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A model of the formation of serrated deformation and propagation of Luders bands during the Portevin-Le Chatelier effect in alloys

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Abstract. A distributed autowave model of the Portevin-Le Chatelier effect has been developed for the region of medium and elevated temperatures in alloys. The model was converted into dimensionless form and the mechanisms of serrated deformation and localization of plastic flow were studied using analytical and numerical approaches. An instability region is found for the rate of plastic deformation and temperature, in the vicinity of which the Portevin-Le Chatelier effect is realized. The critical dimensionless parameters responsible for the variety of spatial-wave solutions of the initial system of equations are determined: the shapes of the load oscillations representing a quasi-periodic sequence of oscillating wave packets; bursts of plastic deformation velocity. The bursts are strictly correlated and form distinct Portevin-Le Chatelier bands under the stochastic deformation regime. Portevin-Le Chatelier bands extend from one end of the crystal to the other, where the reverse band is formed. This process of propagation of deformation bands is periodically repeated.

Keywords: Portevin-Le Chatelier effect; alloys; serrated deformation; high temperatures; stochastic self – oscillation; Luders and Portevin-Le Chatelier bands

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Introduction

Plastic deformation processes are among the most complex processes in materials science, since they lead to various features of the microstructure of the resulting materials and their behavior under loading.

One of such features of metal alloys in the region of medium and elevated temperatures is the instability of plastic deformation in the form of the serrated flow [1–7] known as the Portevin-Le Chatelier effect (PLC), named after French researchers who first observed this phenomenon in 1923 [8].

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The PLC effect consists in the irregular repetition of the load jumps σ_d and the rate of plastic deformation[4,5,9], which correspond to the localization of plastic flow in the form of deformation bands of the Luders type [10,11]. The oscillations of the deformable crystal occur due to the elastic response of the machine-sample system [12,13] and have the form of stochastic relaxation self-oscillations (Fig. 1).

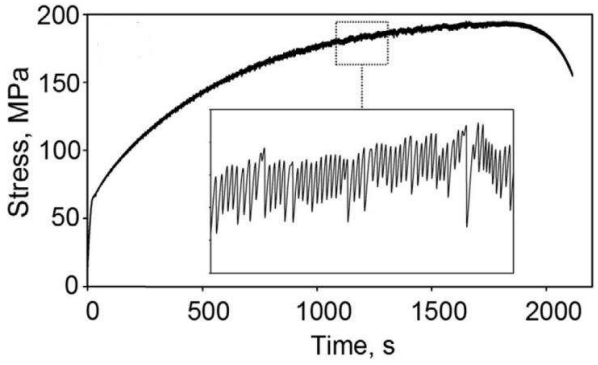

Fig. 1. A typical stress-time curve showing type B stress jumps at a given rate of plastic deformation $\dot{\varepsilon}_0 = 1{,}4 \cdot 10^{-4} s^{-1}$ [12]

There are usually five types of basic jumps of the deforming stress [14,15], but three [13,16] of them are distinguished, which correspond to various features of the occurrence and propagation of deformation bands [4,5].

Jumps of the *A* type occur above a certain average level of deforming stresses at relatively low temperatures. Jumps of the *B* type are irregular in nature and characterized by the relay propagation of deformation bands and their spatial correlation. Jumps of the *C* type occur at elevated temperatures, are located below the average level of deforming stresses and are characterized by high randomness. Jumps of other types are usually less common [14].

In the articles [17,20], an autowave model of the Portevin-Le Chatelier effect has been proposed. The model is described by a system of differential equations for deforming stress, dislocation velocity, concentration of dissolved impurity atoms interacting with moving dislocations and forming a cloud of impurity atoms around them, which is called the Cottrell atmosphere [3]. At low velocities of dislocations the Cottrell atmosphere brakes them strongly. However, as the dislocation velocity increases, the atmosphere decreases, which leads to a weakening of the braking force (there is a negative sensitivity to strain rate) and instability, which is the cause of various spatial-wave solutions.

In [20], within the framework of this model, in the dislocation sliding plane, the formation of a switching wave of the plastic deformation rate was described, interpreted as a Luders band. In the article [17], a solution was obtained in the form of relaxation self-oscillations of the deforming stress and the plastic deformation rate, which can be considered as a manifestation of the Portevin-Le Chatelier effect. However, in [17], the oscillatory process is considered in a homogeneous approximation, which does not allow for the localization of sliding in the form of deformation bands.

