ISSN 0021-8944, Journal of Applied Mechanics and Technical Physics, 2018, Vol. 59, No. 6, pp. 1078–1084. © Pleiades Publishing, Ltd., 2018.
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ENTROPY INTERPRETATION OF THE ELASTIC–PLASTIC STRAIN INVARIANT

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UDC 622:223; 530:3

Abstract: An interpretation of the nature of the relation between elastic and plastic strains, called the elastic–plastic strain invariant, is proposed which takes into account the change in the entropy of the system during autowave generation at the stage of linear strain hardening. It is shown that this approach consistently explains the nature of the invariant and its role in the description of plasticity.

Keywords: plasticity, elastic deformation, plastic deformation, localization, elastic waves, defects, dislocations.

DOI: 10.1134/S0021894418060135

INTRODUCTION

The results of experimental studies generalized in [1] show that the plastic deformation of solids is localized at the macroscopic level and this deformation determines the yield point and fracture. Localized deformation involves spontaneous layering of the material into alternating volumes: actively deformed at the moment and passive (Fig. 1). The distribution patterns of such volumes in the specimen are determined by the deformation hardening law acting at this stage and are interpreted as autowave modes [2, 3] of the localized plastic flow. In metals and alloys in various structural states (single crystals and polycrystals), switching autowaves, phase autowaves, stationary dissipative structures, and collapse of autowaves have been experimentally observed [1–3]. Phase autowaves of localized plastic flow that arise at linear strain hardening stages, where the deforming stress is linearly dependent on the strain $\sigma(\varepsilon)$, have a length $\lambda \approx 10^{-2}$ m and propagate at a rate 10^{-5} m/s $\leqslant V_{\rm aw} \leqslant 10^{-4}$ m/s. Elastic processes in the medium depend on the distances between atomic planes $\chi \approx 10^{-10}$ m and the propagation velocities of transverse elastic waves $V_t \approx 3 \cdot 10^3$ m/s (reference data). These characteristics are included in the equality $\lambda V_{\rm aw} \approx \chi V_t/2$, whose terms have the dimension of the diffusion coefficient or kinematic viscosity. The purpose of this study is to explain the nature of this equality indicating the relationship between elastic and plastic deformation processes. This is done by experimental verification of the generality of the relation $\lambda V_{\rm aw} \approx \chi V_t/2$ and its interpretation using thermodynamic theory.

EXPERIMENTAL DATA

Generality was verified by increasing the number of materials studied and analyzing the satisfaction of the equality $\lambda V_{\rm aw} \approx \chi V_t/2$ for different materials with different deformation mechanisms. The characteristics of localized plastic strain autowaves λ and $V_{\rm aw} = \lambda/T$ were determined by constructing $(X–t)$ diagrams (Fig. 2) (X is the coordinate of the localized plasticity zone in the specimen, and t is time) [1] with linear strain hardening of

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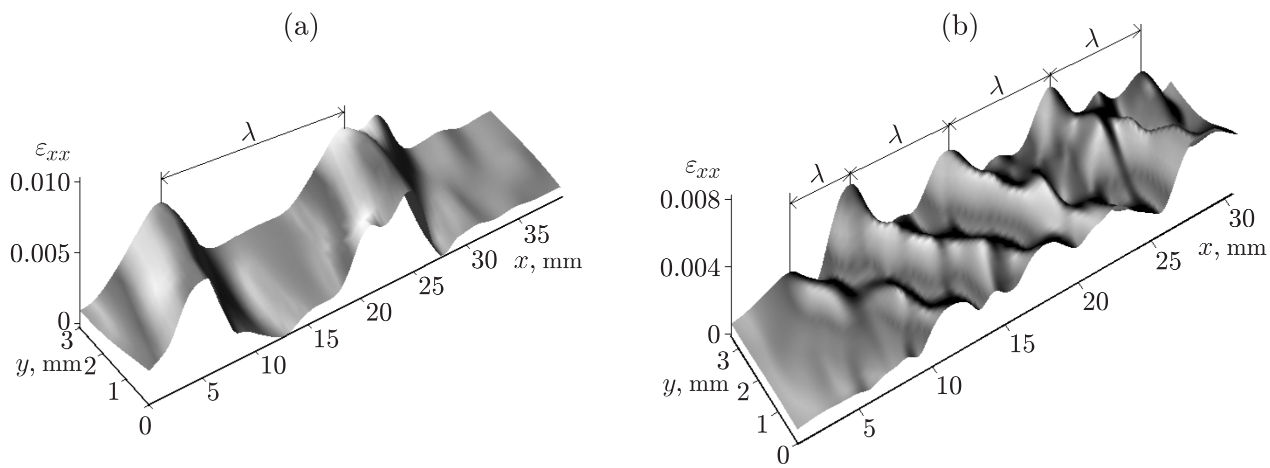

Fig. 1. Plastic strain localization in a specimen of 88/12 Fe/Mn alloy at the stages of easy slip (a) and linear strain hardening (b).

