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KINETIC THEORY OF CONTINUOUSLY DISTRIBUTED DISLOCATIONS

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Abstract—The paper is devoted to the kinetic theory of continuously distributed dislocations. After defining the particle velocity distribution function and its moments, we derive transport and collision parts of the kinetic equation. Its right hand side is based on the Fokker–Plank long-range interaction for dislocations. The expressions obtained for the diffusion coefficients of this equation are found to be similar to analogous values obtained by others. As a result of a successive procedure of averaging the kinetic equation, the transport equations for dislocation density and flow density tensors are derived. In particular, the first moment equation is found to be similar to the well-known equation of the conservation of the Burgers vector in the continuous theory of dislocations. Some general features of the system are discussed and a one-dimensional example is used for calculating the dislocation drag coefficient in dynamically loaded media.

NOTATION

$\hat{f}(r, v, t)$	distribution function of dislocations in the velocity space
f_0	the same for the equilibrium case
f^s	distribution function for dislocations of a single slip system number s
$\hat{\rho}(r, t)$	dislocation density tensor
ρ	average dislocation density
$\hat{J}(r, t)$	dislocation velocity tensor
v	instantaneous dislocation velocity
u	average dislocation velocity
c	relative dislocation velocity
P_{iln}	the second statistical moment of the distribution function
Q_{mjn}	the third statistical moment of the distribution function
m	effective mass of dislocation
b	Burgers vector
F	external driving force of dislocation
B	dislocation dumping coefficient
D_1	coefficient of dynamic friction in the Fokker–Plank equation
D_2	diffusion coefficient in the Fokker–Plank equation
μ	elastic shear modulus
λ	Lame-elastic coefficient
ρ_0	mass density of material
U	displacement of medium due to dislocation motion
W	plastic distortion tensor
G	Green tensor in the dynamic elasticity theory
k	wave vector
ω	frequency
e_{ikl}	Levi-che-Vitta tensor
σ	stress tensor
τ_r	relaxation time for the velocity distribution function
c_t	transverse sound velocity
c_f	phase velocity for wave propagation in the dislocation medium
δ	decay decrement for stress wave propagation
I_{coll}	collision term in the kinetic equation

1. INTRODUCTION

The continuous theory of dislocations is known to deal with averaged characteristics of dislocations, such as mean density and mean velocity. There are two classes of problems which can be solved by the continuous theory of dislocations. In the first class, space distribution of dislocation density and velocity are given, and the ultimate goal is to find the space distribution of the stress and displacement fields in the medium. This direction of the classical continuous theory of dislocations has been developed in its final form by Kondo (1949), Bilby (1955), Kroner (1955), Mura (1963) and Kosevich (1964).

The second class, on the contrary, proceeds from a knowledge of the stress and displacement fields, while the density dislocation tensor and flow dislocation density tensor are unknown. This direction in dislocation theory has been developed by Head and Wood (1972) and Rosenfield and Hahn (1972). Both cases mentioned deal with static and quasi-static loading and cannot describe the dynamic behavior of dislocations and their ensembles.

The next important step has been the subdivision of the dislocations into slow (gliding, climbing, cross-slipping or even pinned at obstacles) and fast (driven by high stress) dislocations. The reaction–diffusion equations introduced by Aifantis (1983, 1986, 1987) appear to be appropriate for describing the dislocation dynamics, their motion and interactions. This approach results in the method of description of structure instabilities, persistence of dislocation patterns, ladder structures, shear bands and so on.

The statistical behavior of the elementary particles in the mechanics of fluids and gases is known to define the processes which cannot be understood and described on the basis of the average medium characteristics. For example, it describes the decay of the waves in plasma, molecular relaxation in gas flows in lasers, fine structure of shock waves, etc. An analogous situation occurs in the mechanics of solids, where plastic flow results from the motion of the elementary carriers of deformation, such as point defects, dislocations, twins, planar defects and so on. It can thus be argued that their motion may be characterized by some distribution in the velocity space, the character of that distribution being defined not only by the mutual interaction of the elementary carriers but also by their interaction with the medium in which they move. In particular, the kinetic approach to dislocation structures should be developed for the description of transient and non-equilibrium processes in solids. These processes are thought to play a key role in the unsteady wave propagation and dynamic localization of deformation. At the same time, well-known dislocation characteristics such as the density and flow of dislocations can be defined as the statistical moments of the velocity distribution function. The latter can be found from the kinetic equation for dislocations which, in turn, must be self-consistently related to the stress and displacement fields through the equations of the continuous theory of dislocations. The situation is similar to the kinetic plasma theory where, for example, the Vlasov equation describing the evolution of the charged particle velocity distribution function is "locked" with the continuum variables via the Maxwell equations.

A desirable kinetic theory must also satisfy the following requirements.

