

## SOLITON MODELS OF DISLOCATION AND ACOUSTIC EMISSION IN METALLIC MATERIALS

A. PAWELEK

Polish Academy of Sciences  
Aleksander Krupkowski Institute of Metallurgy and Materials Science  
(30-059 Kraków, ul. Reymonta 25, Poland)

S. PILECKI

Polish Academy of Sciences  
Institute of Fundamental Technological Research  
(00-049 Warszawa, Świątokrzyska 21, Poland)

In this paper the analysis of the dislocation models and the possibilities of their application to the description of the acoustic emission (AE) sources, which are acting during plastic deformation of metallic materials are presented. Especially the one-dimensional atomic Frenkel-Kontorova model of dislocation (model FK) has been discussed with particular reference to its nonlinear properties which determine the movement of the dislocation kink along the dislocation line as a solitary wave process. At the same time the equivalence of the FK model with the string model of dislocation (S model) has been demonstrated. In consequence, the FK model has been generalized by the consideration of new terms of higher order responsible for the anharmonic (nonlinear) interaction between the atoms (including also the second coordination zone). A new class of nonlinear partial differential equations (NLPD equations), which may play a role in the theory of lattice vibration of the crystal with dislocation as well as in the theory of dislocations, has been obtained. The results are discussed in the context of rich experimental data (obtained at IMIM) which establish the correlations between the measured AE parameters and the plastic deformation mechanisms as well as microstructure evolution occurring in fcc single and polycrystals subjected to channel-die compression, especially at the liquid nitrogen temperature.

### 1. Introduction

The phenomenon of acoustic emission (AE), occurring particularly at a moderate degree of plastic strain, is generally explained on the basis of various forms of the dislocation movements [1-4]. However, there exists no model, which would be commonly accepted. On the other hand, the experimental data obtained so far at the IMIM, suggest that there exist strong correlations between the AE behaviour and the dislocation mechanisms of plastic deformation [5-9]. In particular, it was suggested in the quoted papers

that the AE phenomenon during channel-die compression of both fcc monocrystalline (Cu, Ag, Cu-2% Al) and polycrystalline (Cu, Cu-30% Zn) metals may be interpreted on the basis of two main dislocation processes. The first one is the acceleration (or deceleration) of the dislocation motion and the other one is the annihilation of dislocations occurring especially during the escape of dislocations to the free surface of a sample.

For these reasons the main aim of this paper is to search for such a model of dislocation which could serve simultaneously as a model of the AE source. To attain this, the existing dislocation models have been briefly reviewed. Especially, the atomic Frenkel-Kontorova dislocation model (FK model) and its equivalent of the model of dislocation as a string (S model) has been reconsidered. As a consequence, the FK model has been generalized by the consideration (including the second coordination zone) of the anharmonic interaction between the atoms.

## 2. Survey of dislocation models

Generally, there are two kinds of dislocation models: the discrete models and continuous ones. The more important models among the discrete ones are: the Peierls-Nabarro model (PN model), the Maradudin static and dynamic models, the Tewary dynamic model and the FK model. These models are discussed in greater detail in [10]. Here we want to note that thanks to the PN model, we are familiar with the concepts of both energetic barriers (PN barriers) and sinusoidal periodic force,  $f$ , commonly called the PN force, which is given by

$$f = b\tau_p \sin(2\pi x/a), \quad (1)$$

where  $\tau_p = U_p/ab$  is called the Peierls stress, and  $U_p$  defines just the energy of the PN barriers;  $a$  is the lattice parameter and  $b$  is the magnitude of the Burgers vector of dislocation.

Other dislocation models are based on the static and/or dynamic properties of the crystal lattice. The simplest of them, at least from the point of view of lattice vibrations, is the atomic FK model of dislocation in a one-dimensional crystal (Fig. 1). In the FK model the PN force is also taken into account, and it is very interesting to note that the FK model is mathematically equivalent to the continuous model of dislocation as an infinite string (S model, Fig. 2), vibrating within two adjacent valleys of the Peierls potential,  $U(x)$ , defined as follows

$$U(x) = - \int f(x) dx = (U_p/2)[1 - \cos(2\pi x/a)]. \quad (2)$$

The movement of the dislocation in a real crystal is the consequence of the dislocation kink motion along the dislocation line. The basic solutions of the governing equation in the FK model, as presented further in Sec. 3, describe clearly the properties of the moving dislocation kinks and particularly also their behaviour as the solitary (nonlinear) wave processes. Moreover, the FK model is, at the same time, a quite good analytical model of the dislocation core, the elastic properties of which are highly nonlinear, and thus their description in terms of the linear theory of elasticity is completely insufficient.

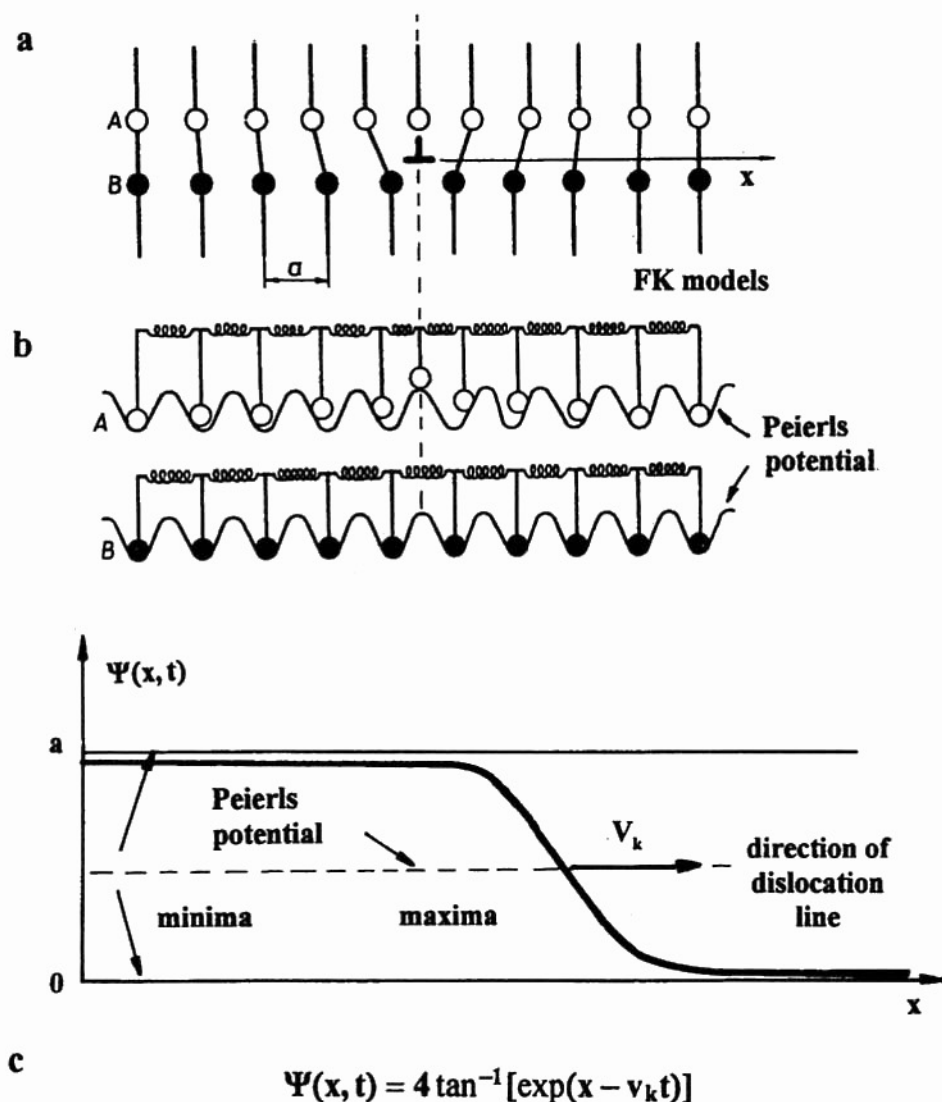


Fig. 1. One-dimensional Frenkel-Kontorova model (FK model) of edge dislocation (a), the corresponding atom configuration in the Peierls potential (b), and the kink motion as a solitary wave process (c).

This strong nonlinearity of the dislocation core determines the solitary wave behaviour of the moving dislocation kink. Since the vibrating motion of the dislocation core as well as the mutual annihilation of the dislocation kinks of opposite signs may be, in our opinion, the real causes of the acoustic waves in plastically deformed crystals, both the FK and the S models will be reconsidered below in greater detail as they now constitute the basis of the dislocation models of AE sources.

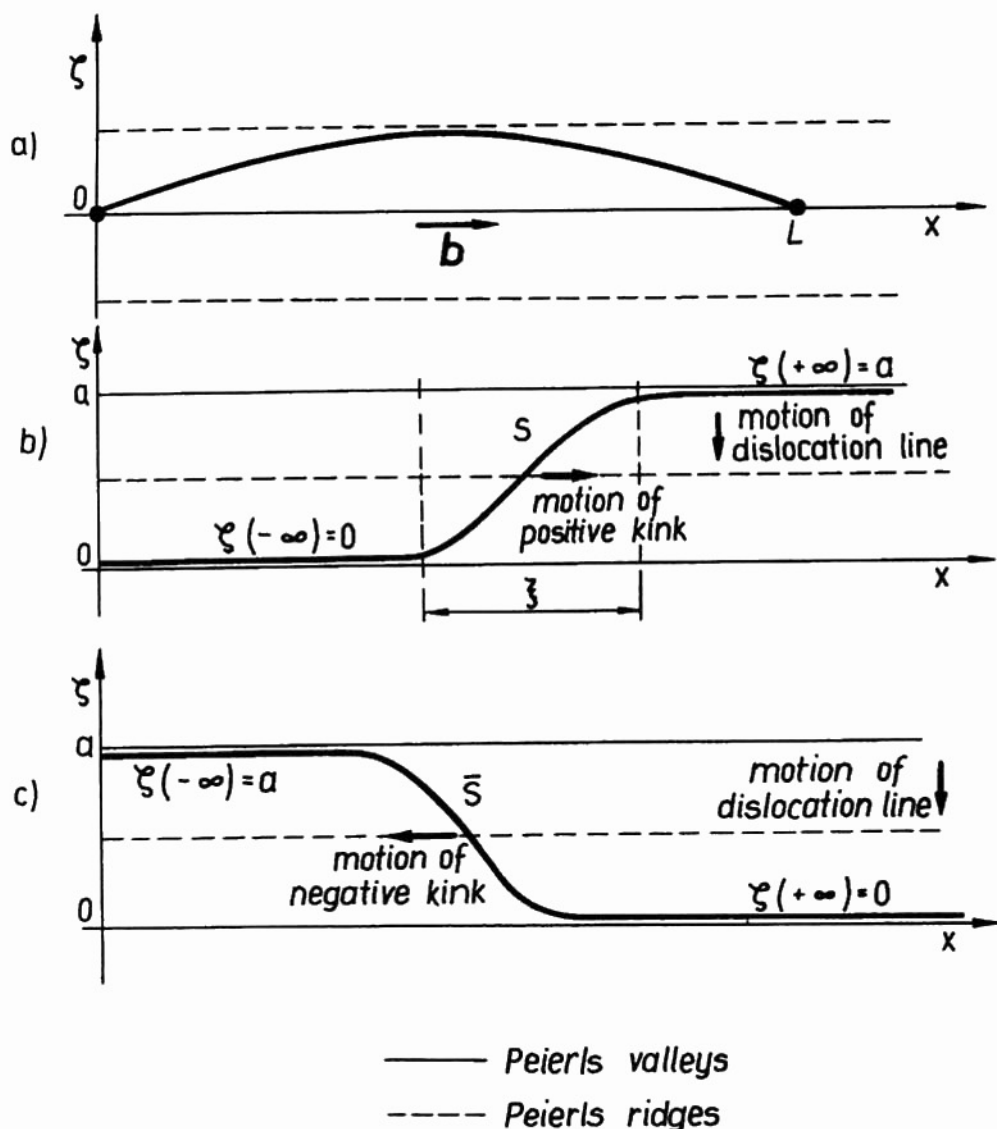


Fig. 2. String model (S model) of dislocation (a) and the kink motion (b), (c) along an infinite dislocation line.

