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Theoretical and Numerical Modeling of Strain-Rate Softening Instabilities: On the Velocity Selection of Propagating Portevin–Le Chatelier Deformation Bands

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ABSTRACT

Uniformly propagating Portevin–Le Chatelier (PLC) plastic deformation bands are studied theoretically and numerically in terms of a model which incorporates the dynamic strain ageing kinetics and the effect of long-range dislocation interactions. PLC deformation banding is traced back to a wave propagation phenomenon, and the problem of propagation velocity selection is addressed for both strain- and stress-controlled tensile tests. According to the control mode, the model reveals fundamental differences in the velocity selection mechanism, which compare favourably with numerical simulations and experimental observations.

1. Introduction

The Portevin–Le Chatelier (PLC) effect, also known as jerky flow, denotes the serrated yielding of solid solutions. The PLC effect represents a strain-rate softening instability (a negative strain-rate sensitivity (SRS) of the flow stress), the microphysical reason of which consists in a repeated break-away of dislocations from, and subsequent recapture by, mobile solute atoms, *i.e.* dynamic strain ageing (DSA).

Recently, a new PLC model has been introduced [1, 2]. Its implications on the velocity selection problem during band propagation are to be discussed in the present work, in particular, as far as tensile tests at constant *stress* rate are concerned ($\dot{\sigma} = \text{const}$). In this case, staircase-type stress–strain curves go along with PLC bands propagating rapidly at virtually constant stress, while quasi-elastic loading intervals separate the nucleation/propagation of successive bands. From the characteristic times involved (the duration of band propagation $t_{\text{prop}} \approx 10^{-1}$ s is much less than the duration of the intermediate loading phases $t_{\text{load}} \approx 10$ s) we conclude that most of ageing occurs during elastic loading. In fact, as the characteristic time of solute diffusion largely exceeds t_{prop}, *dynamic* strain ageing during band propagation is not significant, but *static* ageing occurs during elastic loading transients.

2. DSA-based model of the PLC effect

Consider a plastically-deforming material described by an Arrhenius law for the plastic strain rate $\epsilon_{,t}$, which depends on an effective Gibbs' free activation enthalpy $G = G_0 + \Delta G$, with an additional enthalpy ΔG in proportion to the solute content accumulated at glide dislocations: $\epsilon_{,t} = \nu\,\Omega\,\exp\left[-\frac{G_0+\Delta G}{kT} + \frac{\sigma_{\text{eff}}}{S_0}\right] \equiv \eta\,\Omega\,\exp[-g]\,f$. Here a generalized driving force f and the reduced additional enthalpy g have been defined by:

$$f = \frac{\nu}{\eta}\exp\left[-\frac{G_0}{kT}\right]\exp\left[\frac{\sigma_{\text{eff}}}{S_0}\right]\ , \qquad \text{and} \qquad g = \frac{\Delta G}{kT}\ , \tag{1}$$

where ν is an appropriate attack frequency, Ω is the elementary strain associated with a single activation step, G_0 is the basic activation enthalpy in the absence of DSA, k is Boltzmann constant and T absolute temperature. S_0 denotes the *instantaneous* SRS of the flow stress. By the parameter η we have introduced the ageing rate ($\propto$ solute mobility) as a relevant model time scale (*cf.* Eqs. (2,3)), such that the generalized driving force f and the scaled DSA-related activation enthalpy g are the dimensionless dynamical variables of the model. Expressed in non-dimensional terms the evolution equations of the model read [1, 2]:

$$\dot{f} = \dot{\sigma} f - \theta\,\exp[-g] f^2\ , \tag{2}$$

$$\dot{g} = g'' + (g/g_\infty)^{-(1-n)/n}(g_\infty - g) - f\exp[-g]\,g\ . \tag{3}$$

Here dots stand for differentiation with respect to dimensionless time $\tilde{t} = \eta t$. Dimensionless parameters have been introduced by scaling the external stress rate $\sigma_{\text{ext},t}$ and the strain hardening coefficient h according to $\dot{\sigma} = \sigma_{\text{ext},t}/(\eta S_0)$, $\theta = \Omega h/S_0$, and g_∞ denotes the asymptotic value of g associated with completely aged dislocations (saturation value of g). The exponent n governs the initial ageing kinetics, $g \propto t^n$, well before saturation sets in.