In this paper, the PLC autowave model is generalized to the case of deformation propagation along the sample and investigated numerically for spatial wave solutions, namely stochastic load dynamics and plastic deformation rate.

Note that there are other models for describing the phenomenon of PLC [12,13], the so-called Dynamic Strain Ageing (DSA) models [14]. However, they are mainly phenomenological in nature, unlike our approach.

PLC effect model

Consider the behavior of an ensemble of dislocations in a slip band of width w. Let's choose the direction of dislocation sliding to the $0x'$ axis at some angle to the $0x$ axis of sample stretching. Usually this angle is approximately $\pi/3$ [2]. Let the dislocation distribution in the slip band be considered homogeneous $\rho = \rho_0$. Denote by $v(t,x')$ the velocity of dislocations in the transverse sliding plane. Accordingly, the rate of plastic deformation in the slip band is determined by the Orovan's formula as $\dot{\gamma}(t,x') = b\rho_0 v(t,x')$ (b is the modulus of the Burgers vector). Then the dislocation velocity and the rate of plastic deformation along the loading axis can be approximately written as $v(t,x) \approx \phi v(t,x')$ and $\dot{\varepsilon}(t,x) \approx \phi\dot{\gamma}(t,x')$, where $\phi = 1/2 \div 1/3$ is the orientation factor.

In this case, the process of plastic deformation in the loading regime with a given rate of plastic deformation $\dot{\varepsilon}_0$ can be described along the loading axis by the following system of equations [17]

$$m^* \frac{\partial v}{\partial t} = b(\sigma + \sigma^{int}) - F(v), \tag{1}$$

$$\frac{\partial \sigma^{int}}{\partial t} = -\frac{\sigma^{int}}{t_a} + \gamma_1 \frac{\partial^2 \dot{\varepsilon}}{\partial x^2}, \tag{2}$$

$$\frac{\partial \sigma}{\partial t} = G^*[\dot{\varepsilon}_0 - \frac{b\rho_0}{L}\int_0^L v(x,t)dx]. \tag{3}$$

Here we neglect the orientation factor ϕ, since it has little effect on the nature and shape of the space-wave solutions, making only small corrections to the numerical results.

Equation (1) is the equation of dislocation motion, m^* is the effective mass of a dislocation (per unit length), $\sigma(t)$ is the external stress minus dry friction stresses (which we consider constant) such as Hall-Petch stresses and substructural hardening, σ^{int} is an internal stress field from a system of dislocation charges induced by plastic deformation at grain boundaries, $F(v)$ is a viscous N-shaped braking force per unit dislocation length due to the interaction of dislocations with impurity atoms [3].

Equation (2) takes account for the role of boundaries in the formation and propagation of deformation bands. Due to the elastic correlation of the grains, stresses $\sigma^{int} = \gamma_1 \partial^2_{xx}\varepsilon$ [14, 18] arise, which relax due to accommodation mechanisms [19]. The parameter $\gamma_1 \approx \alpha_g GD^2$ serves as a measure of elastic correlation of grains ($\alpha_g \approx 1$, D is the grain size), t_a is characteristic time of plastic accommodation [20].

Equation (3) is the Gilman-Johnston equation for the active loading mode [21], which takes account for the dynamics of the load change σ under the condition that the strain rate of the crystal sample is constant. Here $\dot{\varepsilon}_0$ is the specified rate of plastic deformation in the slip band, $G^* = \kappa h_0/\zeta S$ is the effective modulus of elasticity, κ is the rigidity of the "machine-sample" system, h_0 and S are the height and cross-section area of the sample, L is the length of the sample, ζ is geometric factor of the order one.