### 2.1. The Frenkel-Kontorova dislocation model (FK model)

In the one-dimensional FK model two series of atoms are considered (Fig. 1, at the top). The lower series (B) is immobile and contains  $n$  atoms which are treated as perfectly rigid and elastic balls lying in the potential valleys and connected by the springs (Fig. 1, at the middle). On the other hand, the higher series (A) contains  $(n+1)$  atoms which

may vibrate along the  $x$ -axis. In this way a system of two such series of atoms forms an object like the nonius of the effective length  $\xi$  in which to  $(n+1)$  marks (atoms) in the higher part there correspond only  $n$  marks (atoms) in the lower one.

Let assume that  $u_k$  is the displacement of the  $k$ -th atom in the higher row in relation to the equilibrium position occupied by its counterpart in the lower row of atoms. In further considerations it will be assumed that the lower row of atoms constitutes a perfect, one-dimensional crystal in which the atom at the position  $x_k$  determines simultaneously the position of the  $k$ -th node of an ideal one-dimensional crystal lattice of the parameter  $a$ . For simplicity it is also assumed that the magnitude of the Burgers vector is  $b \cong a$ . Then the position of the  $k$ -th atom in the higher row can be written as follows

$$x_k = ka + u_k, \quad (3)$$

and the total potential energy,  $\Phi$ , of the atoms in the higher row in relation to those in the lower one may be written in the following form

$$\Phi = A_0 \sum_{k=-\infty}^{\infty} [1 - \cos(2\pi u_k/a)] + (\alpha_0/2) \sum_{k=-\infty}^{\infty} (u_{k+1} - u_k)^2, \quad (4)$$

where  $A_0$  and  $\alpha_0$  are the interaction constants characteristic of the FK model. The first term in Eq. (4) describes the part of potential energy related to the changes in positions of the atoms in the dislocated crystal. On the other hand, the second term describes the energy of the mutual interactions between the vibrating atoms in the higher row. Moreover, this term is derived by using the so-called approximation of the first nearest neighbours (e.g. for the  $k$ -th atom there are atoms in the nodes with the numbers  $(k-1)$  and  $(k+1)$  only). With these assumptions, the equation of motion for the  $k$ -th atom of mass  $m$  has the following form

$$m\partial^2 u_k / \partial t^2 = -\partial\Phi / \partial u_k, \quad (5)$$

or, after differentiation of Eq. (4), the form

$$m\partial^2 u_k / \partial t^2 = -(2\pi \cdot A_0/a) \sin(2\pi u_k/a) + \alpha_0(u_{k+1} + u_{k-1} - 2u_k). \quad (6)$$

Furthermore, in the FK model it is also assumed that the quantities  $u_k$  are continuous functions of the position  $x$  and the time  $t$ , and that the displacements of any two neighbouring atoms from the equilibrium position are not drastically different, i.e. the following relations are satisfied

$$u_{k+1}(x) \cong u_k(x+a) \quad \text{and} \quad u_{k-1}(x) \cong u_k(x-a). \quad (7)$$

Using Eq. (7) and the second order Taylor expansion the next relation can be obtained

$$u_{k+1} + u_{k-1} - 2u_k \cong a^2 \partial^2 u_k / \partial x^2. \quad (8)$$

Finally, putting Eq. (8) into Eq. (7) and denoting for simplicity,  $u_k(x, t) \equiv u(x, t) \equiv u$ , one can obtain the equation which is a governing one in the FK model. This is the nonlinear partial differential equation (NLPD equation) which is very well known in the theory of solitons and is called the sine-Gordon equation (SG equation)

$$m\partial^2 u / \partial t^2 - \alpha_0 a^2 \partial^2 u / \partial x^2 + (2\pi A_0/a) \sin(2\pi u/a) = 0. \quad (9)$$

In physical contexts the SG equation is often written in the form

$$\partial^2 \Psi / \partial t^2 - c_0^2 \partial^2 \Psi / \partial x^2 + \omega_0^2 \sin \Psi = 0, \quad (10)$$

where it is assumed that  $\Psi = 2\pi u/a$  and both the velocity  $c_0$  and the frequency  $\omega_0$  constants, characteristic of the FK model, are given by

$$c_0^2 = \alpha_0 a^2 / m \quad \text{and} \quad \omega_0^2 = 4\pi^2 A_0 / m a^2. \quad (11)$$

In further considerations other notations will be used for the derivatives, e.g.  $\partial^2 \Psi / \partial x^2 \equiv \Psi_{xx}$ . Then the SG equation (10) may be written in a more simple form

$$\Psi_{tt} - c_0^2 \Psi_{xx} + \omega_0^2 \sin \Psi = 0. \quad (12)$$

The basic solutions of the SG equation, reflecting the essence of the FK model, and describing the soliton nature of the movement of dislocations, will be discussed further, in Sec. 3, where the generalization of the FK model is proposed. Below, the reconsideration of the string model of dislocation (S model) and its equivalent of the FK model will be also presented briefly in the new aspect of the dislocation models for AE sources (see also [10]).

## 2.2. The string model of dislocation (S model)

The S model is only one of the continuous models which is reconsidered here in the context of the dislocation models of AE sources. Other types of continuous dislocation models are based on the Somigliano model which was constructed within the theory of continuous media and they will not be considered here.

The dislocation segment in a real crystal, lying in a slip plane (Fig. 2) between two point obstacles (e.g. of the type of forest dislocations), and, at the same time, being potentially the dislocation source of the Frank-Read type (FR source, Fig. 3), can be treated as a string vibrating in a single Peierls potential valley (Figs. 2a and 3a, b). The general equation of the motion of a dislocation as a vibrating string was derived by Koehler and later this equation was considered also by Granato and Lücke in the context of the theory of internal friction (see also [10]).

It appears that in the particular case, when the infinite string is considered and both damping and external forces are neglected, the shape,  $\zeta(x, t)$ , of a freely vibrating dislocation string is described by the following NLPD equation

$$M \partial^2 \zeta / \partial t^2 - T \partial^2 \zeta / \partial x^2 + b \tau_p \sin(2\pi \zeta / a) = 0, \quad (13)$$

where  $M$  is the effective mass of the dislocation unit length,  $T$  is the line tension of the dislocation, and the Peierls stress  $\tau_p$  is defined by Eq. (1). One can see that Eq. (13) is the same as the SG Eq. (12), and that the characteristic constants are now given by

$$c_0^2 = T/M, \quad \omega_0^2 = 2\pi b \tau_p / M a. \quad (14a)$$

The expressions (14a) mean that the FK and S models are mathematically equivalent. There are two kinds of the consequences of this equivalence (see also [10, 11]). First,

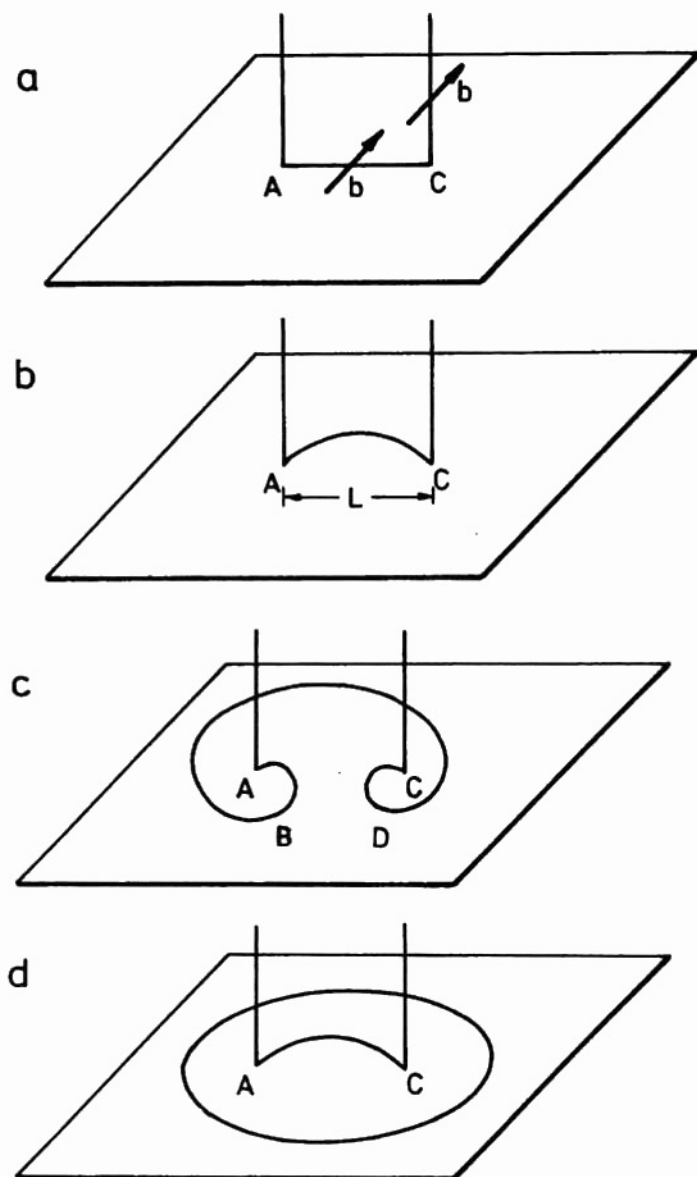


Fig. 3. The model of the Frank-Read dislocation source operation (FR model).

the parameters  $\alpha_0$  and  $A_0$  in the FK model can be expressed by the corresponding parameters  $M$  and  $T$  in the S model because the characteristic constants  $c_0$  and  $\omega_0$ , appearing in the common SG equation (12), are given by

$$c_0^2 = T/M = \alpha_0 a^2 / m, \quad \omega_0^2 = 4\pi^2 A_0 / m a^2 = 2\pi b \tau_p / M a. \quad (14b)$$

More detailed considerations [10, 11] show that the effective mass of the dislocation of a length equal to the lattice parameter  $a$ , is, as a good approximation, equal to the mass of the atom, i.e.  $Ma \cong m$ . Thus, the interaction constants  $\alpha_0$  and  $A_0$  in the FK model may be expressed as

$$\alpha_0 = T/a, \quad A_0 = \tau_p ab/2\pi = U_p/2, \quad (15)$$

i.e. the microscopic parameters  $\alpha_0$  and  $A_0$  may be expressed by the macroscopic parameters of line tension  $T$  and the Peierls stress  $\tau_p$ , which are often estimated as  $T \cong \mu b^2$  and  $\tau_p \cong 10^{-4}\mu$  for fcc and  $\tau_p \cong 10^{-2}\mu$  for bcc crystals;  $\mu$  is the shear modulus for a given crystal.