The theory must first take into account the dissipative character of dislocation motion in the medium, i.e. the equation of dislocation motion must include the interaction of dislocations with the dissipative medium.

Secondly the long range character of the dislocation interaction must be taken into account as well, i.e. the kinetic theory at hand must be able to describe the processes of deformation in which the collective properties of dislocation structures are accounted for.

Thirdly for the description of highly non-equilibrium processes accompanied, for example, by high strain deformation, the kinetic theory must not neglect the internal properties of the elementary carriers of deformation. Inertia is typically ignored in quasistatic dislocation theories, although the importance of this term is probably underestimated.

Last but not least is the question of scale averaging in a kinetic description of dislocation structures. Every elementary volume must contain a lot of dislocation pieces belonging to different dislocation lines in order for their description in terms of distribution functions to be justified from the point of view of the statistical approach. When the considered process assumes dislocation multiplication, the averaging scale must be chosen from the condition that it must be greater than the mean distance between dislocation sources.

The development of the kinetic theory of dislocations includes the following stages:

(i) The definition of the velocity distribution function of dislocations as objects, characterized at every point in space by the tangent direction to the dislocation line and by the Burgers vector; separate segments of the dislocation linc may be of different orientations in space and different velocities.

(ii) The derivation of the kinetic equation for the distribution function. The convective and collision parts of the equation must take into account the dissipative properties of the medium where dislocations move, as well as their mutual long-range interactions. The collision part of the equation, in general, must allow not only the redistribution of dislocations under external stress but also their nucleation and annihilation during the deformation process.

(iii) The definition of equilibrium dislocation functions.

(iv) The derivation of the moment equation system from the kinetic equation. This system must coincide with the well-known equations of the continuous dislocation theory. A different approach based on the statistical dislocation description and the Kirkwood transport equation system has been developed by Zorski (1968).

In this study we follow the above sequence in designing the present kinetic theory of dislocations (sections 3–5). In section 5 a derivation procedure of transport equations is carried out. We have also undertaken an analytic investigation of the kinetic behavior of dislocation structures during unsteady external loading. When applied to stress pulse propagation problems this theory results in an obvious expression for the decay decrement of the stress pulse amplitude reminiscent of the well-known "Landay decay" in plasma (section 6).

2. DEFINITION OF THE DISTRIBUTION FUNCTION

Taking into account the configurational complexity of dislocation lines it is relevant to use a tensorial description of the dislocation continuum. Such descriptions are used in the continuous dislocation theory where the dislocation density is a second rank tensor; the first index characterizes the tangent direction to the dislocation line and the second one is the direction of the Burgers vector. According to this definition $f_{ik}(r, v, t)\,\mathrm{d}r\,\mathrm{d}v\,\mathrm{d}t$ is a mathematical expectation of the number of dislocation segments of type ik in the volume dr at the moment from t to $t+\mathrm{d}t$ with the velocities in the range from v to $v+\mathrm{d}v$. The zero moment of the distribution function obtained by its velocity averaging

$$\rho_{ik}(\vec{r}, t) = \int f_{ik}(\vec{r}, \vec{v}, t)\,\mathrm{d}\vec{v} \tag{1}$$

then gives the dislocation density tensor.

The first statistical moment of the distribution function defines the so-called dislocation velocity tensor or dislocation flow tensor:

$$J_{ij}(\vec{r}, t) = e_{ikl} \int v_l f_{kj}(\vec{r}, \vec{v}, t)\,\mathrm{d}\vec{v}. \tag{2}$$

In such definitions the zero and the first statistical moments of the distribution function coincide with the dislocation density tensor and dislocation velocity tensor introduced in the continuous dislocation theory. Accordingly, an analogous restriction of the continuous theory of dislocations has to be applied to the components of the distribution function:

$$\partial f_{ik}/\partial x_i = 0 \tag{3}$$

which is the conservation condition for the Burgers vector along the dislocation line.

The average flow of dislocations of kind ik in the direction p can be expressed in terms of the dislocation density tensor in the form

$$J_{ik} = e_{ijp} u_p \rho_{jk} \tag{4}$$

where u_p is the p-component of the average dislocation velocity which can be expressed in terms of the instantaneous velocity v and the relative velocity c as follows:

$$c_p = v_p - u_p. \tag{5}$$

By analogy with the kinetic theory of fluids, one can introduce the subsequent moments of the distribution function in the form:

$$P_{iln} = e_{ijk} \int c_l c_k f_{jn} \, \mathrm{d}\vec{v} \tag{6}$$

$$Q_{mjn} = e_{ijk} e_{ils} \int c_m c_k c_s f_{ln} \, \mathrm{d}\vec{v} \tag{7}$$

where P is analogous to the pressure tensor in the mechanics of fluids and Q can be identified with the energy of chaotic dislocation motion.

