies a very large strain-rate dependence. This arises from the assumption of dynamic break-away first introduced in the earlier model of Takeuchi and Kuramoto [3]. Figure 2 shows the dynamic break-away model.

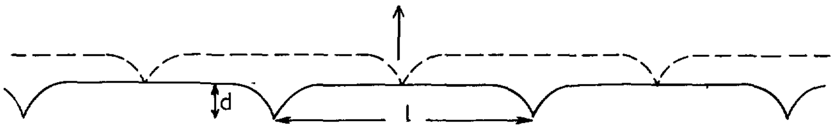

Fig. 2. — Dynamic breakaway model ; dislocation advances with velocity controlled by viscous drag.

The screw dislocation is assumed to advance rapidly in « free flight », the velocity being given by

$$v = \tau b / B \tag{3}$$

where B is the viscous drag damping constant. In the steady state, when the dislocation breaks away from one pinning point (where cross-slip has occurred), after the dislocation has advanced by d, another new pinning point is formed. The steady state condition is

$$\frac{d\ell}{v} f(T, \tau) = 1 \tag{4}$$

where $f(T, \tau)$ = probability/unit length/unit time of cross-slip on (010), and ℓ is the average distance between pinning points. From this it follows that

$$\tau = A \exp - H_\ell / 3\, KT \tag{5}$$

where H_ℓ = activation energy for locking by cross-slip. The PPV expression for H_ℓ explains satisfactorily the orientation dependence and tension/compression asymmetry of τ which was the main objective of the PPV model.

However, the strain rate $\dot{\varepsilon}$ is given by

$$\dot{\varepsilon} = \rho_m b v = \rho_m \tau b^2 / B \tag{6}$$

where ρ_m = mobile dislocation density. In an instantaneous change of strain-rate test, if we assume $\rho_m \sim$ constant, $\dot{\varepsilon} \propto \tau$ which is inconsistent with the small strain-rate dependence found in the experiments. Also using reasonable estimates for $B(\sim 5 \times 10^{-5}\ \mathrm{Nm^{-2}\,s})$, and $\tau(\sim 200\ \mathrm{MPa})$, for $\dot{\varepsilon} \sim 10^{-4}\ \mathrm{s^{-1}}$, we find $\rho_m \sim 1/25\ \mathrm{cm^{-2}}$. This is of course far too small to be realistic. The basic reason for the discrepancy between the observed strain-rate dependence and that implied by the PPV model is that the dynamic break-away model could apply only at much greater stresses than those experimentally observed. It was now necessary to develop a new formulation for the yield stress anomaly, consistent with the small strain-rate dependence observed below the peak. Such a theory could have wider application ; e.g. the temperature dependence of the strain-rate sensitivity of the yield stress for TiAl [4] is similar to that for $Ni_3(Al, X)$.

The question arose as to whether the basic cross-slip blocking mechanism in the PPV model should be retained in any new formulation. A number of different mechanisms had been proposed in the literature, based on post deformation TEM observations :

(1) Interaction between dislocations on octahedral and cube planes [2, 5]. It would seem difficult, however, to account for the observed reversibility of the yield stress with temperature on this mechanism. Professor Kirchner reported that Dr. Korner now felt that this mechanism is more likely to affect workhardening than the yield stress.

(2) Motion controlled by edge segments (superkinks) on (111) planes [6, 7]. The problem is

that it is difficult to deduce the mechanism controlling the dynamics of plastic flow from post-deformation structural observations. Nevertheless, while not necessarily rate controlling, mobile edge segments are potential sources for slip, and the Kear-Wilsdorf locks may be relevant to workhardening.

(3) Exhaustion of octahedral glide by cross-slip and subsequent bending of screws on (010) [8]. This is related to mechanism (2), the idea being that the greater the bowing of the screws on (010) planes, the greater the applied stress has to be to activate the glissile superkinks.

There is however as yet no detailed formulation for the yield stress on any of the above mechanisms.

On the other hand the *in situ* TEM observations provided important evidence on mechanisms controlling the dynamics of dislocation motion. The experiments of Molenat and Caillard [9] on motion of screws in Ni_3Al at 300 K, presented at the conference, showed clearly that long sessile configurations of screws on (111) exist, and that the dislocation advances from one sessile configuration to another (e.g. Fig. 3), exactly as expected from the sessile configurations described in the PPV (1984) paper. The experiments also imply that since the transformation from one sessile configuration to the next appears instantaneous, the jogs on the $(1\bar{1}1)$ or (010) cross-slip planes must be highly mobile during the transformation. Professor Hirsch raised the question however whether the observed mechanism of motion of the screws is necessarily the controlling one ; there might be faster mechanisms which control movement in the bulk.