Secondly, the equivalence of the FK and S models means also that their common Eq. (12), and particularly its solutions, can be, in a sufficiently satisfying way, referred to a three-dimensional real crystal in which the movement of dislocation is, after all, a very complex process perturbed by various internal interactions, and in general, it proceeds also under the perturbations of external forces. In this way, the SG equation and its solutions, when related to an idealized case, describe the basic unperturbed forms of the dislocation motion which have been extracted from the real more or less perturbed and chaotic movement. The simplest cases of such solutions will be further discussed in detail in Sec. 3.

### 3. Generalization of the FK model

The generalization of the FK model, proposed in this paper, consists in taking into account new assumptions. The first one is the interaction between atoms in the second coordination zone and the second one is the nonlinear (anharmonic) interaction between the atoms in both the coordination zones.

The starting point is the expression for the potential energy of a simple ideal crystal of regular structure. This expression contains the terms of the Taylor expansion including those of fourth order [12]. Thus, instead of Eq. (4), the following formula will be considered now

$$\begin{aligned} \Phi = & \Phi_p + (1/2) \sum_k \left\{ (1/2!) \sum_{mn} \Phi_{\alpha\beta}^{(2)}(\mathbf{m}, \mathbf{n}) u_\alpha(\mathbf{m}) u_\beta(\mathbf{n}) \right. \\ & + (1/3!) \sum_{mnp} \Phi_{\alpha\beta\mu}^{(3)}(\mathbf{m}, \mathbf{n}, \mathbf{p}) u_\alpha(\mathbf{m}) u_\beta(\mathbf{n}) u_\mu(\mathbf{p}) \\ & \left. + (1/4!) \sum_{mnpq} \Phi_{\alpha\beta\mu\nu}^{(4)}(\mathbf{m}, \mathbf{n}, \mathbf{p}, \mathbf{q}) u_\alpha(\mathbf{m}) u_\beta(\mathbf{n}) u_\mu(\mathbf{p}) u_\nu(\mathbf{q}) \right\}, \quad (16) \end{aligned}$$

where the vectors

$$\mathbf{m} = \mathbf{l} - \mathbf{k}, \quad \mathbf{n} = \mathbf{l}' - \mathbf{k}, \quad \mathbf{p} = \mathbf{l}'' - \mathbf{k}, \quad \mathbf{q} = \mathbf{l}''' - \mathbf{k}, \quad (17)$$

are lattice vectors related to the corresponding components,  $u_\alpha$ , of the vectors of relative displacements of the atoms in the positions defined by the respective vectors  $\mathbf{k}$  and  $\mathbf{k} + \mathbf{m}$ ,



etc. These components are determined by

$$u_{\alpha}(\mathbf{m}) \equiv u_{\alpha}(\mathbf{l}) - u_{\alpha}(\mathbf{k}) = u_{\alpha}(\mathbf{k} + \mathbf{m}) - u_{\alpha}(\mathbf{k}). \quad (18)$$

Instead, the quantities,  $\Phi_{\alpha\beta\dots}^{(i)}$ , where  $i = 2, 3, 4$ , are the force constants of the second, third and fourth order, respectively. They are defined as the values of the respective second, third and fourth order derivatives calculated with respect to the corresponding components  $u_{\alpha}(\mathbf{m})$ . For most crystals, the values of the force constants are known and are not given here.

In the one-dimensional case, considered here, we have  $\alpha = \beta = \mu = \nu \equiv x$ ,  $u_{\alpha}(\mathbf{m}) = u(\mathbf{l}) - u(\mathbf{k}) \equiv u_{k+m} - u_k$ ,  $\Phi_{\alpha\beta\dots}^{(i)}(\mathbf{m}, \mathbf{n}) \equiv \Phi_{mn}$ , and  $\Phi_p = (U_p/2)[1 - \cos(2\pi u_k/a)]$ . Then all the expressions become simpler and one can obtain the following formula for the potential energy of a one-dimensional crystal with a dislocation

$$\begin{aligned} \Phi = & (U_p/2)[1 - \cos(2\pi u_p/a)] + (1/2) \left\{ \sum_{k=-\infty}^{\infty} (1/2!) \sum_{mn} \Phi_{mn} (u_{m+k} - u_k)(u_{n+k} - u_k) \right. \\ & + (1/3!) \sum_{mnp} \Phi_{mnp} (u_{m+k} - u_k)(u_{n+k} - u_k)(u_{p+k} - u_k) \\ & \left. + (1/4!) \sum_{mnpq} \Phi_{mnpq} (u_{m+k} - u_k)(u_{n+k} - u_k)(u_{p+k} - u_k)(u_{q+k} - u_k) \right\}, \quad (19) \end{aligned}$$

where the summation proceeds over  $m, n, p$  and  $q$ , as including the second coordination zone, and should be taken from  $-2$  up to  $+2$ . In this way the final form of the equation of motion for the  $k$ -th atom may be written as follows

$$\begin{aligned} m\partial^2 u_k / \partial t^2 = & -\partial\Phi/\partial u_k = -b\tau_p \sin(2\pi u_k/a) \\ & + A_1 [(u_{k+1} - u_k) - (u_k - u_{k+1})] + A_2 [(u_{k+2} - u_k) - (u_k - u_{k+2})] \\ & + B_1 [(u_{k+1} - u_k)^2 - (u_k - u_{k+1})^2] + B_2 [(u_{k+2} - u_k)^2 - (u_k - u_{k+2})^2] \\ & + C_1 [(u_{k+1} - u_k)^3 - (u_k - u_{k+1})^3] + C_2 [(u_{k+2} - u_k)^3 - (u_k - u_{k+2})^3], \quad (20) \end{aligned}$$

where the constants  $A_i$ ,  $B_i$  and  $C_i$ , ( $i = 1, 2$ ) may be expressed by the force constants  $\Phi_{mn}$ , and by the force constants of higher orders, i.e. the third  $\Phi_{mnp}$  and fourth  $\Phi_{mnpq}$  ones. Consequently, like in the case of the FK model, we use the continuous approximation and the fourth order Taylor expansion, i.e. it is assumed that

$$u_{k+n}(x) \cong u_k(x + an), \quad (21)$$

and

$$\begin{aligned} u_{k+n} - u_k = & (an)\partial u_k / \partial x + (1/2!)(an)^2 \partial^2 u_k / \partial x^2 \\ & + (1/3!)(an)^3 \partial^3 u_k / \partial x^3 + (1/4!)(an)^4 \partial^4 u_k / \partial x^4, \quad (22) \end{aligned}$$

where the index  $n$  proceeds over  $\pm 1, \pm 2$ . In this way a new NLPD equation is obtained governing in the generalized FK model. Namely, after the replacements,  $\Psi = 2\pi u/a$  and  $u \equiv u_k$ , and using a simple notation of the derivatives, it has the following form

$$\Psi_{tt} - c_0^2 \Psi_{xx} + \omega_0^2 \sin \Psi = c_1^3 \Psi_x \Psi_{xx} + c_2^4 \Psi_x^2 \Psi_{xx} + c_3^4 \Psi_{xxxx}, \quad (23)$$

where the constants  $c_i$  ( $i = 0, 1, 2, 3$ ) and the  $\omega_0$  are expressed by the formulae

$$\begin{aligned} c_0^2 &= \alpha a^2/m, & c_1^3 &= \beta a^3/m, & c_2^4 &= \gamma a^4/m, \\ c_3^4 &= \delta a^4/m, & \omega_0^2 &= 2\pi^2 U_p/m a^2, \end{aligned} \quad (24)$$

in which the  $\alpha, \beta, \gamma$  and  $\delta$  constants depend only on the force constants  $\Phi_{mn} \dots$ . Below the most important cases of the general Eq. (23) will be briefly considered.

### 3.1. A non-dislocated crystal ( $\omega_0 = 0$ )

This case is mostly discussed in the theory of crystal lattice vibrations. FLYTZANIS *et al.* [13] have shown that it leads to the type of the NLPD equation well known in the theory of solitons as the Boussinesq equation. Namely, after the substitution  $\Theta = \Psi_x$  Eq. (23) with  $\omega_0 = 0$  becomes the so-called generalized Boussinesq equation in which both kinds of anharmonicity (cubic and quartic) are taken into account

$$\Theta_{tt} - c_0^2 \Theta_{xx} = (c_1^3/2)(\Theta^2)_{xx} + (c_2^4/3)(\Theta^3)_{xx} + c_3^4 \Theta_{xxxx}. \quad (25)$$

On the other hand, considering only the cubic anharmonicity (in Eq. (25)  $c_2 = 0$ ) we obtain the NLPD equation which is known simply as the Boussinesq equation, whereas the consideration of the quartic anharmonicity only, i.e. the nonlinearity of the fourth order (in Eq. (25)  $c_1 = 0$ ), leads to the NLPD equation which is called the modified Boussinesq equation. The explicit forms of these NLPD equations are not given here, though it is worth of notice that all the NLPD equations of Boussinesq type are of very great importance in the theory of crystal lattice vibrations.