3. THE KINETIC EQUATION

The common form of the kinetic equation can be written as

$$\frac{D\hat{f}}{Dt} = I_{\text{coll}}. \tag{8}$$

The left hand side of this equation represents the convective part of the distribution function change and the right hand side part is the so-called collision integral of the kinetic equation. In the one-dimensional case, the convective part of this equation has the form:

$$\frac{\partial f}{\partial t} + v_x \cdot \frac{\partial f}{\partial x} + \frac{\partial v_x}{\partial t} \cdot \frac{\partial f}{\partial v_x} + f \frac{\partial \dot{v}_x}{\partial v_x} \tag{9}$$

where the components of dislocation acceleration $\partial v/\partial t$ can be obtained from the equation of dislocation movement:

$$m \partial v/\partial t = F - Bv. \tag{10}$$

Here m is the "effective" dislocation mass, F is the well-known Peach–Kochler force due to external action onto dislocation lines and B is the dislocation damping coefficient which takes into account the interaction of moving dislocations with the medium. Then the kinetic equation [eqn (8)] becomes:

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + \left(\frac{F}{m} - \frac{B}{m} v_x \right) \frac{\partial f}{\partial v} + \frac{B}{m} f = I_{\text{coll}}. \tag{11}$$

One can see that the convective part of the kinetic equation, due to the dependence of the acceleration of dislocations on their velocity, differs from that in the classical mechanics of fluids and gases where the particles interact with each other only. Both additional terms $(B/m)v_x$ and $(B/m)f$ show the sequence of the dependence of dislocation motion on their dissipative interaction with the medium through the damping coefficient B.

In our theory, the collision part of the kinetic equation I_{coll} is introduced in the so-called Fokker–Plank collision term, the common form of which is as follows:

$$\left.\frac{D\hat{f}}{Dt}\right|_{F-P} = -\nabla_v \times (\hat{D}_1 \times \hat{f}) + \tfrac{1}{2}\nabla_v\nabla_v : (\hat{D}_2 \times \hat{f}). \tag{12}$$

Here D_1 and D_2 are Fokker–Plank coefficients. D_1 is the dynamic friction coefficient and D_2 is the coefficient of diffusion in velocity space. Their dependence on the dislocation medium parameters will be given in section 5 but now we write the expression for the equilibrium form of the distribution function. For this we will use the Fokker–Plank form of the collision integral. Combination of eqns (11) and (12) gives:

$$\frac{\partial^2}{\partial v^2}(D_2 f) - 2\frac{\partial}{\partial v}(D_1 f) - 2\left(\frac{F}{m} - \frac{B}{m}v\right) + 2\frac{B}{m}f = 0. \tag{13}$$

We shall assume in this analysis that the velocity dispersion determined by the diffusion coefficient D_2 does not depend on the dislocation velocity itself. This means that for the equilibrium distribution of dislocations, the diffusion coefficient remains constant in the velocity space, which makes it possible to write the equilibrium equation in the form:

$$\frac{\partial^2 f}{\partial v^2} - \frac{2}{D_2}\cdot\left(\frac{F}{m} - \frac{B}{m}v\right)\frac{\partial f}{\partial v} + \frac{2B}{D_2 m}f = 0. \tag{14}$$

This equation can be integrated and if the integration constant is determined from the condition of the constant in the time average dislocation density $\rho(x)$ the solution of eqn (14) becomes:

$$f_0(x,v) = \left(\frac{B}{D_2 m}\right)^{1/2}\rho(x)\exp\left[-\frac{B}{D_2 m}\left(v - \frac{F}{m}\right)^2\right]. \tag{15}$$

The above expression characterizes the quasi-equilibrium velocity distribution of dislocations for one-dimensional movement. This equilibrium distribution has a mean dislocation velocity:

$$u = F/B \tag{16}$$

and a velocity dispersion:

$$(\Delta v)^2 = D_2 m/B. \tag{17}$$

4. DIFFUSION COEFFICIENTS

The coefficient $D_1 = \langle\Delta\vec{v}\rangle/\Delta t$ in eqn (12) is called the dynamic friction coefficient. The vector with the components $m\langle\Delta\vec{v}\rangle/\Delta t$ is a friction force directed opposite to the mean dislocation velocity $\bar{u}$. The collision integral I_{coll} of the Fokker–Plank equation includes only the mutual interaction of dislocations. The breaking force arriving due to this interaction has a fluctuative nature. The breaking force due to the interaction of dislocations with the medium, where they move, is taken into account in the convective part of the kinetic equation.