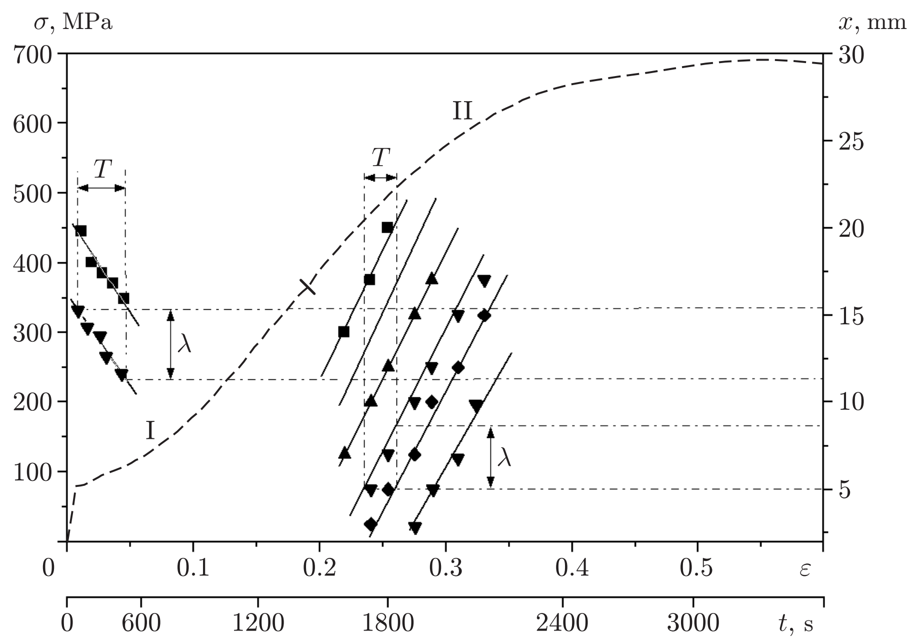

Fig. 2. Determination of the values of λ and t using a $(X–t)$ diagram for 88/12 Fe/Mn alloy specimens for the case shown in Fig. 1 at the autowave velocity $V_{\rm aw} = \lambda/T$: the dashed curve corresponds to the dependence $\sigma(\varepsilon)$; I correspond to the easy slip stage, and II to the linear strain hardening stage; the points are the coordinates X of localized strain zones.

metals, easy slip in metal single crystals, compression of alkali halide single crystals, compression of rock specimens, deformation resulting from phase transformation in a NiTi single crystal.

For 18 metals studied, the values of $\lambda V_{\rm aw}$ (see Tables 1 and 2) differ insignificantly, and the average value $\langle \lambda V_{\rm aw} \rangle_{lwh} = (2.52 \pm 0.36) \cdot 10^{-7}$ m^2/s.

Table 1. Values of χV_t and $\lambda V_{\rm aw}$ for linear strain hardening of metals

Metal	$\lambda V_{\rm aw} \cdot 10^7$, m^2/s	$\chi V_t \cdot 10^7$, m^2/s	$\lambda V_{\rm aw}/(\chi V_t)$
Cu	3.60	4.8	0.75
Zn	3.70	11.9	0.30
Al	7.90	7.5	1.10
Zr	3.70	11.9	0.30
Ti	2.50	7.9	0.30
V	2.80	6.2	0.45
Nb	1.80	5.3	0.30
α-Fe	2.55	4.7	0.54
γ-Fe	2.20	6.5	0.34
Ni	2.10	6.0	0.35
Co	3.00	6.0	0.50
Mo	1.20	7.4	0.20
Sn	2.40	5.3	0.65
Mg	9.90	15.8	0.63
Cd	0.90	3.5	0.20
In	2.60	2.2	1.20
Pb	3.20	2.0	1.60
Ta	1.10	4.7	0.20
Hf	1.00	4.2	0.25

Table 2. Values of χV_t and $\lambda V_{\rm aw}$ for easy slip in metal single crystals

Metal	$\lambda V_{\rm aw} \cdot 10^7$, m^2/s	$\chi V_t \cdot 10^7$, m^2/s	$\lambda V_{\rm aw}/(\chi V_t)$
α-Fe	7.4	6.5	1.1
γ-Fe	2.9	6.0	0.5
Cu	1.9	4.7	0.4
Zn	1.0	5.0	0.2
Ni	1.3	6.0	0.2
Sn	3.3	4.9	0.7