### 3.2. A dislocated crystal with cubic ( $c_2 = 0$ ) and quartic ( $c_1 = 0$ ) anharmonicities

The consideration of the cubic anharmonicity only in the generalized FK model is described by Eq. (23) with the constant  $c_2 = 0$ , i.e. by a new type of the NLPD equation

$$\Psi_{tt} - c_0^2 \Psi_{xx} + \omega_0^2 \sin \Psi = c_1^3 \Psi_x \Psi_{xx} + c_3^4 \Psi_{xxxx}. \quad (26)$$

Instead, the consideration of the anharmonicity of the fourth order only (Eq. (23) with the constant  $c_1 = 0$ ) also leads to a new type of the NLPD equation

$$\Psi_{tt} - c_0^2 \Psi_{xx} + \omega_0^2 \sin \Psi = +c_2^4 \Psi_x^2 \Psi_{xx} + c_3^4 \Psi_{xxxx}. \quad (27)$$

In this way, we have obtained a new class of NLPD equations not discussed so far in the theory of solitons. It is very probable that they have solitary wave solutions which also (like in the case of the Boussinesq equations) may play a role not only in the theory of dislocated lattice crystal vibrations, but also in the very theory of dislocations. To our knowledge, any solutions of these equations are not known and some efforts to solve them are undertaken now by using both the analytical and numerical methods. These attempts are limited rather to literature studies, though the computer simulation of numerical solutions is sufficiently advanced now.

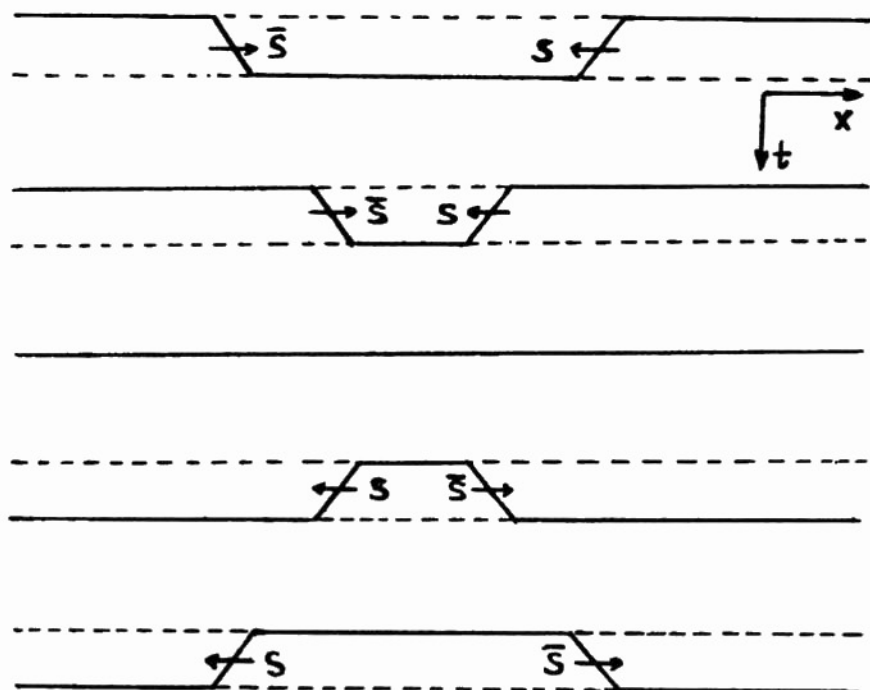


Fig. 4. A schematic illustration of the annihilation and creation of dislocation kinks described by the two-soliton solution of the SG equation in the FK model.

### 3.3. A harmonic crystal with dislocation ( $c_1 = c_2 = c_3 = 0$ )

It appears that the harmonic vibrations of atoms within the first coordination zone in a one-dimensional crystal with a dislocation is still the case best recognized. It is described by Eq. (23) with  $c_1 = c_2 = c_3 = 0$ , i.e. just by the well known SG equation (12)

$$\Psi_{tt} - c_0^2 \Psi_{xx} + \omega_0^2 \sin \Psi = 0, \quad (28)$$

which is the fundamental equation in the FK model. The SG equation was discussed sufficiently in Sec. 2.1, and here we present its simplest solutions which was found for the first time by SEEGER *et al.* [14] (see also [10]). These solutions can serve as the basic dislocation models for the elementary acoustic emission events.

The fundamental one-soliton solution of the SG equation (28) may be written in the form

$$\Psi(x, t) = 4 \tan^{-1} \{ \exp[\pm(x - vt)/\xi] \}, \quad (29)$$

where  $\xi = \xi_0(1 - v^2/c_0^2)^{1/2}$  is the width of the dislocation kink and  $v$  is its velocity;  $\xi_0$  is the kink rest width. The solution (29) describes the movement of the dislocation kinks, i.e. both the positive (sign "+" in expression (29)) and the negative (sign "-" in (29)) kinks as a solitary wave process (or simply as the soliton,  $s$ , and the antisoliton,  $\bar{s}$ , respectively; Fig. 2b, c;  $\xi = \Psi$ ).

The simplest two-soliton solution of SG equation, given by the formula

$$\Psi(x, t) = \tan^{-1}[c_0 \sinh(vt/x)/v \cosh(x/\xi)], \quad (30)$$

describes, in turn, the movement of a system of two dislocation kinks of opposite signs which are approaching each other from infinity, and, at first, they are annihilated and next created in subsequent Peierls potential valley, and in the further evolution they run away again in opposite directions to infinity. Thus, this solution describes the elementary dislocation annihilation process inside the crystal as a solitary wave process. There exists another two-soliton solution of the SG equation, i.e. the so-called pulson

$$\Psi(x, t) = 4 \tan^{-1} \left\{ (\omega_0^2 - \omega_p^2)^{1/2} \sin(\omega_p t) / \omega_p \cdot \cosh \left[ x(1 - \omega_p^2/\omega_0^2)^{1/2} / \xi_0 \right] \right\}, \quad (31)$$

which is a stable system of two dislocation kinks of opposite signs vibrating at the frequency  $\omega_p$ . Similarly, the kinks here are also approaching each other, and after anni-

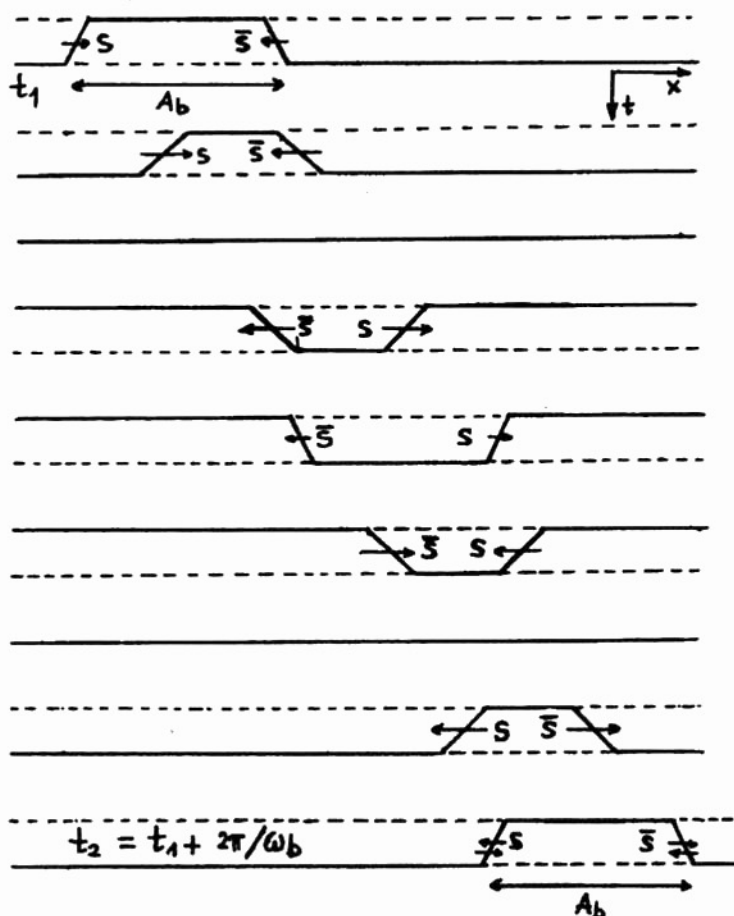


Fig. 5. A schematic illustration of the stable vibrating system of a pair of dislocation kinks (the so-called pulson) as described also by a two-soliton solution of the SG equation in the FK model.

hilation and creation they are again running away in opposite directions, but now only by a finite distance  $A_b$  (Fig. 5). Then the process is repeated in the same way.

#### 4. Dislocation models of the acoustic emission sources (AE models)

A concept is proposed below saying that the basis of the acoustic emission phenomenon, observed during the plastic deformation of regular crystals, are elementary dislocation processes, the description of which is given in the three above mentioned simplest soliton solutions of the SG equation as the one governing both the FK and S dislocation models.

##### 4.1. AE models based on changes in the dislocation velocity

The starting point is here the theory in which ESHELBY [15], considered the vibrations of a dislocation kink (Fig. 6a) and derived, as the first, the formula shows that the rate,  $P$ , of the acoustic energy emitted by the vibrating kink is proportional to the mean value of the square of the time derivative of its velocity

$$P = m_k \gamma_k \langle \dot{v}^2 \rangle, \quad (32)$$

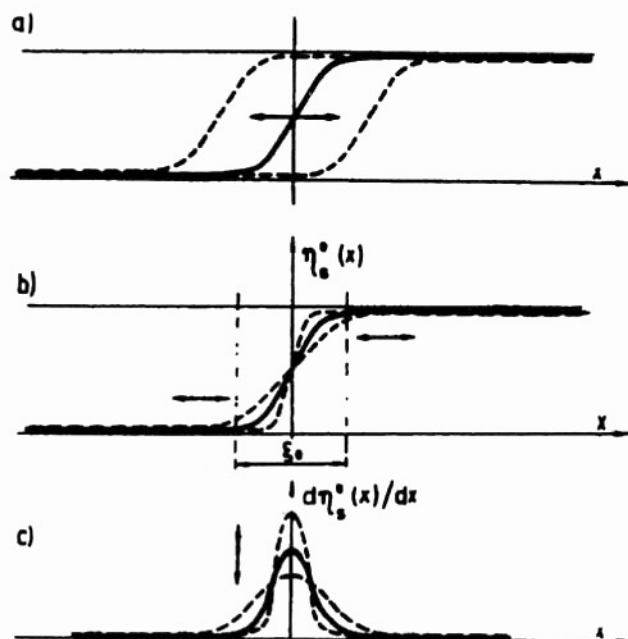


Fig. 6. Scheme illustrating the dislocation kink vibrations: (a) the rigid kink vibrating as a whole along the dislocation line, (b) the kink vibration as related to the changes in its width, and (c) the changes in the derivative of the kink shape.