It has been shown by Hubburd and Thompson (1960) that the relation between the first and the second diffusion coefficients of the Fokker–Plank equation has the form:

$$D_1 = \frac{1}{2}\frac{\partial}{\partial v}\left[\frac{\langle\Delta\vec{v}\Delta\vec{v}\rangle}{\Delta t}\right] = -\frac{1}{2}\frac{\partial}{\partial v}(D_2). \tag{18}$$

Then the collision integral can be modeled in a more explicit form:

$$I_{\text{coll}} = \frac{\partial^2}{\partial v^2}(D_2 \hat{f}) \tag{19}$$

and our main problem now is to obtain the obvious expression for D_2. The latter can be obtained with the help of the stress correlation function according to the following general relation:

$$D_2 = \frac{\langle \Delta \vec{v} \Delta \vec{v} \rangle}{\Delta t} = \frac{b^2}{m^2} \int_{-\infty}^{+\infty} \langle \hat{\sigma}(0,0)\, \hat{\sigma}(\vec{v}\tau, \tau) \rangle \, \mathrm{d}\tau$$

where $\langle \sigma\sigma \rangle$ is a stress correlation function.

Derivation of the stress correlation function is based on the use of the continuous dislocation theory in the form developed by Mura (1963) and Kosevich and Nacik (1966):

$$\begin{gathered} \rho_0 \frac{\partial^2 U_{\mathrm{m}}}{\partial t^2} = \frac{\partial \sigma_{mn}}{\partial X_n}; \quad v_m = \frac{\partial U_m}{\partial t}; \\ \frac{\partial W_{mn}}{\partial t} = \frac{\partial v_m}{\partial X_n} + J_{mn}; \quad \sigma_{ik} = \lambda_{iklm} W_{lm}; \\ e_{ikl} \frac{\partial W_{lm}}{\partial X_m} = \rho_{ik}. \end{gathered} \tag{20}$$

Here $\hat{W}$ is the distortion, U is the displacement, ρ_0 is the mass density of the medium, ρ_{ik} are the dislocation density tensor components, σ_{ik} are the stress tensor components and λ_{iklm} are the elastic moduli. This system allows the stress correlation function of the velocity dislocation tensor $\hat{J}$ to be stated as follows:

$$\langle \hat{\sigma}(\vec{k}_1, \omega_1) \hat{\sigma}(\vec{k}, \omega) \rangle = \frac{\hat{\eta}\hat{\eta}}{\omega} \langle \hat{J}(\vec{k}_1, \omega_1) \hat{J}(\vec{k}, \omega) \rangle \tag{21}$$

where

$$\eta_{pqij} = \lambda_{pqmn} \lambda_{ijkl} (G_{km} k_l k_n - \delta_{mi} \delta_{nj}). \tag{22}$$

$\hat{G}$ is the Green tensor in the dynamic theory of elasticity (Kosevich and Nacik, 1966), and $\hat{J}(\vec{k}, \omega)$ is the Fourier transformation of the dislocation velocity tensor.
Omitting the intermediate steps of the calculation, one can obtain the final result in the form:

$$\hat{D}_2 = \frac{1}{2\pi} \cdot \frac{b^4}{B^2} \mu^2 \hat{\rho}. \tag{23}$$

The expression is very similar to that obtained by Alekseev and Strunin (1975) using an entirely different method.

We are now in a position to write down the final form of the kinetic equation for the dislocation structure:

$$\begin{aligned} \frac{\partial \hat{f}}{\partial t} + \nabla_r \times (\vec{v} \times \hat{f}) + \nabla_v \times (\dot{\vec{v}} \times \hat{f}) &= -\nabla_v \times (\hat{D}_1 \times \hat{f}) \\ &\quad + \frac{1}{2} \nabla_v \nabla_v : (\hat{D}_2 \times \hat{f}) + \alpha \vec{v} \times \hat{f} - \beta \hat{f} \cdot \int \hat{f}(\vec{v}_1)\, \mathrm{d}\vec{v}_1. \end{aligned} \tag{24}$$

The last two terms in eqn (24) account for the processes of multiplication and annihilation of the dislocations respectively.

5. STRESS IMPULSE DECAY IN THE DISLOCATION CONTINUUM

Using the kinetic approach we make an attempt to describe the decay of short compression impulses in solids. There is considerable interest in predicting dissipative effects stipulated by the dislocation structure only. Now it is well known (Johnston *et al.*, 1970) that the one-dimensional phenomenological dislocation theories based on relaxation equations of the Gilman–Johnston type cannot describe the decay of precursors in shock-loaded solids. This is due to the fact that these theories take into account only independent movement of dislocations in the expression for the general strain rate, whereas the collective interaction of dislocations during the wave passage is neglected.