Table 3. Values of χV_t and $\lambda V_{\rm aw}$ for compression of alkali halide crystals [4] and rock specimens [5]

Substance	$\lambda V_{\rm aw} \cdot 10^7$, m^2/s	$\chi V_t \cdot 10^7$, m^2/s	$\lambda V_{\rm aw}/(\chi V_t)$
KCl	3.00	7.0	0.4
NaCl	3.10	7.5	0.4
LiF	4.30	8.8	0.5
Marble	1.75	3.7	0.5
Sandstone	0.60	1.5	0.4

In the case of easy slip in Cu, Ni, α-Fe, γ-Fe, Zn, and Sn single crystals, where there is also a linear stress–strain relation $\sigma(\varepsilon)$ and a phase autowave is observed, $\langle \lambda V_{\rm aw}\rangle_{eg} \approx (2.95 \pm 1.05) \cdot 10^{-7}$ m^2/s (see Tables 1 and 2).

The stages of linear strain hardening and phase autowaves of localized plasticity were also observed during compression of specimens of alkali halide crystals and rocks [4, 5]. According to the results of these experiments (see Table 3), $\langle \lambda V_{\rm aw}\rangle_{ahc} = (3.44 \pm 0.49) \cdot 10^{-7}$ m^2/s and $\langle \lambda V_{\rm aw}\rangle_{\rm rock} = (1.44 \pm 0.34) \cdot 10^{-7}$ m^2/s.

Plastic deformation of TiNi intermetallic compound of equiatomic composition results from phase transformation [6]. In the case of a localized plasticity autowave, a value $\langle \lambda V_{\rm aw}\rangle_{pt} \approx 0.85 \cdot 10^{-7}$ m^2/s was obtained using experimental data.

The elementary mechanism of plastic deformation is the slip of individual dislocations. This process is usually characterized by the dislocation path length l and the dislocation velocity $V_{\rm disl}$, which are determined by analyzing available experimental data on the mobility of individual dislocations in different single crystals [7–11]. Known data on the velocities of quasi-viscous motion of dislocations for a linear relationship between the dislocation velocity and stress $V_{\rm disl}(\sigma)$ were used [12]. The product of the quantities l and $V_{\rm disl}$ was estimated using the relation $lV_{\rm disl} \approx V_{\rm disl}^2\tau$ (τ is the duration of the load pulse acting on the crystals during loading). The results of these calculations presented in Table 4 show that $\langle lV\rangle_{\rm disl} = (3.20 \pm 0.35) \times 10^{-7}$ m^2/s.

The empirical data given in Tables 1–4 lead to the relations

$$\langle \lambda V_{\rm aw}\rangle_{lwh} \approx \langle \lambda V_{\rm aw}\rangle_{eg} \approx \langle \lambda V_{\rm aw}\rangle_{pt} \approx \langle \lambda V_{\rm aw}\rangle_{ahc} \approx \langle \lambda V_{\rm aw}\rangle_{\rm rock} \approx \langle lV_{\rm disl}\rangle. \quad (1)$$

Table 4. Values of χV_t and $lV_{\rm disl}$ determined by adding individual dislocations in single crystals

Single crystal	$lV_{\rm disl} \cdot 10^7$, m^2/s	$\chi V_t \cdot 10^7$, m^2/s	$lV_{\rm disl}/(\chi V_t)$
NaCl [7]	4.1	7.3	0.60
LiF [8]	4.1	8.6	0.50
CsI [9]	1.9	4.0	0.50
KCl [10]	4.1	6.8	0.60
Zn [11]	1.8	4.0	0.45

The quantities included in (1) were compared in pairs by calculating Student's t-criterion [13]. It has been found that the obtained values differ slightly, i.e., belong to one population.