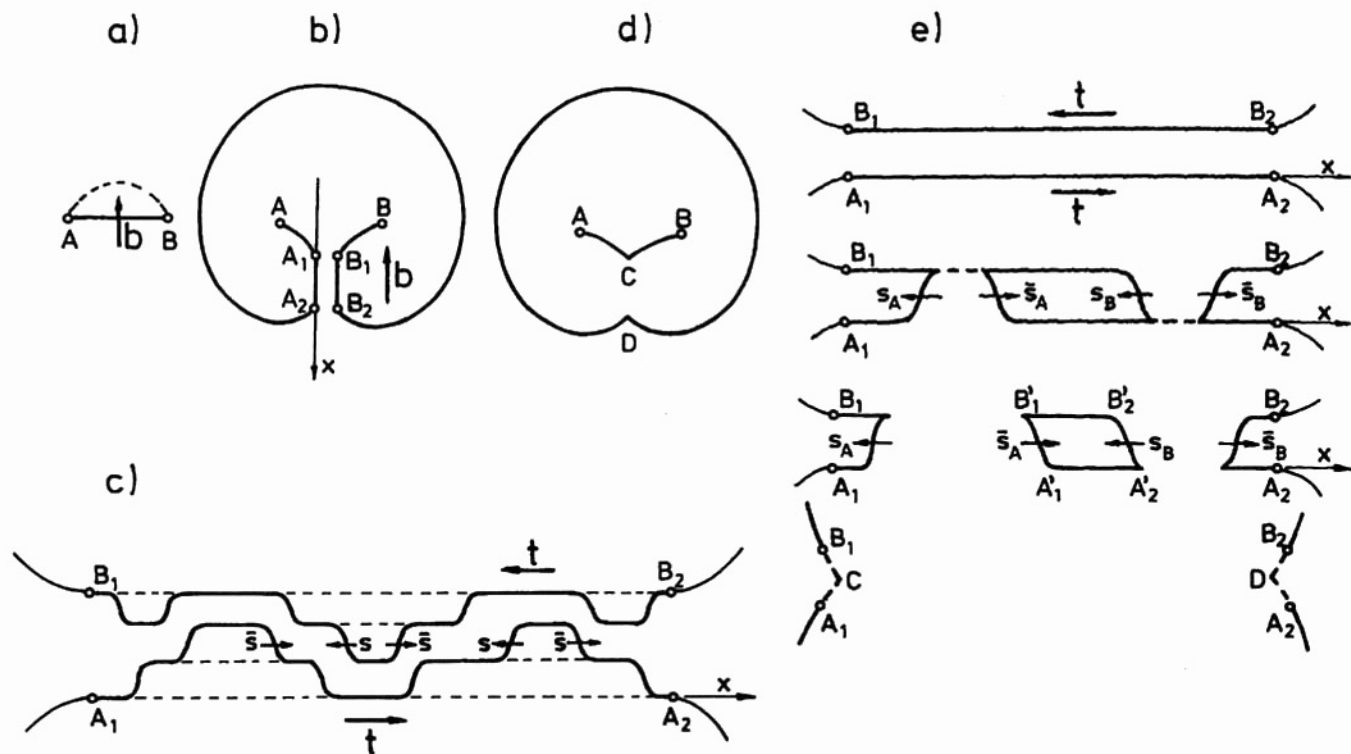


Fig. 7. The mechanism of the Frank-Read dislocation source operation (FR model) as the dislocation model of the source of elementary AE events.

where  $m_k$  is the kink effective mass,  $\gamma_k = \mu a^2 / 10 \pi m_k c^3$  with  $c^{-3} = c_t^{-3}(1 + c_t^5/3c_l^5)$ , where  $c_t$  and  $c_l$  are the transverse and longitudinal velocities of the sound, respectively. It should be noted, on the other hand, that the expression (29) says also that the changes in the kink velocity,  $v$ , result in corresponding changes of its width  $\xi$ . Namely, the shape of the accelerating kink becomes more sharp, whereas the shape of the decelerating one is more soft, thus the kink vibrations can occur also in a way illustrated schematically in Fig. 6b. In terms of the derivative of the function of the kink shape it means that the "hump" is more sharp or more broadened, respectively (Fig. 6c). In consequence, the solution (29) and the formula (32) constitute a dislocation model for the source of elementary acoustic emission events, related generally to the changes in the dislocation kink velocities (or simply in the dislocation velocities) including also those changes of various kinds of their vibrating movement.

It should be also stressed here that the result, similar to Eq. (32), but describing the dislocation mechanism of AE sources in a macroscopic scale, was obtained later by KOSEVICH [16]. In general, he used the methods of the continuous theory of dislocations in reference to the dynamics of any system of moving dislocation loops, and particularly to the system of dislocation loops emitted by sources of the Frank-Read type (Figs. 3 and 7). In a general way, KOSEVICH [16] stated that the density of the elastic energy flux,  $I$ , is proportional to the mean value of the square of the second time derivative of the so-called dislocation moment,  $\mathbf{D}$ , for the system of moving dislocation loops

$$I \approx \langle \ddot{\mathbf{D}}^2 \rangle, \quad (33)$$

where  $\mathbf{D}$  is the dislocation moment tensor which, e.g. for a single dislocation loop, is defined as  $\mathbf{D} = \mathbf{A} \mathbf{b}$ , i.e. as the diadic product of the vector  $\mathbf{A}$  of the area of the expanding loop by the Burgers vector  $\mathbf{b}$  of the dislocation. Though in the case of a system of dislocation loops, the soliton behaviour is not completely recognized as yet (some suggestions given in Figs. 12 and 13 are discussed also in [17, 18]), the formula (32), and similarly, the expression (33) describe the same large class of dislocation models of AE sources related to the dislocation acceleration.

#### 4.2. AE models based on the dislocation annihilation

The starting point is the basic two-soliton solution of the SG equation, given by (30), which describes the annihilation of dislocations in a completely analytical way. This solution is referred to the unperturbed case when after an annihilation event there occurs a creation, and next the dislocation kinks move in opposite directions (Fig. 4). However, in fact, such perturbations as lattice friction and/or various obstacles to the dislocation motion (e.g. forest dislocations, solute atoms, etc.) do not favour the repeated creation of kinks and the whole elastic energy revealed in the annihilation process can be transferred into the energy,  $E$ , of the acoustic wave.

The energy,  $E$ , was estimated for the first time by NATSIK and CHISHKO [19] by the methods of the linear theory of elasticity of continuous media. Their result says that the energy,  $E$ , is proportional to the square of the relative velocity  $V$  of the annihilating

dislocations of unit length. For screw dislocations, it is given by the expression

$$E = (\rho b^2/8\pi)V^2 \ln(L/b), \quad (34a)$$

whereas for edge dislocations by the formula

$$E = (\rho b^2/8\pi)V^2(1 + \gamma_c^4) \ln(L/b), \quad (34b)$$

where  $L$  is the linear dimension of the crystal,  $\gamma_c = c_t/c_l$ , and  $\rho$  is the medium density. It is often assumed that  $\ln(L/b) \cong 4\pi$ ,  $\gamma_c \ll 1$ , and  $\rho b^2 \cong M$ , i.e. the quantity  $\rho b^2$  is equal in the order of magnitude to the effective mass of a dislocation unit length. From the above estimations and from the formula (34) it follows that the energy,  $E$ , at the approximation of the linear theory of elasticity, has the form

$$E = MV^2/2, \quad (35)$$

which implies a simple physical interpretation, saying that during the annihilation, only the kinetic energy of the relative motion of dislocations is transferred into acoustic energy.

On the other hand, a similar expression, though only in the sense of an additive term, can be derived on the basis of two-soliton solution (30) of the SG equation: the energy,  $E_k$ , of a single dislocation kink of the effective mass  $m_k$  may be written as a "non-relativistic" approximation (when the kink velocity is  $v \ll c_0$ ; see also [10]) in the following form

$$E_k = E_0 + m_k v^2/2, \quad (36)$$

where the kink rest energy,  $E_0$ , (energy of the dislocation core) as well as the kink effective mass,  $m_k$ , can be expressed by the characteristic constants  $c_0$  and  $\omega_0$  in the SG equation, or by the parameters  $\alpha_0$  and  $A_0$  in the FK model, or by the parameters  $\tau_p$  and  $T$  in the S model (such an expressions has been derived and analysed in more details in [10]). In consequence, for the energy,  $E$ , revealed during the annihilation of two dislocation kinks, the following expression was obtained

$$E = 2E_k = 2E_0 + m_k V^2/2, \quad (37)$$

where  $V = 2v$  is the relative velocity of the annihilating kinks; for the unit length of dislocation it was assumed that it is equal to the kink width  $\xi$ . The formulae (35) and (37) differ only by the term  $2E_0$  (the quantities  $M$  and  $m_k$  are of the same order of magnitude). The explanation for this difference is quite simple. In the linear theory of elasticity, the very strong nonlinear effects appearing due to the existence of the dislocation core cannot be taken into account. On the contrary, in the FK model, which, at the same time, is a dislocation core model, these effects are considered. They are reflected in the solitary wave properties of the dislocation kinks. Thus, the quantity  $E_0$ , given by the formula

$$E_0 = 2a(2U_p T)^{1/2}/\pi, \quad (38)$$

as an additive term in Eq. (37), does not change the quantitative physical interpretation: the AE caused by the dislocation annihilation is proportional to the square of their relative velocity. Perhaps, the term  $E_0$  can play a role in the qualitative estimations of the number of AE events.



As a result of the above considerations, one can say that the formulae (30) and (37) constitute the basic dislocation model of the source of elementary AE events which, in general, are related to the dislocation annihilation processes. It should be emphasized that this model can also serve as a model of AE sources related to the dislocation annihilation processes occurring at the free surface of the sample due to the escape of dislocations from the crystal because, from the mathematical point of view, the problem is in this case equivalent to the annihilation of a dislocation with its virtual image of opposite sign in respect to this surface. However, it should be strongly emphasized that the models (29), (30) and (31) describe the soliton behaviour of dislocation kinks in a conservative, closed system in that the energy and velocity remain unchanged, thus they cannot be related immediately to a deformed sample which is an open system. Nevertheless, these models are useful for the qualitative understanding of the operation of AE sources in deformed metals where the perfect soliton behaviour is perturbed by external and local stresses.

#### 4.3. Other AE models

First of all, the mixed models based, in an inseparable way, on both the dislocation velocity changes and the dislocation annihilation processes should be mentioned here. The two-soliton solution of the SG equation, given by Eq. (31), i.e. the so-called pulson illustrated schematically in Fig. 5, may serve as an example of such a model on a microscopic level. According to the formula (29), the stably vibrating pulson generates acoustic waves due to the continuous changes in the linear velocity of its kinks. On the other hand, the total destruction of the pulson results also in the generation of acoustic waves related, in turn, to the annihilation of its kinks according to formula (37). Such a situation is very probable because repeated creations of the kinks may be often impossible, for example due to strong local perturbations.

