Two-component model of localized plasticity autowaves and quantum properties of the same

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Abstract: A new approach to plastic flow in crystals is proposed. This is based on investigations of the macrolocalization patterns of plastic deformation, which are regarded as autowave processes of different types involved in the self-organization of structural defects. A two-component model is used to account for autowave formation; built into the model is the notion of interaction between a dynamic and an information subsystem of the deforming medium. The existence of a quazi-particle is hypothesized which is responsible for the propagation of localized plastic deformation autowaves.

Key-Words: - localized plastic deformation autowaves, active medium, two-component model, autowave quantization

1 Introduction

Investigations into the nature of plastic deformation in solids were carried on during recent 25 years. The investigators arrived at an important conclusion that the plastic flow would exhibit an inhomogeneous behavior at the micro-, meso- and macro-scale levels [1-4]. It is maintained that by plastic flow the deformation is prone to localization at all the stages from yield limit to fracture, with the micro-, meso- and macro-scale localization events being almost simultaneously involved in the plastic flow processes. The macrolocalization phenomenon would occur in all deforming materials in any loading conditions, no matter what crystal lattice type and material phase composition and granular structure [3]. The evolution of macrolocalization patterns would cause autowaves to originate.

The types of localized plasticity autowaves are determined by the deformation hardening law, i.e. each type of autowaves corresponds to the respective flow stage on the loading curve. This observational result enabled Zuev [5] to propose a correspondence rule, which holds that a changeover in the type of localized plasticity autowaves is determined by a changeover in the plastic deformation hardening stages. One can single out a particular flow stage on the stress-strain curve [3, 5] using the respective value of deformation hardening exponent from the Ludwick – Hollomon equation (1), which in a general case applies to any kind of deformation curves, i.e.

$$\sigma = \sigma_0 + K\varepsilon^n . \qquad (1)$$

In this case, the correspondence rule is formulated as follows.

- For n = 0, yield plateau or easy glide stage is observed; it corresponds to the occurrence of a single localized deformation front (Chernov – Luders band) traveling at a constant velocity V_{aw}, which can be regarded as a self-excited wave (Fig. 1 a).
- For n = 1, linear work hardening stage begins; this is distinguished by the occurrence of a set of equidistant localized deformation nuclei propagating synchronously at a constant rate in the same direction. This pattern can be treated as a phase autowave of deformation localization, which has a constant rate λ and a propagation rate V_{aw} (Fig. 1 b).
- For n = ½ the stage of parabolic work hardening (Taylor stage) [6] sets in; the emergent autowave pattern is a stationary and equidistant one having a spatial period λ (Fig. 1 c).
- For n < ½, the prefracture stage is observed; it is characterized by the occurrence of a prominent stationary localization zone in which the deformation amplitude would grow steadily. The remaining nuclei are traveling towards the latter zone, the father away from the zone a nucleus is, the higher

its motion rate. With growing degree of tension, necking would occur within the stationary zone which is followed by fracture. This process is defined in [3] as collapse of localized plasticity autowave (Fig. 1 d).

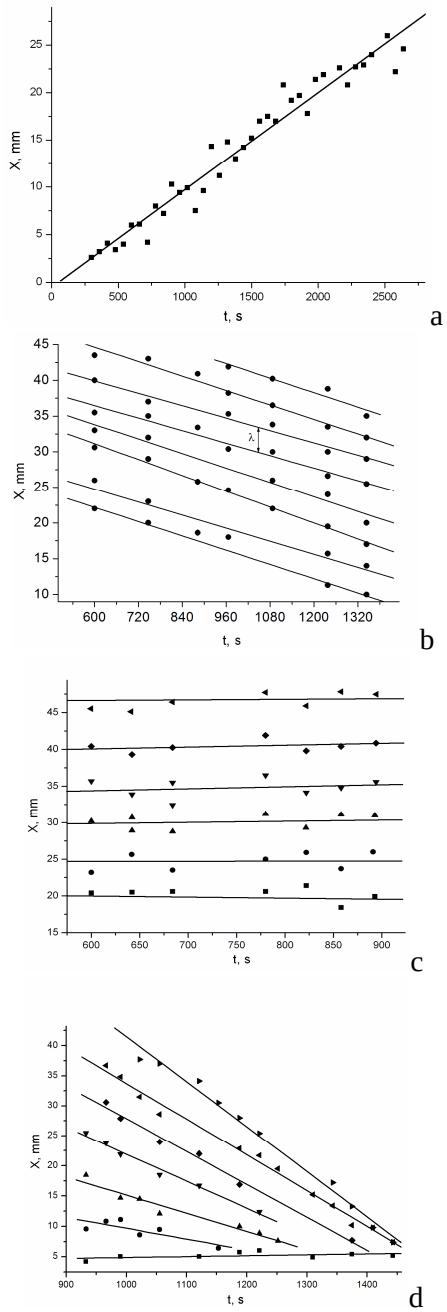

Fig. 1. Typical localized plasticity patterns: (a) yield plateau in a high manganese steel monocrystal, (b) linear work hardening stage in a vanadium alloy sample, (c) Taylor's parabolical stage in a silicon iron alloy sample, (d) prefracture stage in a zirconium alloy sample. Localization nuclei' positions plotted against time of loading