The outlined formulation permits us to overcome this deficiency. We shall see that the distribution of the dislocations in velocity space plays an important role in the decay of the stress waves. We consider the propagation of submicrosecond stress impulses by way of a dislocation structure having some velocity distribution. Again we shall begin from the equations of the continuous theory:

$$\rho_0 \frac{\partial v_k}{\partial t} = \frac{\partial \sigma_{ik}}{\partial X_i}; \quad \frac{\partial v_k}{\partial X_i} = \frac{\partial W_{ik}}{\partial t} - J_{ik} \tag{25}$$

where ρ_o is the density of material. Their combination results in the following equation:

$$\nabla_i \nabla_l \sigma_{ik} - \rho_o \lambda_{iklm} \frac{\partial \sigma_{im}^2}{\partial t^2} + \rho_o \sum_s J_{ik}^s = 0. \tag{26}$$

Here sign Σ_s means summarizing all the slip planes of the crystal. Making use of the definition of the velocity dislocation tensor via the velocity distribution function of the kind s in the form:

$$J_{ik}^s = e_{ilm} \tau_l b_k \int v_m f^s \, \mathrm{d}\vec{v}. \tag{27}$$

One can find the components of the distribution function from a kinetic equation of the relaxation type:

$$\frac{\partial f^s}{\partial t} + v_i \frac{\partial f^s}{\partial X_i} + e_{ikl} \tau_l b_k \sigma_{im} m_{mn}^{-1} \frac{\partial f^s}{\partial v_n} = \frac{f_0^s - f^s}{\tau_r}. \tag{28}$$

Here τ_r is the relaxation time of the distribution function towards an equilibrium state and $\hat{m}$ is the dislocation mass tensor. When represented as a sum $f = f_0 + f_1$, where $f_0 \gg f_1$, the distribution function appears to be described by an equation whose Fourier's form reads:

$$i\omega f_1^s + ikv f_1^s + \frac{1}{\tau_r} f_1^s = \sigma b m^{-1} \frac{\partial f_0^s}{\partial v}$$

from where:

$$f_1^s = i\sigma b m^{-1}\frac{\partial f_0^s}{\partial v}\left[\omega - kv - \frac{i}{\tau}\right].$$

For the one-dimensional case this value defines the dislocation velocity tensor according to:

$$J^s = b\int_{-\infty}^{+\infty} v f_1^s \, dv$$

and eqn (27) becomes:

$$k^2 - \frac{\rho_0}{\mu}\omega^2 + \frac{b^2}{m}\rho\omega\int_{-\infty}^{+\infty}\frac{\partial f_0^s}{\partial v}\left(\omega - kv - \frac{i}{\tau_r}\right)^{-1} dv = 0.$$

Using the equilibrium distribution function given in eqn (15), one can transform this equation to the form:

$$1 - \frac{\omega^2}{k^2 c_t^2} + \frac{c_f}{c_t^2}\cdot\frac{\omega^2}{v^3}\int_{-\infty}^{+\infty}\frac{v(v-\bar{u})\cdot\exp\left[-(v-\bar{u})^2/v_0^2\right]}{\omega - kv - i/\tau_r}dv - \frac{c_f^2}{c_t^2} = 0. \qquad (29)$$

It is convenient to present the integral as a sum of two integrals each of which is an average of the values $v^2(\omega - kv - i/\tau_r)^{-1}$ and $v(\omega - kv - i/\tau_r)^{-1}$ along the equilibrium distribution [eqn (15)]:

$$1 - \frac{\omega^2}{kc_t^2} + \frac{c_f^2}{c_t^2}\cdot\frac{\omega^2}{v_0^2}\left[\langle y_2\rangle - \bar{u}\langle y_3\rangle\right] - \frac{c_f^2}{c_t^2} = 0,$$

where

$$\langle y_2\rangle = \frac{1}{\sqrt{\pi k v_0}}\int_0^{\infty}\frac{v^2\exp\left[-(v-\bar{u})^2/v_0^2\right]}{(\omega - kv - i/\tau_r)}dv$$

$$\langle y_3\rangle = \frac{1}{\sqrt{\pi k v_0}}\int_0^{\infty}\frac{v\exp\left[-(v-\bar{u})^2/v_0^2\right]}{(\omega - kv - i/\tau_r)}dv.$$

After averaging, one obtains;

$$\langle y_2\rangle = \frac{\omega^2}{k^2}\left\{\frac{\pi}{kv_0}\exp\left[-\left(\frac{\omega}{kv_0} - \frac{\bar{u}}{v}\right)^2\right]\right\} + \frac{1}{\omega}\left[1 + \frac{1}{2}\frac{1}{\left(\frac{\omega}{kv_0} - \frac{\bar{u}}{v}\right)}\right]$$

$$\langle y_3\rangle = 0.$$

and the dispersion equation [eqn (29)] becomes:

$$1 - \frac{\omega^2}{k^2 c_t^2} + 2i\sqrt{\pi}\left(\frac{\omega_0}{kv_0}\right)^2\exp\left[-\left(\frac{\omega}{kv} - \frac{\bar{u}}{v}\right)^2\right] + \frac{c_f^2}{c_t^2} = 0.$$

where $c_t = \sqrt{\mu/\rho}$ is the transverse sound speed in the solid, $c_f = \omega_0/k$ is the phase velocity of the wave, $v_0 = \sqrt{Dm/B}$ is the average velocity of the fluctuation motion of dislocations and $\omega_0 = \sqrt{\mu b^2 \rho / m}$ is the frequency of the collective oscillations of the dislocation structure.