Normalizing the terms of relation (1) by the corresponding products of the elastic characteristics of the deformable medium χV_t (see Tables 1–4), we obtain the dimensionless quantities

$$\frac{\langle \lambda V_{\rm aw}\rangle_{lwh}}{\langle \chi V_t\rangle_{\rm el}} = \hat{Z}_{lwh}, \quad \frac{\langle lV\rangle_{\rm disl}}{\langle \chi V_t\rangle_{\rm el}} = \hat{Z}_{\rm disl}, \quad \frac{\langle \lambda V_{\rm aw}\rangle_{eg}}{\langle \chi V_t\rangle_{\rm el}} = \hat{Z}_{eg},$$

$$\frac{\langle \lambda V_{\rm aw}\rangle_{pt}}{\langle \chi V_t\rangle_{\rm el}} = \hat{Z}_{pt}, \quad \frac{\langle \lambda V_{\rm aw}\rangle_{ahk}}{\langle \chi V_t\rangle_{\rm el}} = \hat{Z}_{ahc}, \quad \frac{\langle \lambda V_{\rm aw}\rangle_{\rm rock}}{\langle \chi V_t\rangle_{\rm el}} = \hat{Z}_{\rm rock}.$$

From calculations, we have

$$\hat{Z}_{lwh} \approx \hat{Z}_{\rm disl} \approx \hat{Z}_{eg} \approx \hat{Z}_{pt} \approx \hat{Z}_{ahc} \approx \hat{Z}_{\rm rock} \approx 1/2,$$

whence we finally obtain the relation

$$\left\langle \frac{\lambda V_{\rm aw}}{\chi V_t} \right\rangle = \hat{Z} \approx \frac{1}{2} \qquad (2)$$

called the elastic–plastic strain invariant [14].

The fact that relation (2) is valid for various materials and deformation mechanisms proves its universality. Generally, the elastic–plastic invariant (2) formalizes the relationship between two wave processes occurring during plastic deformation of a medium. The first of these (the propagation of elastic waves with velocity V_t) is due to the rapid decay and formation of elastic stress concentrators in the material, and the second (propagation of autowaves with velocity $V_{\rm aw}$) is the consequence of slow redistribution of plastic strain localization zones in the material.

INTERPRETATION OF EXPERIMENTAL DATA

To explain the nature of the elastic–plastic invariant, we will take into account the point of view developed in recent years [15], according to which plastic strain localization is the result of self-organization (structure formation) in an active deformable medium consisting of nonlinear structural defects [16, 17]. The main indicator of self-organization processes in a thermodynamically open system such as a deformable specimen is a reduction in its entropy [18]. This condition is satisfied for the formation of localized plastic flow autowaves [19]. Therefore, the use of entropy for a detailed description of plastic deformation localization is reasonable and promising.

Plastic flow is accompanied by space-time transformation of the stress $\sigma(x, y, t)$ and plastic strain $\varepsilon(x, y, t)$ fields [1]: stress relaxation results in strain, whose change leads to a change in the stress field. The kinetics of these processes is determined by the velocities included in the invariant (2): the propagation velocity of transverse elastic waves V_t and the propagation velocity of phase autowaves $V_{\rm aw}$.

Assuming that the transformations of the fields are due to displacements of particles of the medium, we consider the relationship between elastic (reversible) and plastic (irreversible) displacements with a small deviation of the deformable system from the equilibrium state in whose neighborhood the displacement velocities during transformations of strain and stress fields to within first-order small quantities can be assumed to be linearly dependent on the plastic and elastic strain gradients: $\dot{u}_{\rm pl}^{(p)} \approx D_{\varepsilon\varepsilon}\nabla\varepsilon_{\rm pl}$ and $\dot{u}_{\rm el}^{(p)} \approx D_{\sigma\sigma}\nabla\varepsilon_{\rm el}$ ($\lambda V_{\rm aw} \equiv D_{\varepsilon\varepsilon}$ and $\chi V_t \equiv D_{\sigma\sigma}$).

The substantial nonlinearity of the strain–stress relationship makes it necessary to take into account the occurrence of additional velocities $\dot{u}_{\rm el}^{(ad)} \approx D_{\varepsilon\sigma}\nabla\varepsilon_{\rm pl}$ and $\dot{u}_{\rm pl}^{(ad)} \approx D_{\sigma\varepsilon}\nabla\varepsilon_{\rm el}$. Then, similarly to [20], the system of equations for the plastic and elastic components of the displacement velocities can be written as

$$\dot{u}_{\rm pl} = D_{\varepsilon\varepsilon}\nabla\varepsilon + D_{\varepsilon\sigma}\nabla\varepsilon_{\rm el}, \qquad \dot{u}_{\rm el} = D_{\sigma\varepsilon}\nabla\varepsilon_{\rm el} + D_{\sigma\sigma}\nabla\varepsilon. \tag{3}$$

The coefficients of equations (3) can be represented in the form of the matrix

$$D = \begin{pmatrix} D_{\varepsilon\varepsilon} & D_{\varepsilon\sigma} \\ D_{\sigma\varepsilon} & D_{\sigma\sigma} \end{pmatrix},$$

in which, in accordance with the principle of symmetry of the Onsager kinetic coefficients [21, 22], the off-diagonal components are equal: $D_{\varepsilon\sigma} = D_{\sigma\varepsilon}$. The diagonal coefficients $D_{\varepsilon\varepsilon}$ and $D_{\sigma\sigma}$, which are the coefficients of the autowave equations of localized plasticity obtained in [1] do not have to be equal; for example, it has been shown [23] that $D_{\varepsilon\varepsilon} \ll D_{\sigma\sigma}$.