The formation of localized plasticity autowaves can be approached in the framework active medium model; the basic assumption of the model is that an active medium incorporates two subsystems, i.e. an information and a dynamic one [7]. An idea about the quantum nature of autowaves has been advance recently. In what follows the above two problems are considered.

2 The main concept and experimental evidence

The above two-component model is proposed for the acquisition of the physical notion of the nature of autowaves in question [8, 9]. The basic assumption of the given model is that a deforming medium is subdivided into dynamic and information subsystems: (i) various processes involving motion of dislocations and of dislocation ensembles, which are responsible for form changing proper, play the role of dynamic subsystem; (ii) the acoustic emission signals emitted by elementary relaxation acts in the course of plastic deformation are assigned the role of information subsystem. According to Kadomtsev [7], the interaction between these two subsystems is liable to cause self-organization of the active medium, which might involve autowave propagation.

The mathematical treatment of the problem is to represent the two-component model by a system of two differential parabolic equations of reaction-diffusion type [3], i.e.

$$\dot{\varepsilon} = f(\varepsilon,\sigma) + D_{\varepsilon}\varepsilon'', \qquad (2)$$

$$\dot{\sigma} = g(\sigma,\varepsilon) + D_{\sigma}\sigma''. \qquad (3)$$

Equations (2) and (3) are derived for the rate of variations in the dynamic and information subsystems, respectively. The non-linear functions $f(\varepsilon,\sigma)$ and $g(\varepsilon,\sigma)$ which describe the point kinetics have the meaning of the rates of stress and strain variation on the micro-scale level. In particular, the non-linear function $f(\varepsilon,\sigma)$ from (2) is equivalent to the Taylor-Orowan equation of dislocation kinetics. This function can be rewritten as $\dot{\varepsilon} = b\rho_d V_d$ (here b – Burgers vector; ρ_d – mobile dislocation density and V_d – rate of dislocation motion over local barriers). Alshits and Indenbom [10] pointed out that dislocation motion over local barriers would be retarded by the phonon and electron gases. The phonon gas density would vary only insignificantly for different metals at the same temperatures, while the electron gas density might vary considerably for different metals. The contribution of electron gas to the retardation of dislocation motion is significantly

lower relative to the phonon gas. However, it is the contribution of electron gas, which determines the point kinetics of the dynamic subsystem described by the function $f(\varepsilon,\sigma)$ from (2) for a given metal. Since both the phonon and the electron gas in metals have a quantum nature, it is expected that the autowaves of plastic deformation localization might exhibit certain quantum features.

The idea of adopting a quantum approach to describe the localized plasticity autowaves was introduced at the beginning of this century [11-13]. This consists in substitution of the autowave characteristics λ and V_{aw} into the de Broglie equation (4):

$$p = \frac{h}{\lambda}, \qquad (4)$$

where $p = mV_{aw}$ and h – the Planck constant. It is evidently required that the experimental values λ and V_{aw} be determined simultaneously. For this reason, one can only use λ and V_{aw} data obtained for the stage of linear deformation hardening. Indeed, at the yield plateau a single mobile localization nucleus would occur; therefore, one cannot determine the value λ as a spatial period. At Taylor's stage the nuclei are immobile; hence $V_{aw} = 0$. At the prefracture stage collapse of the autowave occurs, with its length and rate being variable values.