Then subdividing the frequency into real and imaginary parts, $\omega = \omega_0(1+i\delta)$, where δ is the decrement of decay, one can obtain for the latter,

$$\delta = \sqrt{\pi}(\omega_0/kv_0)^3 \exp\left[-\left(\frac{\omega_0}{kv_0} - \frac{\bar{u}}{v_0}\right)^2\right]\frac{c_f}{c_t}. \tag{30}$$

Now we consider two limit situations to the absence of drag $B = 0$ and to large values of the drag coefficient $B \to \infty$. For the first case we have

$$\frac{\bar{u}}{v_0} = \frac{\sigma b}{B}\left[\frac{2B}{D_2 m}\right]^{1/2} \to \infty,$$

and thus

$$\frac{\omega_0}{kv} = \frac{\omega_0}{k}\left[\frac{2B}{D_2 m}\right] \to 0.$$

As a result, $\delta \to 0$ and decay is absent. For the second case $\bar{u}/v_0 \to 0$ and $\omega_0/kv_0 \to 0$ and decay equals to zero again. With increasing diffusion velocity v_0 the decay decrement δ decreases, indicating that the velocity distribution of dislocations leads to a decrease in the impulse decay. The intermediate situation is obviously related to a non-monotonous sharp decay increase. From eqn (30) one can find the value of the dynamic viscosity B of dislocations, using the experimental data from the short compression impulse decay. The result for aluminum is 2×10^{-4}Pa·c. Thus, discounting a collective interaction of dislocations gives the possibility of describing the short impulse propagation of solids in a more correct manner. What is the physics of this phenomenon? In dynamic compressive waves the dislocations can have velocities both greater and lower than the phase velocity c_f. It is known that in ensembles of particles distributed according to eqn (15) the number of particles with velocities lower than the given phase velocity is greater then the number of those with greater velocities. Therefore the number of dislocations which are carried away by the stress wave exceeds the number of dislocations which give their energy to the wave. As a result, there is a stress wave decay similar to the well-known "Landau decay" in plasma. This is an essential collective effect. Thus, an account of the collective interaction of dislocations leads to the necessity of including the inertial characteristics of dislocation structure, which define both the frequency of their collective oscillations and the average velocity of chaotic motion v_0 of dislocations. It should be recalled that previous investigations devoted to the inertial behavior and acceleration of individual dislocations have concluded that their influence on stress pulse propagation is negligible in comparison to that of the exact shape of the stress pulse, as follows from Gillis and Kratochvil (1970). This is true only for individual dislocations. In reality the inertial features of dislocations define their velocity distribution in the kinetic meaning and thereby define the character of flowing high-velocity processes in solids.

6. TRANSPORT EQUATIONS

The next step in our formulation is the derivation of moment equations from the kinetic equation using a standard procedure of averaging. Making use of the definitions of $\hat{\rho}$ and $\hat{J}$ in terms of the distribution function after multiplying the kinetic equation by zero degree velocity i.e. by unity, and after integrating in velocity space one can obtain the zero moment of the kinetic equation. During formal procedures, both the tensor character of the distribution function, and the prohibition of the dislocation motion along itself should be overlooked. The convective part of the kinetic equation gives:

$$\int \frac{\partial \hat{f}}{\partial t} \mathrm{d}\vec{v} = \frac{\partial}{\partial t} \int \hat{f} \mathrm{d}\vec{v} = \frac{\partial}{\partial t} \hat{\rho}$$

$$\int \nabla_{\vec{v}} \times (\dot{\vec{v}} \times \hat{f})\, \mathrm{d}\vec{v} = 0$$

$$\int \nabla_{\vec{r}} \times (\vec{v} \times \hat{f})\, \mathrm{d}\vec{v} = \nabla_{\vec{r}} \times \int (\vec{v} \times \hat{f})\, \mathrm{d}\vec{v} = \nabla_{\vec{r}} \times \hat{J}. \tag{31}$$

The second term gives zero because the distribution function aspires to zero on the integration limits. For the collision term I_{coll} one has:

$$\int \alpha \cdot (\vec{v} \times \hat{f})\, \mathrm{d}\vec{v} = \alpha \cdot \hat{J}$$

$$\int \beta \cdot \hat{f}(\vec{v}_1) \cdot \int \hat{f}(\vec{v})\, \mathrm{d}\vec{v}\, \mathrm{d}\vec{v}_1 = \beta \cdot \hat{\rho} \cdot \hat{\rho}. \tag{32}$$