In equation (1) the function

$$F(v) = F_1(v) + F_2(v) \tag{4}$$

consists of two terms. The force $F_1(v)$ is due to the interaction of impurity atoms with a dislocation moving at some speed v and is determined by the formula [3]

$$F_1(v) = -\int_{-\infty}^{\infty} c \frac{\partial W}{\partial x'} dx', \tag{5}$$

where c is the concentration of impurity atoms, which is determined from the stationary diffusion equation [17]

$$D_c \frac{\partial^2 c}{\partial x'^2} + \frac{D_c}{kT}\frac{\partial}{\partial x'}(c\frac{\partial W}{\partial x'}) + v\frac{\partial c}{\partial x'} = 0. \quad (6)$$

Here D_c is the diffusion coefficient of dissolved atoms,

$$W = \frac{\beta}{(b^2 + x'^2)^{1/2}} \quad (7)$$

is the energy of interaction of dislocations with impurity atoms in the one-dimensional approximation, similar to the interaction energy in the two-dimensional case in the Cottrell theory [1, 3].

Analysis of solution for the braking force $F(v)$ shows that the deceleration force first increases, reaching a maximum at a certain value $b\sigma_{max}$ at a speed $v_a = D_c kT/\beta$ [22], and then decreases. This is due to the fact that as the velocity increases, the dislocation gradually loses the atmosphere of dissolved atoms and at some critical velocity [3]

$$v_c = D_c\beta/kTb^2 \quad (8)$$

the atmosphere disappears and the braking is caused only by statistically distributed atoms of the dissolved substance. In this region $(v > v_c)$ the deforming stress linearly depends on the velocity [3, 22], i.e. $F_2 = Bv$, where the mobility is defined as $B = \alpha c_0\beta^2/(D_c bkT)$ [22]. Here, parameter $\alpha < 1$ takes account for the features of the movement of dislocations in the field of uniformly distributed impurity atoms.

Analyzing the mathematical structure of the equation (6), it can be seen that its solution is determined by two dimensionless quantities: velocity $u = bv/D_c$ and parameter $a = W_c/kT$, which is inversely proportional to temperature. Here $W_c = \beta/b$ is the maximum binding energy of the dislocation with impurity atoms [3].

Numerical solution for $F(u)$ by taking account for equations (4)-(6) and $F_2 = B'u$ (where $B' = \alpha c_0 W_c a$), leads to the dependency shown in Fig. 2.

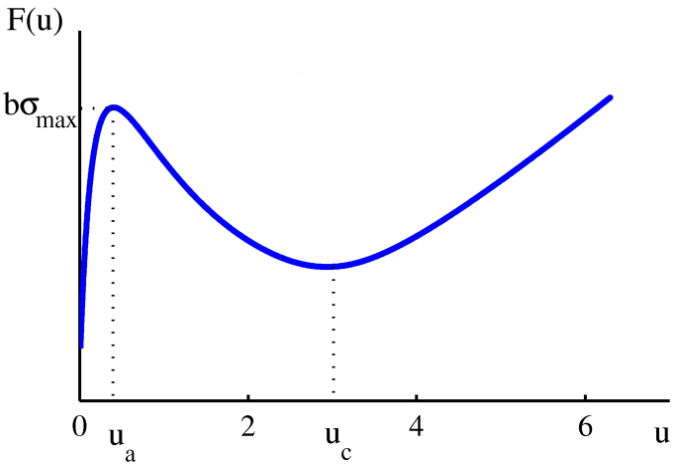

Fig. 2. Dependence of the N – shaped braking force $F(u)$ on the dimensionless dislocation velocity $u = vb/D_c$, where $b\sigma_{max} = 3ac_0\beta$. The calculations were performed at the values of the parameters $a = 3$ and $\alpha = 0.7$

It can be seen that $u_c = v_c b/D_c = a$ and $u_a = v_a b/D_c = a^{-1}$. Since a typical value of the binding energy is $W_c = 0.1\text{eV}$, then at room temperature $T = 300K$ (temperature kT in energy units is 0.025 eV) parameter $a = 4$, the value $a = 3$ corresponds to the temperature $T = 400K$.

Let us determine the region of instability of plastic deformation at which $F'(u) < 0$. By analyzing the curve $F(u)$ we find that the condition $F'(u) < 0$ is satisfied for the velocity interval in the range $[a^{-1}, a]$. For example, at temperature $T = 400K$, this is $[0.33,3]$.Cottrell noticed [1] that the Portevin-Le Chatelier effect is experimentally observed at $(D_c/\dot{\varepsilon}_0)^{1/2} \approx 10^{-5}\,\text{cm}$.