In Eq. (2), the lengths χ, $\lambda \gg \chi$ are the spatial scales of the transformation of the elastic and plastic strain fields, and the velocities V_t and $V_{\rm aw} \ll V_t$ characterize the transformation kinetics. The elastic–plastic strain invariant (2) is written as a ratio of the scales λ/χ and the kinetic quantities $V_t/V_{\rm aw}$:

$$\frac{\lambda V_{\rm aw}}{\chi V_t} = \frac{\lambda}{\chi}\,\frac{V_{\rm aw}}{V_t} = \frac{\lambda/\chi}{V_t/V_{\rm aw}} = \hat{Z} < 1, \tag{4}$$

where λ/χ is interpreted as the number of zones in which the initiation of a localized plastic strain autowave is possible, $V_t/V_{\rm aw}$ characterizes the autowave velocity in the range of possible velocities in the solid $0 \leqslant V_{\rm aw} \leqslant V_t$. Then the ratios $\lambda/\chi \gg 1$ and $V_t/V_{\rm aw} \gg 1$ can be considered as thermodynamic probabilities [22].

Using Eq. (4), we can obtain a numerical estimate of $\hat{Z}$ by calculating the change in entropy of the system during the spontaneous formation of localized plastic flow autowaves. Because of the additivity of the entropy, the expression for its complete change during autowave generation is written in the form of the sum of the scale and kinetic contributions

$$\Delta S = \Delta S_{\rm scale} + \Delta S_{\rm kin} < 0. \tag{5}$$

To satisfy the condition $\Delta S < 0$, which implies a reduction in entropy during the formation of plastic flow localization autowaves [18, 19], at least one term in Eq. (5) must be negative.

Using the Boltzmann formula and taking into account that $\lambda/\chi \gg 1$, we obtain

$$\Delta S_{\rm scale} = k_{\rm B} \ln(\lambda/\chi) > 0 \tag{6}$$

($k_{\rm B}$ is the Boltzmann constant). Assuming the kinetic contribution to be negative, we have

$$\Delta S_{\rm kin} = -k_{\rm B} \ln(V_t/V_{\rm aw}) = k_{\rm B} \ln(V_{\rm aw}/V_t) < 0. \tag{7}$$

The quantities $\Delta S_{\rm scale} > 0$ and $\Delta S_{\rm kin} < 0$ in Eqs. (6) and (7) have different signs; therefore, the scale and kinetic factors differently affect the development of localized plastic deformation. Equations (5)–(7) imply that

$$\ln(\lambda/\chi) - \ln(V_t/V_{\rm aw}) = \Delta S/k_{\rm B} < 0,$$

and hence

$$\hat{Z} = \frac{\lambda V_{\rm aw}}{\chi V_t} = \frac{\lambda/\chi}{V_t/V_{\rm aw}} = \exp\Big(\frac{\Delta S}{k_{\rm B}}\Big).$$

We finally obtain

$$\hat{Z} = \exp(\Delta S/k_{\rm B}) \approx 1/2,$$

from which it follows that the increment $\Delta S = k_{\rm B} \ln(1/2) \approx -0.7k_{\rm B}$ in an elementary act of relaxation [24].

CONCLUSIONS

Estimates were obtained for the experimentally found elastic–plastic strain invariant for various materials and mechanisms of plastic deformation, and it was shown that the relation $\langle \lambda V_{\text{aw}}/(\chi V_t)\rangle = \hat{Z} = 1/2$ holds for all investigated materials whose flow curve has a linear section of strain hardening.

It is established that the existence of an elastic–plastic strain invariant is determined not only by the dependence of the stress σ on the strain ε, but also by the mutual influence of the plastic and elastic deformation mechanisms. Thus the elastic–plastic invariant describes the development of macroscopically localized plasticity of materials.

The nature of the elastic–plastic invariant is explained based on the idea that plastic deformation is a self-organization process in the defective structure of a deformable medium and is accompanied by a decrease in the entropy of this medium. This self-organization is a form of the development of the deformation structure of the deformable medium during plastic flow.

This work was supported by the Russian Science Foundation (Grant No. 16-19-10025).

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