Another example of the mixed AE models is the Frank-Read mechanism of the dislocation source operation (FR model, Figs. 3 and 7). In this case the annihilation of many dislocation kinks takes place in each time interval when the closing of the dislocation loop occurs (along the sections C and D of the dislocation line in Fig. 3c; see for more details Fig. 7b and c). This leads, according to formula (36), to the generation of elementary AE events. On the other hand, each of the just closed dislocation loops which is still expanding, e.g. under external stresses, is undergoing the acceleration and thus it generates an acoustic wave according to Eq. (29); see also [4, 10, 18].

Also the dislocation pole mechanism of the twin formation (Fig. 8, T model) is another example of mixed models of the AE source. The increase of the velocity of twinning dislocations, which is especially high just in the twinning processes, is the main cause of the acoustic wave generation according to the formula (29). Similarly, during the escape of the twins from a crystal to its free surface, i.e. the annihilation of twinning dislocations, elastic energy is released and transformed into the acoustic wave energy according to Eq. (37).

All the AE models discussed have their more or less immediate origin in the corresponding (governing) type of the equation of the dislocation motion. In most of the

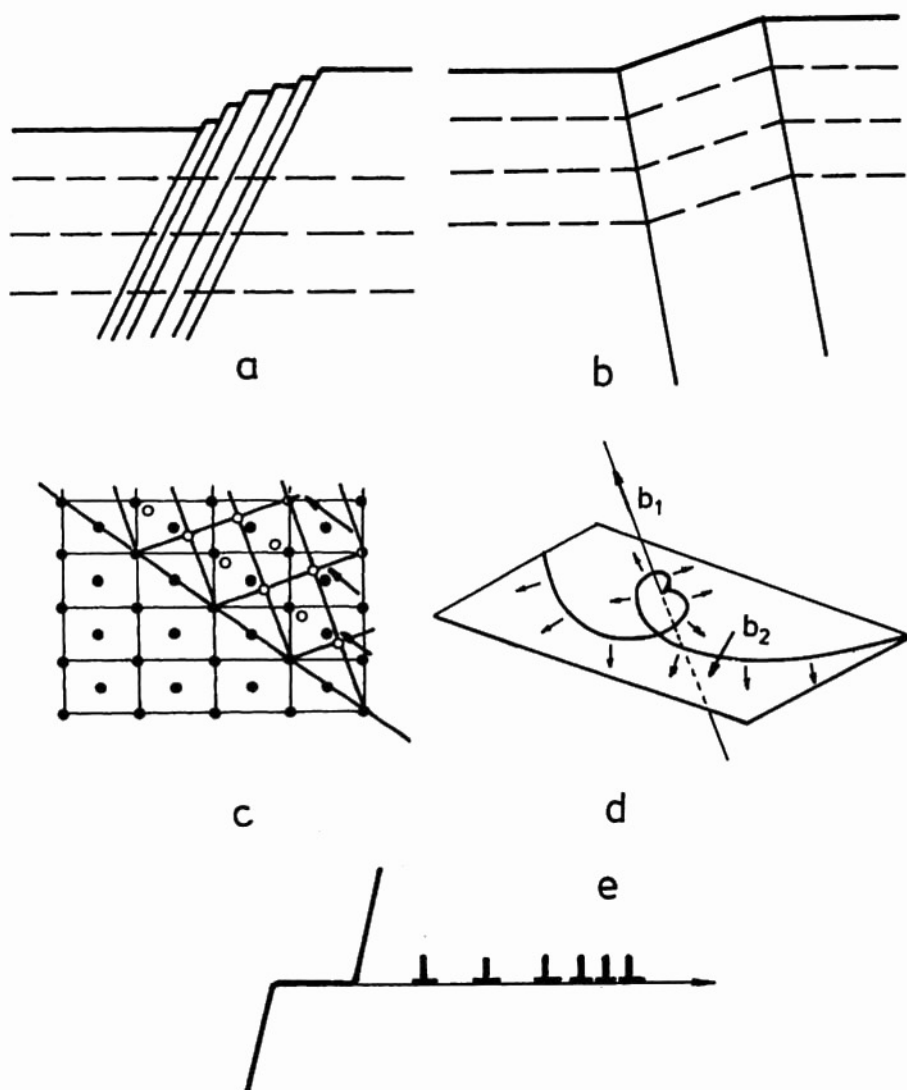


Fig. 8. A schematic illustration of the twinning process: the dislocation pole mechanism (d) leads to the mirror positions of atoms (c), and the final deformation of the crystal (b) differs from the step formed only due to the slip (a); both cases, at a one-dimensional approximation, are equivalent to the dislocation pile-up (e).

cases considered here, it is the SG equation that can be qualified as the equation of *string* type. Thus it is worthy of pointing out that also equations of the *diffusion* (or *heat transfer*) type may have solutions of the solitary wave type (see e.g. [18]), and they can serve too as possible dislocation models of AE sources. Such a suggestion, just in a new context of AE, is briefly reconsidered below.

#### 4.4. AE models based on a "diffusion" equation of the dislocation motion

Starting from the equation of continuity for a coplanar array of moving dislocations (e.g. generated by the FR source and distributed continuously), we consider the dynamics of dislocations in terms of a concept of the dislocation flux which would obey the equation formally similar to those describing the diffusion or heat transfer processes. In a one-dimensional space, we may define the dislocation flux in the form

$$J(x, t) = \rho(x, t)v(x, t), \quad (39)$$

which satisfies the equation of continuity

$$\partial \rho(x, t) / \partial t = -\partial J(x, t) / \partial x, \quad (40)$$

where  $\rho(x, t)$  is the linear density, and  $v(x, t)$  is the mean velocity of dislocations (see e.g. [21, 22]). For simplicity, we restrict our treatment to the one-dimensional case, i.e. we consider a dislocation flux in only one direction corresponding to the single active slip system. Using the results of our earlier papers [18, 23] on the thermally activated motion of dislocations, the following expression, analogous to that for heat conduction or diffusion processes, may be obtained

$$J(x, t) = -D \partial \rho(x, t) / \partial x, \quad (41)$$

and finally, using Eq. (40) we get the evolution equation for the density of activated dislocations which is analogous to the Fourier law of heat transfer or to the second Fick law of diffusion

$$\partial \rho(x, t) / \partial t = D \partial^2 \rho(x, t) / \partial x^2. \quad (42)$$

This equation is the simplest version of that one discussed earlier [24, 25] in the form

$$\partial \rho / \partial n = D \Delta \rho + k_1 \rho - k_2 \rho^2, \quad (43)$$

where, additionally,  $n$  is the number of the imposed load cycles in the fatigue process considered there, and the constants  $k_1$  and  $k_2$  are the multiplication and annihilation coefficients, respectively;  $\Delta$  is the laplacian. In this way, Eq. (42) is related to the ideal extracted case of the dislocation motion, where the terms responsible for both the multiplication and annihilation of dislocations are neglected (i.e. in Eq. (43)  $k_1=0$  and  $k_2=0$ ).

In order to determine the flux,  $J(x, t) = \rho(x, t)v(x, t)$ , of activated dislocations, it is necessary to find the evolution equation for the dislocation velocity  $v(x, t)$ . Assuming that the mean value of the dislocation flux is,  $J = \rho v/2$ , Eq. (41) may be written in the following form (see also in [18, 23])

$$\rho(x, t)v(x, t)/2 = -D \partial \rho(x, t) / \partial x. \quad (44)$$

It is, perhaps, very interesting to note that this equation has the form of the Cole-Hopf transformation which is known in the mathematical theory of solitons, and is usually given by

$$v(x, t) = -2D \rho_x / \rho. \quad (45)$$

This transformation maps solutions of the diffusion type equation (42) onto solutions of the NLPD Burgers type equation, the form of which may be written as follows

$$\partial v(x, t)/\partial t + v(x, t)\partial v(x, t)/\partial x - D\partial^2 v(x, t)/\partial x^2 = 0, \quad (46)$$

or simply in the form

$$v_t + vv_x - Dv_{xx} = 0. \quad (47)$$

One of the analytical well-known solutions of the Burgers equation is of the solitary wave character, the form of which is the Taylor shock profile given by [26] (see also in [18, 23])

$$v(x, t) = \alpha D \{1 - \tanh[(x - \alpha Dt)/2]\}, \quad (48)$$

where  $2\alpha D = v$  is the velocity at  $x \rightarrow -\infty$ , and  $\alpha v_\infty/2 \equiv w$  is the rate of changes in the dislocation velocity during their propagation. These changes are of the step-like front character and they are localized within a narrow region of the space [26].

In agreement with the above considerations we can now treat the motion of a group of dislocations as a nonlinear wave process, i.e. during each local movement of the dislocation group inside the crystal (related e.g. to the FR mechanism of the dislocation source operation in the simplest case, or in a more general case to the slip and/or shear band propagation), the mean velocity of the group changes in space and time like a solitary wave impulse. Thus, in the sense of changes in the dislocation velocities with time, the movement of a dislocation group can be considered as the AE source of the type described by the formula (32) or (33). Finally, it is worthy of pointing out that there exist also the periodic solutions of the SG equation. Such solutions, for example, were discussed elsewhere [27] in the context of the behaviour of the moving dislocation kink as the soliton on the background of a quasi-periodic process.

## 5. Discussion and conclusions

Firstly, we present some chosen most representative experimental data which illustrate the existence of strong correlations between the behaviour of the acoustic emission (AE) and the mechanisms of plastic deformation in mono- and polycrystalline metals of a fcc lattice that undergoes a channel-die compression at both the ambient and liquid nitrogen temperatures [5–9].