The effective stress in Eq. (1) is defined as the externally applied stress σ_{ext} (flow stress) minus the internal stress σ_{int} (athermal back stress), $\sigma_{\text{eff}} = \sigma_{\text{ext}} - \sigma_{\text{int}}$. Accordingly, the driving force f changes owing to the external stress rate $\sigma_{\text{ext},t}$ diminished by the contribution from strain hardening, $\sigma_{\text{int},t} = h\epsilon_{,t}$. Eq. (2) then expresses the balance between external loading and strain hardening of the specimen. The term $g_\infty - g$ in Eq. (3) describes the effect of ageing: g approaches the saturation value at unit rate on the non-dimensional time scale $\tilde{t}$. The last term on the r.h.s. of Eq. (3), which is equivalent to $-g\epsilon_{,t}/(\eta\Omega)$ expresses the loss of solute content g in the glide dislocations owing to thermally activated unpinning at the dimensionless rate $\epsilon_{,t}/(\eta\Omega)$.

The spatial coupling term g'' of Eq. (3) represents a second order gradient with respect to the tensile direction x in terms of the non-dimensional coordinate $\tilde{x} = \sqrt{\eta/D}\,x$. In the present case, the diffusion-like coupling coefficient $D = \beta(\mu/S_0)\epsilon_{\text{b},t}s^2$ (where $\beta \approx 0.1$ is a numerical prefactor, μ the shear modulus) is traced back to long-range dislocation interactions associated with gradients in glide velocity [1].

In the following sections tensile tests at constant strain rate ($\dot{\epsilon} = \text{const}$) and at constant stress rate ($\dot{\sigma} = \text{const}$) will be considered separately. We investigate the problem of propagation velocity selection of solitary deformation bands, *i.e.* uniformly translating strain-rate profiles of the form $\epsilon_{,t} = \epsilon_{,t}(x - c_\text{b}t)$. As we shall see, the solution to this problem depends on the test control mode.

3. Velocity selection for $\dot{\epsilon} = \text{const}$

The plastically deforming solid solution is an excitable medium in which various types of waves may nucleate/propagate. The most regular excitation is a Type-A PLC band, which represents a solitary wave propagating at constant speed c_b. The derivation of the band parameters has been presented in [1]. Here we focus on a qualitative discussion on band speed selection. To this end we note that a PLC band represents a zone of almost unaged dislocations (g small) which propagates into an aged state (g near g_∞). The unpinning of dislocations in the front of the band occurs at near constant f, as this is a comparatively slow variable unable to follow rapid ageing changes. So we may concentrate on the dynamics of a solitary wave in g with $\dot{g} = -c\, g'$ and $c = (D\eta)^{-1/2} c_\mathrm{b}$ denoting the non-dimensional band speed. Consider Eq. (3) rewritten in the form ($n = 1$, for simplicity):

$$g'' + cg' = -\frac{\partial U}{\partial g} \quad \text{with} \quad U = g_\infty g - \frac{1}{2} g^2 + f(g+1)\exp[-g]\ . \tag{4}$$

The dynamical 'potential' U is plotted in Fig. 1 for various f values. For intermediate values $f_\mathrm{min} < f < f_\mathrm{max}$, U exhibits two stationary points corresponding to dynamically stable steady states (the strongly aged state in front of the advancing band and the almost unaged state within the band), separated by a minimum (unstable steady state at intermediate g). The value f_max at which the strongly aged steady state disappears corresponds to the upper yield point associated with the nucleation of a new band. Band propagation occurs as band nucleation goes along with a certain stress drop. The switching of one stable state to the other, which is associated with the passage of the band front, can then be interpreted in terms of a simple mechanical analogue: Eq. (4) is tantamount to the equation of motion of a unit mass particle in the 'potential' U subjected to dynamic friction with 'damping coefficient' c. The solitary wave solution corresponds to a situation where the particle originates from the left maximum at 'time' $\tilde{x} \to -\infty$, moves through the potential valley, and comes to rest again at the right maximum for $\tilde{x} \to \infty$. Obviously, this particular trajectory exists only for a certain value of 'damping coefficient', such that the propagation velocity c is well-defined [1].

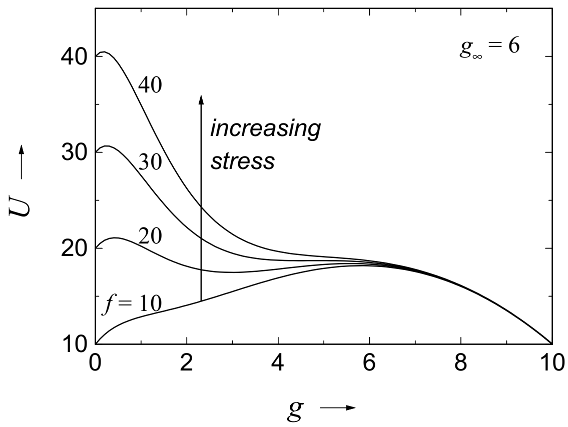

Figure 1: Illustration of the dynamic potential U defined in Eq. (4) for various values of the generalized driving force f (and $g_\infty = 6$).