Metal	$\lambda\times10^3$	$V_{aw}\times10^5$	$\rho\times10^{-3}$	Atomic mass	r_{ion}	N	$m_{eff}\times10^{27}$	d_Ω	d_Ω/r_{ion}	$s\times10^2$
	m	m/s	kg/m^3	a.m.u.	nm		kg (a.m.u.)	nm		
Cu (B)	4.5	8.0	8.9	63	0.072	1	1.84 (1.1)	0.059	0.82	1.74
Zn (B)	7.6	4.85	7.1	65	0.071	2	1.8 (1.08)	0.063	0.89	1.67
Al (A)	7.2	11	2.7	27	0.051	3	0.84 (0.50)	0.068	1.33	1.87
In (A)	4.2	6.1	7.3	115	0.081	3	2.6 (1.6)	0.071	0.88	1.4
Zr (B)	5.5	3.5	6.5	91	0.079	4	3.44 (2.05)	0.081	1.02	2.24
Ti (B)	7	5	4.5	48	0.076	4	1.9 (1.1)	0.075	0.99	2.3
Pb (A)	5.3	6.6	11.3	207	0.084	4	1.89 (1.14)	0.055	0.65	0.55
V (B)	4.0	7.0	6.1	51	0.059	5	2.37 (1.42)	0.069	1.08	2.81
Nb (B)	4.0	4.5	8.6	93	0.069	5	3,68 (2.22)	0.075	1.09	2.39
Sn (A)	4.27	7.3	7.3	118	0.071	4	2.1 (1.28)	0.066	0,93	1.1
γ-Fe (B)	5.0	5.1	7.9	56	0.064	8	2.6 (1.76)	0.069	1.08	2.81
α-Fe (B)	4,3	5,2	7.9	56	0.064	8	2,96 (1.77)	0.072	1.12	3,0
Ni (B)	3.5	6.0	8.9	59	0.069	10	3.16 (1.89)	0.068	0.99	3.24

Table. Characteristics of studied materials and of localized deformation autowaves observed in the same

The calculated value m_{eff} is a sufficiently small one to correlate with the atomic masses of metals. The calculated values m_{eff} are listed in the Table; also tabulated for each metal are the values λ, V_{aw}, atomic masses, density values ρ, number of atoms per unit cell N as well as ionic radii r_{ion} calculated using the Bokii – Belov procedures [14]. As is seen from the Table, the effective masses obtained for all studied materials are in the interval $m_e << m_{eff} \leq 2$ a.m.u. (here $m_e = 5.5\times10^{-4}$ a.m.u. is the electron mass). Evidently, the effective masses m_e obtained for different metals will depend on the atomic masses M_{at} of the same. Therefore, normalization was performed to give dimensionless masses, i.e.

$$s = \frac{m_{eff}}{M_{at}}. \qquad (6)$$

The values s are also tabulated. Finally, the volumes Ω were calculated as $\Omega = m_{eff}/\rho$ and the characteristic distances were obtained for studied metals as $d_\Omega = \sqrt[3]{\Omega}$. The values d_Ω differ from the ionic radii of the respective metals by less than

20%, with the exception of lead and aluminum for which the difference observed is greater than 30%.

In view of the above, the effective mass m_{eff} of the localized plasticity autowave is expected to define the kinetics of individual dislocations by virtue of being an inertial characteristic; consequently, its value would be determined by electron gas density.

The dimensionless mass s against the number of valence electrons N is illustrated for studied metals in Fig. 2. For most metals, this dependence can apparently be interpolated using linear function as

$$s = s_0 + \kappa N, \qquad (7)$$

where $s_0 = 1.5 \cdot 10^{-2}$ and $\kappa = 0.18 \cdot 10^{-2}$. The correlation coefficient is 0.94. The free term s_0 corresponding to the state for $N = 0$ is treated as contribution of the phonon drag to the effective mass of autowaves. The second addend tends to rise with growing electron density; hence it is evidently related to the electron gas contribution.

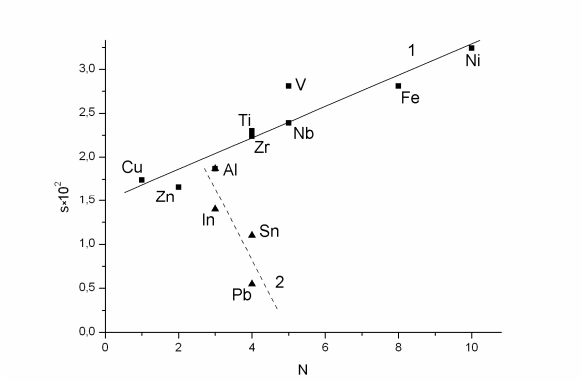

Fig. 2. The dimensionless mass of localized deformation autowave against the number of valence electrons of studied metal

For indium, tin and lead, however, the above regularity does not hold. This might be due to the following causes. (i) The localized plasticity autowaves observed for these metals have significantly lower dimensionless masses relative to the other studied metals, i.e. the value $s = 0.55 \cdot 10^{-2}$ obtained for lead is four times smaller relative to titanium and zirconium, which have the same number of valence electrons as lead does. (ii) With growing number of valence electrons, the dimensionless masses of autowaves obtained for the above three metals decrease (see Fig. 2, line 2). And last but not least, the characteristic size d_Ω obtained for lead differs significantly from its ion radius r_{ion} (see Table).