In Figs. 9–11 the behaviours of AE, i.e. the rate of the AE events,  $\Delta N_z/\Delta t$ , as well as functions of the external compressing force (diagrams at the top) together with the corresponding microstructure (photos at the bottom) are presented. These figures reflect the more significant deformation mechanisms during the channel-die compression which are connected, first of all, with the processes of twinning (Figs. 9 and 10) and with the formation of the primary family of shear bands (Fig. 11). For example, in Fig. 9 it is shown that the formation of exactly three thin plates of twins (in the direction marked on the photo) is accompanied also by exactly three very pronounced peaks of the rate of the AE events (in this case the compression test has been especially stopped at the moment in that the twinning process begins). In Fig. 10 the characteristic steps (see also

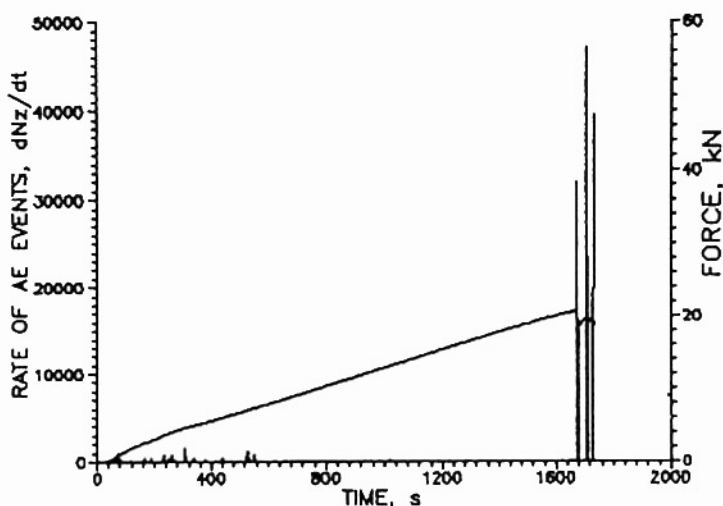


Fig. 9. Acoustic emission (AE), external force (at the top) and the corresponding microstructure (at the bottom) of silver single crystals of  $\{112\}\langle 111 \rangle$  orientation during channel-die compression at ambient temperature (reduction  $\epsilon = 11\%$ , magnification  $\times 10$ ).

the scheme in Fig. 8) formed due to the escape of the twins to the free surface of the sample are shown. On the other hand, in Fig. 11 it was demonstrated that the formation of a primary family of shear bands is related to the creation of the steps at the surface of the sample, the latter being simultaneously strongly correlated to the corresponding AE peaks as well as to the sudden drops of the external compressing force that are accompanying them.

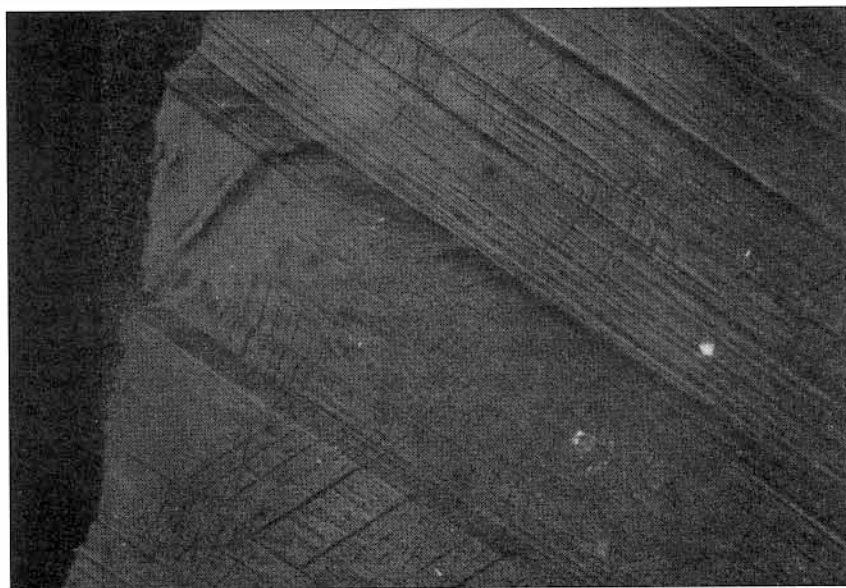
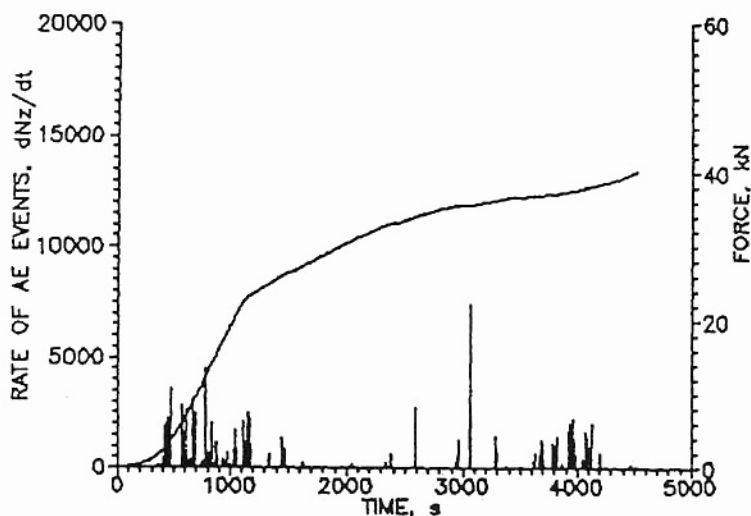


Fig. 10. AE, external force and microstructure of Cu-2%Al single crystals during the channel-die compression ( $T = 77$  K,  $z = 60\%$ , orientation  $\{421\}\{112\}$ ).

The high rate of the AE events during the formation of the particular plates of twins (Fig. 9), attaining the values even of the order of magnitude significantly above  $10^4$ , is in our opinion caused mainly by the escape of the twins to the crystal surface which results in the formation of characteristic steps like those shown in Fig. 10. If we assume the pole mechanism of the twin formation (Fig. 8), such an interpretation is in a qualitative agreement with formulae (35) and (37).

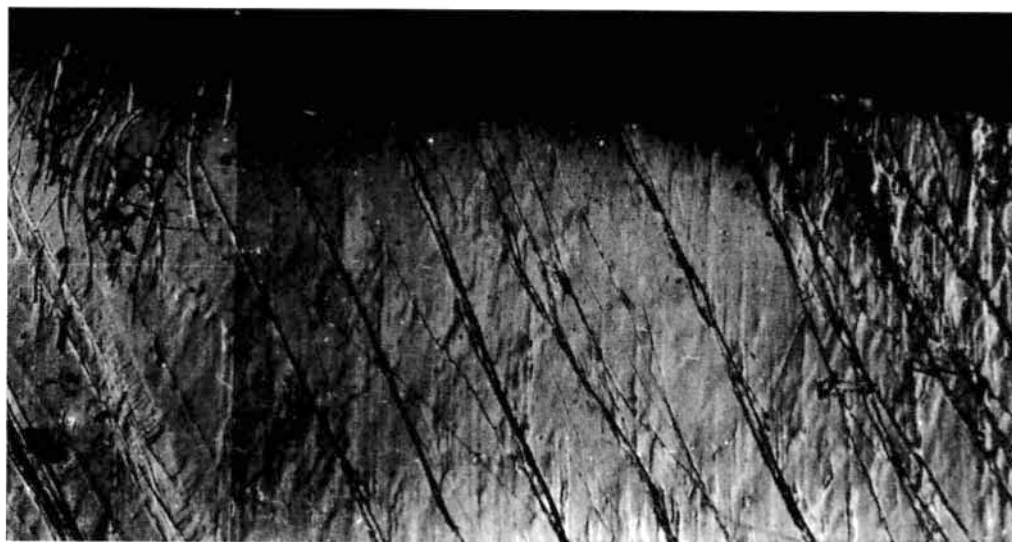
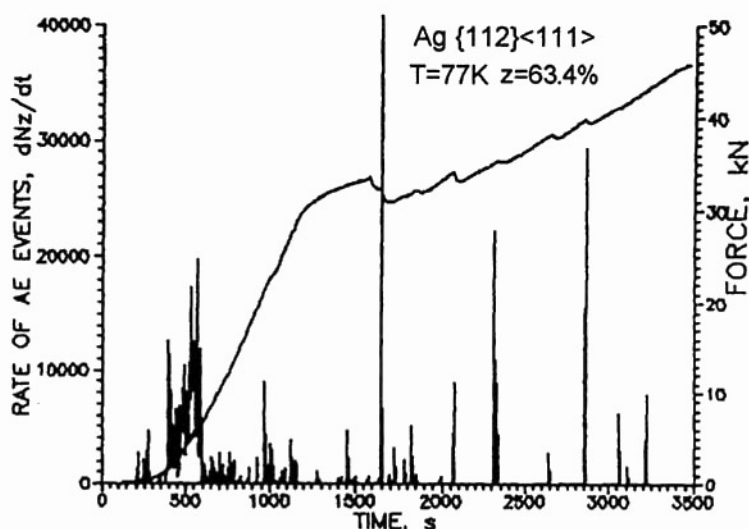


Fig. 11. EA, force and microstructure of Ag single crystals during the channel-die compression ( $T = 77$  K,  $z = 63\%$ ,  $\times 200$ , orientation  $\{112\}\langle 111 \rangle$ ).

A following attempt of the quantitative estimation of the rate of AE events during the formation of a single twin plate can be made. Let us assume that an elementary AE event is connected with the escape to the surface of the twinning dislocations moving within the range of one atomic plane. For simplicity, it is assumed that the lattice parameter  $a$  is of the order of Burgers vector, i.e.  $a \cong b \cong 10^{-4} \mu\text{m}$  (for Cu  $b \cong 2.8 \text{ \AA}$ ). The observed width of the twin lamellae oscillates within the limits  $10^2$  to  $10^3 \mu\text{m}$  which,