Fig. 3. — Example of sessile to sessile transformation for screw with APB on (111).

Professor Hirsch then introduced a new quasi-static jerky flow model, which retained some of the basic features of the PPV model, but replaced the dynamic break-away model by one in which both locking and unlocking are controlled by thermally activated processes. Figure 4a shows the steady state structure in the model. The structure consists of sessile dislocations on (111) (cross-slipped on (010)) of finite length connected by glissile edge dislocation. The assumption is made that the jogs at the ends of the sessile configurations (e.g. at A) ar locked when they are stationary. The glissile edge on (111) has to overcome the obstacle at A by thermal activation and then causes the sessile configuration to shrink as shown in figures 4b, c, or to be bypassed (not shown). The freed glissile dislocation then bows out to the extent controlled by the stress to position 2, where it cross-slips into a sessile configuration 3. The length of the sessile configuration depends on the difference in energy between the glissile and sessile configurations. The jog in the cross-slipped configuration 3 is assumed to be glissile during the transformation but to become sessile when it stops. The steady state structure requires rate of unlocking at A $\leqslant$ rate of locking of bowed out dislocation at B. The strain-rate is controlled by the rate of unlocking, which is determined by an activation enthalpy G, which in turn is controlled by an activation volume $v \sim db^2$. The small strain-rate sensitivity is then due to a large activation volume, i.e. a large d. With increasing stress the scale of the structure (i.e. ℓ, d) is expected to decrease, resulting in an increase in the strain rate sensitivity with increasing stress below the peak. This model has not yet been developed because the factors determining the scale of the structure (ℓ), and the details of the jog

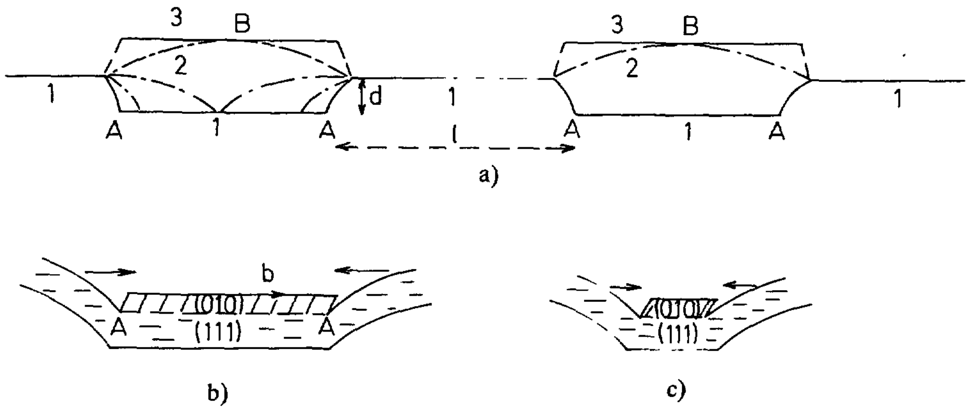

Fig. 4. — Unlocking at A by recombination of kinks on (010). (a) Initial configuration 1, intermediate configuration 2 and final configuration 3 after locking at B. Intermediate configurations between 1 and 2 are also shown. (b, c) Recombination of kinks on (010) after unlocking at A.

unlocking mechanism, are not yet understood. The assumption that the jogs, e.g. at A, are sessile has also to be justified.

Professor Vitek then introduced his new model which is similar in outline but differs in important respects. The crucial point in his new model is that in the steady state the distance ℓ between pinning points is given by

$$\frac{b}{\ell} = \exp - H_\ell/KT \tag{7}$$

where H_ℓ = activation energy for pinning in the PPV model. The sessile configuration is considered not to be much longer than the critical length at the saddle point, because expansion of the sessile configuration is prevented by the bowing out of the glissile segments of the dislocation line. The steady state configuration is shown in figure 5. The strain rate $\dot{\varepsilon}$ is given by

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \exp - (H_{u\ell} - v\tau)/KT \tag{8}$$

Fig. 5. — Steady-state configuration (Vitek).

where $H_{u\ell}$ is the activation enthalpy for unpinning $\dot{\varepsilon}_0$ is a constant. Hence .