For obtaining the moment equation from the Fokker–Plank part of the collision term we multiply eqn (12) by the arbitrary function $\phi(\vec{v})$ and integrate in velocity space, i.e.

$$\int \phi(\vec{v}) \left[-\frac{\partial}{\partial v_\mu} (D_{1\mu} f_{ij}) + \frac{1}{2} \frac{\partial}{\partial v_\mu} \cdot \frac{\partial}{\partial v_\nu} (D_{2\nu\mu} f_{ij}) \right] \mathrm{d}\vec{v}$$

$$= \int \frac{\partial \phi}{\partial v_\mu} (D_{1\mu} f_{ij})\, \mathrm{d}\vec{v} - \frac{1}{2} \int \frac{\partial}{\partial v_\mu} \cdot \frac{\partial}{\partial v_\nu} (D_{2\nu\mu} f_{ij})\, \mathrm{d}\vec{v}. \tag{33}$$

All terms on the right hand side equal zero due to the correlation between diffusion coefficients [eqn (18)]. Conversion into zero of all terms of the Fokker–Plank collision term during integration means that long-range interactions between individual dislocations do not affect the macroscopic convection of dislocations. This convection is thought to be related only to the first part of the collision term I_{coll}. Summing up eqns (32) and (33) one obtains the zero moment of the kinetic equation:

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla_{\vec{r}} \times \hat{J} = \alpha \cdot \hat{J} - \beta \cdot \hat{\rho} \cdot \hat{\rho}. \tag{34}$$

When sources and channels are absent the right hand side of this equation equals to zero and then the left hand side of the equation leads to the equation of "Burgers vector conservation" which is well known in the continuous theory of dislocations. Thus, this equation can be obtained from first principles, that is, from the kinetic theory of dislocations.

The next step is the derivation of the first moment of the kinetic equation. To do this, we need to multiply the latter with $\vec{v}$ and integrate over the velocity space. The first item on the right hand side gives:

$$\int \vec{v} \times \frac{\partial \hat{f}}{\partial t} \mathrm{d}\vec{v} = \frac{\partial}{\partial t} (\vec{v} \times \hat{f})\, \mathrm{d}\vec{v} - \int (\dot{\vec{v}} \times \hat{f})\, \mathrm{d}\vec{v}.$$

To find the acceleration $\dot{\vec{v}}$ in the second term one can use the equation of dislocation motion [eqn (10)]. Then we obtain:

$$\int \vec{v} \times \frac{\partial \hat{f}}{\partial t} d\vec{v} = \frac{\partial}{\partial t}\hat{J} - \frac{1}{m}\hat{\sigma} \dot{\times} \hat{\rho} + \frac{B}{m}\hat{J}$$

$$\int \vec{v} \times (\nabla_{\vec{r}} \times \hat{f})) d\vec{v} = \nabla_{\vec{r}} \cdot \hat{P} - \nabla_{\vec{r}} \cdot [\vec{u}(\vec{u} \times \hat{\rho})]$$

where $\hat{P}$ is the pressure tensor determined by eqn (6) and $\vec{u}$ is the average dislocation velocity. Taking into account eqn (10), the third term of the convective part of the equation gives:

$$\int \vec{v} \times (\nabla_{\vec{v}} \times (\vec{v} \times \hat{f})) d\vec{v} = \frac{2}{m}\hat{\sigma} \dot{\times} \hat{\rho} - \frac{2B}{m}\hat{J}.$$

The collision part, after vector multiplying by $\vec{v}$ and integrating, gives:

$$\alpha \int \vec{v} \times (\vec{v} \times \hat{f}) d\vec{v} = \alpha(\hat{S} + \vec{u} \times \hat{J})$$

$$\beta \int \vec{v} \times \hat{f}(\vec{v}_1) \int \hat{f}(\vec{v}) d\vec{v} d\vec{v}_1 = \beta \hat{J} \cdot \hat{\rho}$$

where

$$\hat{S} = \int \vec{c} \times (\vec{c} \times \hat{f}) d\vec{v}.$$

Summing the right and the left terms of the equation, one obtains for the first moment of the kinetic equation:

$$\frac{\partial \hat{J}}{\partial t} - \nabla(\hat{P} + \vec{u}\hat{J}) + \frac{1}{m}(\hat{\sigma} \dot{\times} \hat{\rho} - B\hat{J}) = \alpha(\hat{S} + \vec{u} \times \hat{J}) - \beta \hat{J} \cdot \hat{\rho}. \quad (35)$$