3 Discussion of results

According to A. Scott [15], a description of autowave processes in active media has to take into account the interaction between the autocatalytic and the inhibiting factor. By the deformation, the strain ε and the stress σ play the roles of catalyst (2) and damper (3), respectively. The members in (2) and (3), which have second spatial derivatives, describe the diffusion redistribution of strains and stresses, i.e. the autocatalytic and inhibiting factors, respectively. Therefore, the coefficients D_ε and D_σ for the latter factors must have the dimension of diffusion coefficient (m^2s^{-1}). It is pointed out in [9, 16] that the diffusion coefficients $D_\varepsilon \approx \lambda V_{aw}$ and $D_\sigma \approx dV_\perp$ are determined, respectively, by the processes occurring on the macro- and micro-scale levels (here d is the distance between the most closely packed crystallographic planes and $V_\perp$ is the rate of transverse sound waves). However, the coefficient D_σ, determines the effective phonon mass as $m_{ph} = h/dV_\perp$; consequently, the effective mass $m_{eff} = h/\lambda V_{aw}$ could be ascribed to another quasi-particle, i.e. an autolocalizon [17]. The quasi-impulse $p = h/\lambda$ and the energy $E = hV_{aw}/\lambda$ of autolocalizon are also determined by the autowave characteristics. This approach agrees with the conventional implementation of quasi-particles in the theory of solids [18]. An additional argument in favor of the quantum approach to plastic flow description is the dispersion relation of quadratic form derived for the localized plasticity autowaves [19].

Today at least two macroscopic phenomena are known which can be addressed exclusively in the framework of quantum theory; these are superfluidity and superconductivity. The latter phenomena, together with localized plastic flow, have similar elementary excitation spectra involving respective quazi-particles. The thesis proposed in the monograph [3] is that the entire deformation process, from yield point to fracture, would involve condensation of respective quazi-particles. Thus condensation of long-wavelength phonons generates plastic flow quanta (dislocations). Due to the condensation of elementary plastic shear carriers, various self-organization ensembles having different degrees of complexity would form. The condensation of plastic flow quanta would cause macro-scale autowaves of plastic flow localization. Finally, autolocalizons would appear whose condensation is manifested as collapse of localized plasticity autowaves and subsequent fracture. The latter process may be represented as formation of a

fracture quantum, i.e. a crackon, which was introduced by Fiedman and co-workers [20].

The effective mass of autolocalizon is taken to be about equal to two effective masses of phonon [16]. In this case, however, the normalized (dimensionless) mass *s* would be equal for all studied materials. The results obtained in this investigation suggest that the above contention is true provided the data is averaged for all studied metals. In point of fact, the value *s* increases with growing number of valence electrons. Consequently, proper allowance must be made for the electronic component of the kinetics of deformation defects. This is sustained by the fact that dependence (7) does not hold for lead, tin and indium, which might be due to the fact that these metals belong to A-subgroup of Mendeleyev's periodic table (see the Table). Thus, by addressing the nature of localized plastic deformation autowaves, one has to take account of the contribution to the kinetics of micro-scale deformation events of electronic component. As is seen from the Table, aluminum also belongs to A-subgroup; its characteristic distance d_Ω adopted in quantum mechanics exceeds significantly its ionic radius. The above four metals make up an individual group characterized by the decreasing dimensionless mass of autolocalizon with growing number of valence electrons (Fig. 2). The only valid explanation of this fact is as follows. The electron configuration of atoms in an element determines its metalloid properties. Thus *p*-electron shell population corresponds to enhanced metalloid properties; the reverse situation is observed for *d*-electron shell population. The above four metals belong to the former group.

4 Conclusion

1. The plastic flow in solids is evolution of regular patterns of localized plasticity autowaves. The type of autowaves is determined by the law of work hardening acting at the corresponding flow stage of the stress-strain diagram.
2. The deforming system separates into a dynamic and an information subsystem, which interact with one another to cause origination of localized plastic deformation autowaves.
3. The localized plasticity autowaves are quantum phenomena; these can be addressed in terms of a hypothetical quazi-particle which has been given the name 'autolocalizon'. The autolocalizon characteristics, i.e. effective mass, quazi-impulse and energy, are determined by the properties of autowaves.
4. The effective mass of autolocalizon depends on the density of phonon and electron gases. With growing number of valence electrons in metals having *d*-electron shell population, the effective mass of autolocalizon increases, while in metals having *p*-electron shell population the same value decreases.
5. The deformation process occurring in a solid from yield point to fracture can be described as a series of condensation events involving respective quasi-particles. Thus the condensation of long-wavelength phonons would cause formation of dislocations, which are plastic shear quanta. Due to the condensation of plastic shear quanta, autolocalizons will form which are quanta of localized plasticity autowaves. The last flow stage involves condensation of the autolocalizon, i.e. collapse of the autowave, with a resultant formation of a fracture quantum, so-called crackon, which is responsible for the main crack development.

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