$$\tau = \frac{1}{v}\left(H_{u\ell} + KT \ln \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right). \tag{9}$$

With $v = b^2 \ell$, and using equation (7)

$$\tau = \frac{1}{b^3}\left(H_{u\ell} + KT \ln \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right) \exp - H_\ell/KT. \tag{10}$$

Assuming $H_{u\ell}$ to be independent of orientation, the dependence of τ on temperature, orientation, tension/compression is controlled by H_ℓ as in the PPV model (note that in this new model the controlling parameter is H_ℓ ; in the PPV model it is $H_\ell/3$). The strain rate dependence is very small but increases near the peak, because of the exponential decrease of ℓ (and therefore of v) with increasing temperature (see Eq. (7)). Professor Vitek showed that there is good agreement with recent load relaxation experiments by Baluc *et al.*, presented at the conference.

Professor Hirsch argued that there is no physical basis for equation 7 ; H_ℓ controls the *rate* at which cross-slip might occur, but not the steady state concentration. Professor Nabarro supported this view and Professor Vitek agreed that there is a difficulty.

Professor Hirsch wondered whether a model of the type presented by Professor Vitek might be more plausible if the length ℓ is determined by the equilibrium concentration of constrictions. Clearly the basis for such models requires further consideration.

Dr. Caillard responded to the suggestion that dislocation motion observed in TEM *in situ* experiments might not correspond to the motion controlling the strain-rate in a three dimensional structure. He pointed out that e.g. for prismatic glide in Be, the motion of totally enclosed loops in the foil is similar to that of dislocations ending at the surface (provided these are sufficiently long), and that the local stress-velocity temperature measurements reproduce the yield stress anomaly measured in the bulk. In this case the jerky flow observed appears to be controlled by the same mechanism over the whole temperature range, i.e. by a sessile-glissile-sessile transformation of long lengths of screws by a mechanism of homogeneous nucleation along the dislocations. The increase in yield stress with increasing temperature is interpreted as resulting from a decrease in stacking fault energy with increasing temperature [11], making it more difficult for the dislocation to cross-slip from the basal into the prismatic plane, even though the temperature increases. Dr. Caillard stated that similar behaviour appeared to apply for cube slip in Ni_3Al, and although it was too early to claim that the same mechanism applied to octahedral slip in Ni_3Al, there is now a distinct possibility that the origin of the yield stress anomaly in metals and alloys is generally due to the same cause — i.e. an increasing difficulty for transformation from a sessile to a glissile configuration, due essentially to an increase in activation energy with increasing temperature of this process. In the case of $Ni_3(AlX)$ this could arise for example from a decrease of the complex stacking fault energy with increasing temperature. It was noted however that Dr. Caillard had not yet established the relation between strain-rate $\dot{\varepsilon}$ and the proposed mechanism in $Ni_3(AlX)$.

In the discussion some doubts were expressed about the interpretation of the jerky flow observed in the *in situ* TEM experiments ; Dr. Veyssière reported on some calculations due to Mills who showed that any screw superpartials in Ni_3Al meeting the surface would have their cores constricted in (111) on one foil surface and extended on the other (essentially the effect identified by Hazzledine *et al.* [12] using elasticity calculations). Dr. Caillard made it clear that such effects were not relevant to observations of screw dislocations wholly contained in the specimens, and observations on dislocations ending at the surface were only relevant if the foil thickness exceeds a critical length depending on the behaviour studied (e.g. several radii of curvature for friction stresses). Observations were always made to check whether the behaviour of dislocations ending at the surface is identical to that of dislocations wholly contained within the specimen. Professor Hirsch found the experiments and interpretation of the yield stress anomaly in Be very convincing, but he warned against assuming that all anomalies resulted from the same cause.