If $u = bv/D_c$ is converted to the form $bv\rho_0/D_c = \dot{\varepsilon}_0/D_c$, then the above mentioned instability region for $(\dot{\varepsilon}_0/D_c)^{1/2}$ takes the form $0.57 < \rho^{1/2} < 1.73$, i.e. approximately $(D_c/\dot{\varepsilon}_0)^{1/2} \approx \rho^{-1/2}$. If we take the typical value $\rho = 10^{10}\,\text{cm}^{-2}$, then we get Cottrell's experimental result.

Numerical study of the PLC effect

In [17], a regular self-oscillating solution of $\sigma(t)$ was obtained for the homogeneous case. Such solution, however, does not correspond to experimental results, because the load fluctuations have a pronounced stochastic character.

To identify the spatial-wave solutions of the original model, a numerical study of the original system of equations (1)–(3) was carried out. At the same time, the system of equations was transformed to a dimensionless form. It was found out that solutions of the system are controlled by temperature via the parameter $a = W_c/kT$ and a given plastic deformation rate $\dot{\varepsilon}_0$. In addition, dimensionless parameters play an essential role:

$$\kappa = \frac{G^* b\rho_0 v_a t_0}{\sigma_{max}}, \quad K = \frac{\gamma_1 b\rho_0 t_0 v_a}{L^2 \sigma_{max}}, \quad \gamma_a = t_0/t_a, \tag{9}$$

which characterize, respectively, the rigidity of the sample-machine system, the elastic correlation of grains and the intensity of plastic accommodation. Here $t_0 = v_a m^*/b\sigma_{max}$.

The analysis shows that the parameters (9) have a large range of possible values. Therefore, in this paper we will limit ourselves to the following values: the length of the plastic zone is chosen equal to $L = 20\text{cm}$, grain size $D = 10\mu\text{m}$, and

$$\kappa = 1, \quad \gamma_a = 0.01, \quad a = 3, \quad \dot{\varepsilon}_0 = 10^{-4} s^{-1}. \tag{10}$$

The parameters κ, K and γ_a characterize, respectively the rigidity of the sample-machine system, the elastic correlation of grains and the intensity of plastic accommodation.

For small values of $K < 10^{-6}$, a regular mode is realized in the system. In this case, there is a in-phase mode of velocity fluctuations in the areas of the plastic flows (along the x coordinate), but already at $K = 10^{-5}$, the deformation process acquires an irregular stochastic character (Fig. 3).

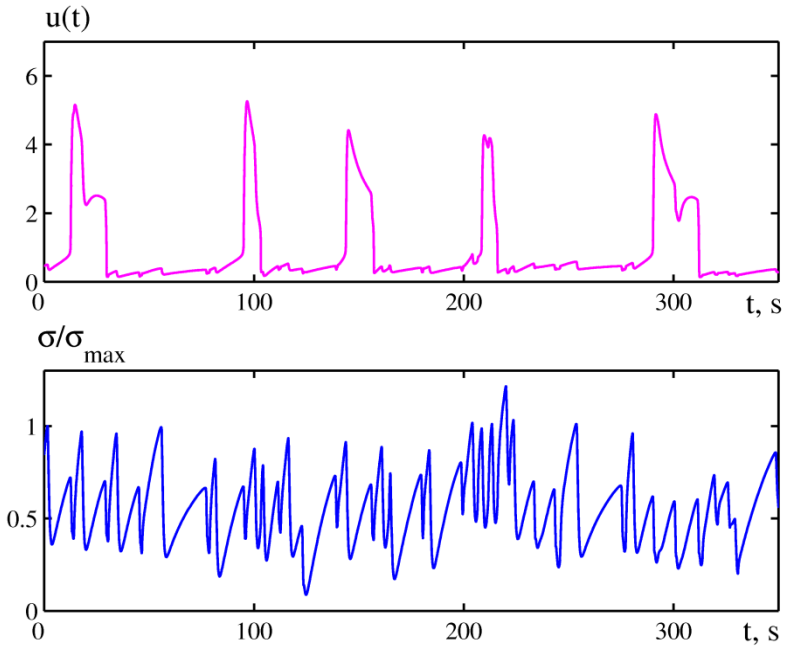

Fig. 3. Change of dislocation velocity $u(t,x)$ (in section $x=10$cm) and load $\sigma(t)$ depending on time. Numerical results are obtained at a temperature of 400K and the values of the parameters given in (10) and $K = 10^{-5}$

At the same time, the pulses of the plastic deformation rate are strictly correlated and form clear Portevin-Le Chatelier bands, which are shown in Fig. 4. This figure shows the wave pattern of the propagation velocity of dislocations $u(t,x)$ in a crystal sample.