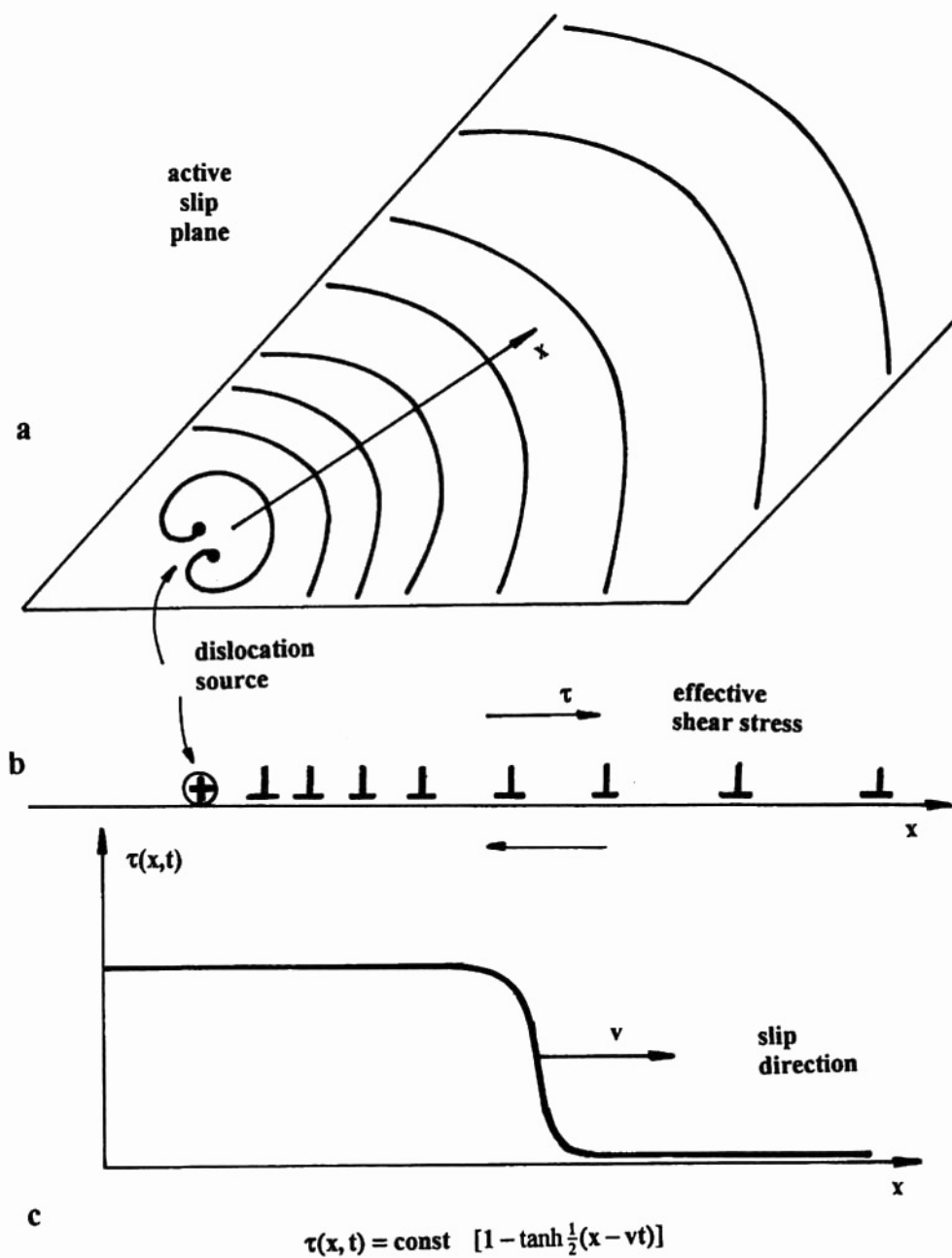


Fig. 12. Schematic illustration of the dynamics of dislocations generated by the source (a), the corresponding dislocation configuration at a one-dimensional approximation (b), and the solitary wave-like character of the dislocation propagation (c).



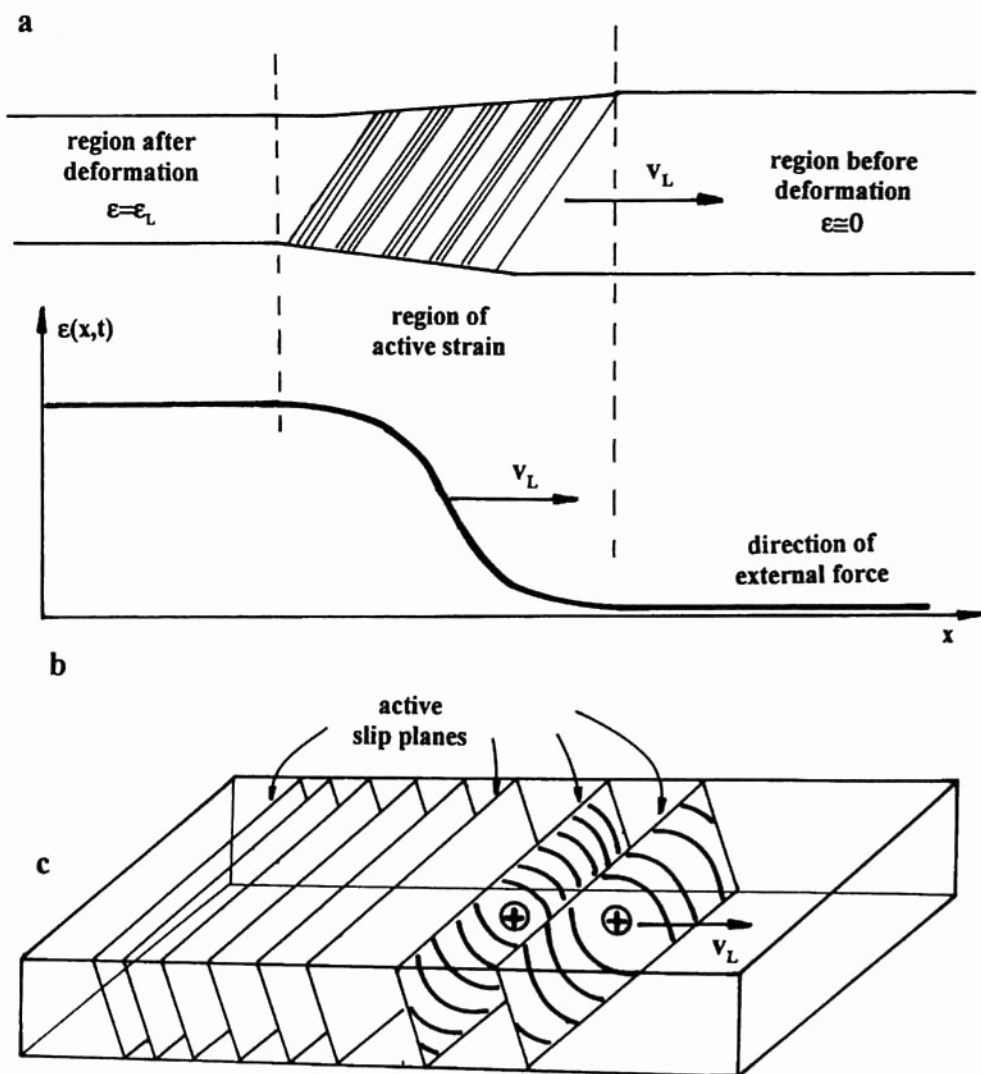


Fig. 13. Schematic illustration of a simple model of slip band propagation (a), its solitary wave representation (b), and the dislocation dynamics in active slip systems (c).

at the applied magnifications of the order of 10 to 100, places the value of the actual width of a twin lamella, at a rough approximation, in the interval from 1 to 100  $\mu\text{m}$ . Hence, the number of engaged atomic planes, and thereby the number of elementary AE events comprising an AE peak originated from a single lamella, is of the order of  $10^4$  to  $10^6$  which is satisfactorily consistent with the magnitude of the observed values. As known and has been mentioned earlier, the dislocations may develop very high velocities during the twinning process (of the order of the speed of sound). Thus, it should be

remembered that great dislocation accelerations are also possible which means that the AE sources of the type defined by the formulae (32) or (33) may be of vital importance in the case of the twinning processes.

In consequence, proceeding in a similar way as in the case of the twinning, we can discuss the formation of shear bands (Fig. 11). The steps on the sample surface (clearly seen in the photo) are formed as a result of the strain localization in the generated shear bands, each being accompanied by a rapid drop of the external force and a corresponding AE peak the value of which falls within the limits  $10^4$  to  $4 \times 10^4$ . Assuming that a single elementary AE event corresponds to the escape of a single gliding dislocation to the surface (a step of the order of magnitude of Burgers vector  $b$ ), it can be estimated that the real size of such steps as shown in Fig. 11 ( $\cong 2$  mm at the magnification  $\times 200$ ) is of the order of  $10 \mu\text{m}$ . Next we assume that the number of dislocations generated by a single FR source, forming a slip line, is of the order of  $10^2 - 10^3$  (in the literature values closer to about  $10^3$  are often assumed [28]; see also [29]). Thus, it can be expected that the formation of a step of size of  $\sim 10 \mu\text{m}$  on the sample surface is accompanied by the escape of dislocations from very many slip planes, that can be of the order of  $10^2$ ; each single source of the plane (e.g. of the FR type) has produced so many dislocations that nearly  $10^3$  of them became annihilated on the sample surface. In this way the formation of a step of the order of 1 to  $10 \mu\text{m}$  in size would be associated with the generation of  $10^4$  to  $10^5$  elementary acoustic events forming a single AE peak. Such an estimation of the order of magnitude is in accordance with the values observed (from  $10^4$  to  $4 \times 10^4$  in Fig. 11).

It should be also pointed out that the contribution to the values of the AE peaks observed may originate also from the annihilation processes during the operation of the FR sources (Figs. 3 and 7) when the dislocation loops are closing as well as from the acceleration of the dislocation loops already generated by these sources. It can be seen that a more significant role of these effects corresponds rather to the beginning stage of the plastic deformation when the yield point (the range of dynamic formation of slip lines) is exceeded. On the other hand, when the shear band formation process is beginning (the creation of the marked steps at the sample surface), the effects of surface annihilation of dislocations are rather prevailing.

To sum up the discussion, it should be emphasized that a new model of dislocation, i.e. the generalized FK model, has been proposed here and that the governing differential equations for the dislocation motion in this model constitute a new class of NLPD equations which, to our knowledge, have not been sufficiently recognized so far in the theory of solitons. Moreover, literature studies of the analytical methods of the solution of NLPD equations have been started, and, at the same time, good progress has been made in preparing a computer programme for their numerical solutions. On the other hand, the FK dislocation model is reconsidered and it has been shown that the basic soliton solutions of the SG equation, being the governing NLPD equation in the model, can be used as basic elements for the dislocation models of the acoustic emission sources since they are very useful for the qualitative understanding of the dislocation annihilation and acceleration processes in a micro-scale. It has also been shown that the proposed dislocation models of the AE sources describe qualitatively the behaviour of AE during

the channel-die compression of fcc metals in a quite satisfactory way. In particular, on the basis of these models the order of magnitude of the values of the peaks of the rate of AE events have been estimated in good agreement with the values observed. Consequently, the most significant results obtained can be formulated in the following final conclusions:

— The differential equations for the dislocation motion, governing in the generalized FK model, are new NLPD equations which can play a role in the theory of the dislocated crystal lattice vibration as well as in the theory of dislocations.

— The SG equation, being the governing NLPD equation in the FK dislocation model, has the analytical solutions which are of the soliton type and which describe the dislocation annihilation processes as well as the vibrating movement of the dislocation kinks.

— The basic soliton solutions of the SG equation, given by Eqs. (29), (30) and (31), as well as the expressions (32) and (37), constitute the main elements of the proposed dislocation models of the acoustic emission (AE) sources related to both the annihilation and acceleration of dislocations.

— The proposed dislocation models of the AE sources allow to estimate the values of the peaks of the rate of AE events accompanying the slip line formation, twinning and shear banding processes during the channel-die compression of fcc metals; the orders of magnitude of these values, are in a quite good agreement with the observed ones for AE peaks.

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