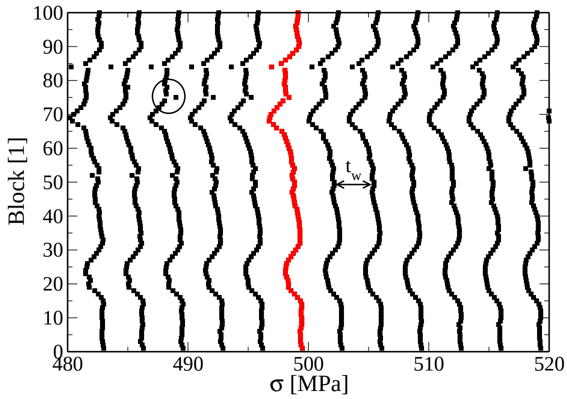

Figure 2: Spatio-temporal band correlation for a numerical tensile test at constant stress-rate: $n = 1/3$, $\dot{\sigma} = 0.5$ MPa/s.

4. Velocity selection for $\dot{\sigma} = $ const

As compared to strain control ($\dot{\epsilon} = $ const), the description of stress controlled tests with $\dot{\sigma} = $ const is formally simplified by the fact that the 'machine equation' does not affect the dynamics. The non-local feedback provided by the tensile machine may induce additional deformation modes, i.e. intermittent bands of Type B and randomly nucleating bands of Type C [1, 2]. Therefore $\dot{\sigma} = $ const tests do not reveal analogues of Types B and C. Also, the propagation velocity of strain-controlled Type-A bands is determined by the imposed deformation rate $\dot{\epsilon}$, while it is not clear what controls velocity in a $\dot{\sigma} = $ const test. In principle, the strain bursts could propagate at any speed. Experimental investigations show that the band velocities c_{b} may significantly exceed those observed for $\dot{\epsilon} = $ const. Moreover, one notes two important differences. Firstly, for $\dot{\sigma} = $ const, the stress rise occurring between two successive PLC bands goes along with quasi-elastic deformation, until a critical stress level for the next nucleation is reached. As band nucleation occurs without stress drop, the specimen is prepared in a marginally stable state (the horizontal inflection point for $f \approx 30$ in Fig. 1), into which the band propagates. This is to be distinguished from the propagation into a metastable state as it was discussed in Section 3. Secondly, most of ageing occurs *statically* during quasi-elastic loadings, while *dynamic* strain ageing is negligible during short propagation periods. The PLC band dynamics depends on the degree of static ageing that the specimen in front of the band was subjected to and, hence, on the applied stress rate $\dot{\sigma}$: the shorter the elastic loading phase, *i.e.* the higher $\dot{\sigma}$, the less ageing has occurred.

Again, Fig. 1 can be invoked to illustrate the velocity selection problem. Now the solution in question (the particle originates from the dynamically stable unaged state associated with the left maximum and comes asymptotically to rest at the horizontal inflection point corresponding to the marginally stable state in front of the band) exists for any 'damping' $c > c^*$. Apart from this lower limit velocity c^* (corresponding to the marginally stable case where group velocity and phase velocity of the plastic wave coincide), a particular propagation speed does not exist. Accordingly, we expect a less regular space-time correlation of deformation bands exhibiting a spectrum of propagation velocities.

That was confirmed by numerical simulations of the model, with specimen discretized in 100 segments ('blocks'). Fig. 2 shows a typical space-time(stress) correlation pattern of the local extrema of the plastic strain rate. One notes that the deformation bands propagate at any velocity (the slope of the space-time trajectories). Hence the propagation velocity is no longer a well-defined quantity, while the recurrence time still is, as in the case of solitary Type-A bands under strain control. Owing to that well-defined recurrence time, however, one observes a regular stair-case type stress-strain curve, which must not be confused with solitary wave propagation at constant speed. This has also been confirmed experimentally by laser-extensometric monitoring of stress-controlled tensile tests on a Cu-Al alloy [3].

References

[1] P. Hähner, A. Ziegenbein, E. Rizzi, H. Neuhäuser, *Spatiotemporal Analysis of Portevin–Le Chatelier Deformation Bands: Theory, Simulation and Experiment*, Phys. Rev. B **65** (2002) 134109.

[2] E. Rizzi, P. Hähner, *On the Portevin–Le Chatelier Effect: Theoretical Modeling and Numerical Results*, Int. J. Plast. **20** (2004) 121.

[3] F. Klose, these proceedings.