Professor Kubin asked what critical experiments were necessary to identify unambiguously the origin of the anomaly in Ni_3Al. Professor Hirsch thought that it would be very useful to carry out computer simulations of the motion of dislocations which undergo a localised

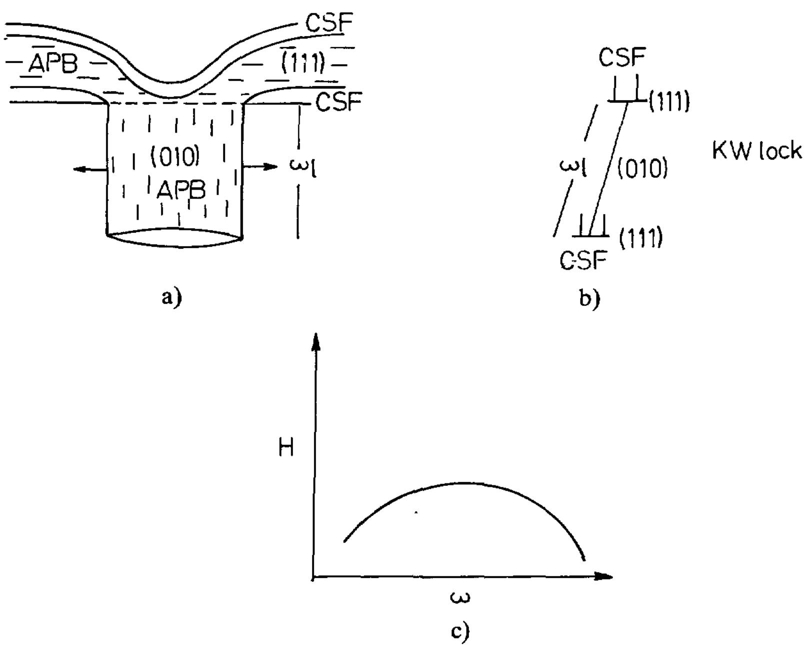

Fig. 6. — (a) Saddle point configuration for cross-slip jump to form Kear-Wilsdorf lock. (b) Kear-Wilsdorf lock. (c) Variation of activation energy H with cross-slip distance w.

locking mechanism by cross-slip, to gain insight on the mode of propagation of such dislocations, and the dependence on the probability of locking and unlocking, and to identify the steady state configuration and motion at the yield stress. Others made the point that the conclusions from such simulations would depend very much on the nature of the input and on the initial assumptions made, and that direct observations were very important to distinguish between mechanisms. There was no doubt that the observations of Molenat and Caillard [9] represent a distinct advance in that they prove unambiguously the transformation from one sessile configuration on (111) to another in screw dislocations in Ni_3Al.

Another outstanding problem concerns the mechanism by which Kear-Wilsdorf locks are formed. Professor Hirsch suggested that a mechanism is possible whereby a Kear-Wilsdorf lock could be formed in one thermally activated jump by cross-slip from (111) to (010) over a distance equal to the equilibrium separation of the screws in the lock. Figure 6a shows the critical configuration at the saddle point, where the distance w_ℓ on (010) is equal to the equilibrium separation of the screws in the lock (Fig. 6b). An approximate expression for the activation energy H is

$$H \sim W_c + Aw \ln \left(\frac{w}{w_0} \right) - B\tau_{\text{eff}}^{1/2} w^{3/2} \tag{11}$$

where $\tau_{\text{eff}} \sim \tau_{010} + \frac{1}{b}(\gamma_{111} - \gamma_{010})$, $W_c =$ constriction energy, and A, B, w_0 are constants ; $w =$ distance cross-slipped. This expression ignores contributions to H from bowing of the second partial on (111) at the saddle point (Fig. 6a) ; the Yoo torque term [13] has no effect under these conditions. Equation (11) shows that for large w the activation energy should decrease with increasing w. For intermediate configurations, with w between $b/2$ for the PPV model and $w = w_\ell =$ Kear-Wilsdorf lock distance, the expression for H is more complex, as the Yoo torque term has to be included, but the dependence of activation energy on w is likely to be of the form shown in figure 6c. It is therefore possible in principle that the activation energy for formation of the Kear-Wilsdorf lock may be less than that for the PPV lock ($w = b/2$), but detailed calculations would be needed to decide whether such a mechanism is plausible. It would be consistent with the original observations of Caillard *et al.* [14]. Professor Hirsch also mentioned that mechanisms of bypassing or unlocking a Kear-Wilsdorf lock from its ends, equivalent to that described in figure 4 for small cross-slip distances on the cube plane, but differing in detail, can be envisaged.

Professor Nabarro stressed that any theory of the yield stress anomaly must explain the behaviour of systems such as Pt_3Al which do not have such an anomaly, and of others in which the yield stress is relatively insensitive to temperature.

The general discussion left little doubt that many points regarding the yield stress anomaly remained unresolved.

Acknowledgements.

The author is grateful to Dr. Dimiduk and Pr. Vitek for their helpful criticisms of the manuscript.

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