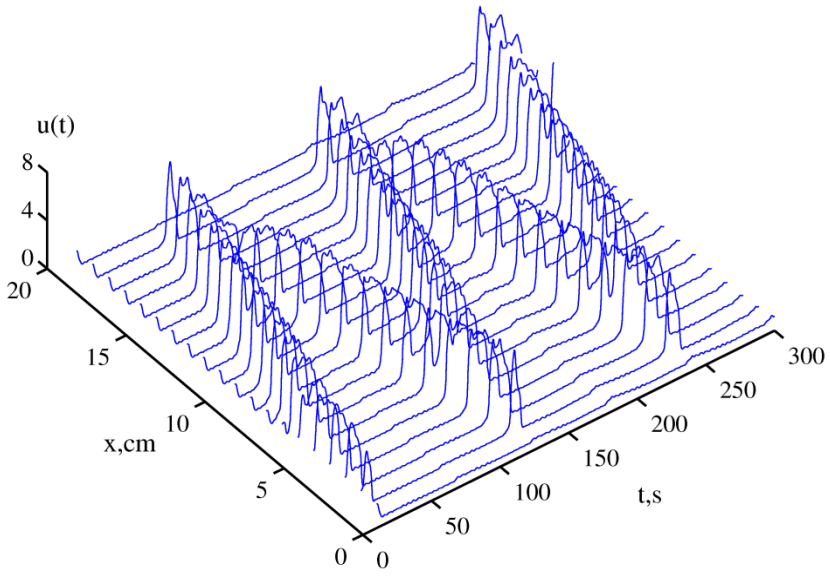

Fig. 4. Wave pattern of propagation of dislocation velocity disturbances $u(t,x)$ in a crystalline sample in the form of PLC bands under stochastic deformation mode

It can be noticed that the PLC deformation bands, which are pulses of plastic deformation, they originate at one of the ends of the crystal and move at a certain speed to the other, where the reverse band is formed. This deformation process is periodically repeated.

Under the given deformation conditions, the PLC bands are strictly correlated. When conditions change, oncoming bands may occur, propagating simultaneously from opposite ends of the crystal. In this case, the bands can annihilate, break up into parts, reappear in other parts, etc. It is necessary at the same time that the total rate of plastic deformation is equal to the specified speed $\dot{\varepsilon}_0$.

In conclusion, we will make some remarks about the Luders bands and PLC bands. In many respects, the mathematical description of these deformation bands differs little, however, the Luders band is a single wave front [20] and occurs above a certain critical load value, while the Portevin-Le Chatelier bands are formed in the instability region $(F'(v)|_{v=v_0} < 0,$ where $v_0 = \dot{\varepsilon}_0/b\rho_0)$ as a quasi -periodic sequence of running waves.

Thus, the original model assumes a wide variety of space-wave solutions, which will be considered in the following work.

Resume

1. The mechanism of plastic deformation instability of crystalline alloys is considered in the autowave model of the Portevin-Le Chatelier effect. Within the framework of the model in the field of medium and elevated temperatures, the mechanisms of serrated deformation and localization of plastic flow in alloys have been studied.
2. An analytical and numerical study of the model was carried out after bringing it to a dimensionless form. An instability region is determined for the rate of plastic deformation and temperature, in the vicinity of which the Portevin-Le Chatelier effect is realized. The critical dimensionless parameters responsible for the variety of wave solutions of the initial system of equations are determined.
3. For given values of the model parameters, the form of stochastic load oscillations is determined, which is a quasi-periodic sequence of oscillating wave arcs, i.e. load surges, as well as bursts of plastic deformation rate, which are strictly correlated and form clear Portevin-Le Chatelier bands under stochastic deformation mode.

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