In the absence of sources and channels, making use of eqn (34), one obtains:

$$\frac{\partial \vec{u}}{\partial t} \times \hat{\rho} - \nabla \cdot \hat{P} - \nabla[\vec{u} \cdot (\vec{u} \times \hat{\rho})] + \frac{1}{m}[(\hat{\sigma} \dot{\times} \hat{\rho}) - B\vec{u} \times \hat{\rho}] = 0.$$

This equation is analogous to that of moment transfer in the mechanics of fluids and gases in a two-phase continuum, and B characterizes the interaction between phases. In the case under discussion one of the phases is the dislocation structure and the other is a crystal lattice. Thus obtained equations can serve as an example of a microscopic basis for the subdivision of media into the two states ("dislocation" and "perfect lattice") introduced by E. C. Aifantis (1983). Omitting all intermediate operations, we may write down the second moment of the kinetic equation (see Appendix):

$$\left(\frac{\partial}{\partial t} - \frac{B}{m}\right)[\hat{S} + \vec{u} \times (\vec{u} \times \hat{\rho})] + \frac{2}{m}[\vec{u} \times (\hat{\sigma} \dot{\times} \hat{\rho})] - \frac{1}{m}\hat{\sigma} \dot{\times} (\vec{u} \times \hat{\rho}) + \nabla(\hat{Q} + \vec{u}[\hat{S} + \vec{u} \times (\vec{u} \times \hat{\rho})] + \hat{P}_1)$$
$$= \alpha(\vec{u} \times [\hat{S} + \vec{u} \times (\vec{u} \times \hat{\rho})] + \hat{T} - 2\vec{u} \cdot \hat{P}) - \beta[\hat{S} + \vec{u}(\vec{u} \times \hat{\rho})] \cdot \hat{\rho}. \quad (36)$$

The tensor quantities $\hat{S}$, $\hat{Q}$, $\hat{T}$, and $\hat{P}$ are different order moments of the dislocation distribution function.

If $\hat{S} = \int \vec{c} \times (\vec{c} \times \hat{f}) d\vec{v}$ is the energy of the chaotic motion of dislocations in a random stress field, the sum $[\hat{S} + \vec{u} \times (\vec{u} \times \hat{\rho})]$ may be related to the total energy transferred by moving dislocations. After multiplying by the mass, the second term gives the kinetic energy of dislocations. Since $\hat{Q}$ characterizes the transfer of energy due to the chaotic motion of dislocations (analog of the heat flow vector in the mechanics of fluids and gases), eqn (36) reflects the balance of energy in the continuum of dislocations moving within a continuous medium. The interaction of dislocations with this media is described by the term $(B/m)[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]$. The action of the internal interaction forces is reflected in the term:

$$\frac{2}{m}[\vec{u}\times(\hat{\sigma}\times\hat{\rho})]-\frac{1}{m}\hat{\sigma}\times(\vec{u}\times\hat{\rho}).$$

Finally, let us write down the single-dimension variant of the energy transfer equation in the case of absence of sources and channels of dislocations:

$$\frac{\partial}{\partial t}(S+u^2\rho)+\frac{1}{m}\sigma b\rho u-\frac{B}{m}(S+u^2\rho)+\nabla[Q+u(S+u^2\rho)+P_1]=0. \tag{37}$$

The term $(S+u^2\rho)$ is the total energy of the dislocation motion, S is the relative chaotic motion energy and $u^2\rho$ is the kinetic energy of convective motion with average velocity u. Thus, eqn (37) suggests that the energy of the moving dislocations is converted over to the work of external forces, dissipation due to the ductile drag exerted on the dislocations by the medium, and to work for overcoming the interaction forces and heat transfer.

The system of transport equations for the dislocations obtained above is not closed until the correlation between the pressure P and the dislocation density is established. This is analogous to constitutive equations in the mechanics of fluids and gases. In our theory the appropriate equation for this purpose has a form which accounts for the long-range interactions of dislocations in terms of the Cauchy-integral

$$\hat{P}(\vec{r},t)=-D\oint\frac{\hat{\rho}(\vec{s},t)}{\vec{r}-\vec{s}}\,\mathrm{d}\vec{s}. \tag{38}$$

Thus, this equation along with two transport equations:

$$\frac{\partial\rho}{\partial t}+\nabla(\rho u)=0 \tag{39}$$

$$\rho\frac{\partial u}{\partial t}+\rho u\Delta u+\Delta P-\frac{2}{m}(\sigma b-Bu)=0$$

constitute the desired closed system. The simulation of stress impulse propagation in the ductile medium has been carried out for the one-dimensional case. The space and temporal profiles of dislocation density were calculated for different moments after the beginning of loading and for different viscosity coefficient values B. Some of these profiles are shown in Figs 1–3. The calculations result in specific values for the drag coefficient (e.g. for aluminium and other materials). One of the interesting results obtained from these simulations is a non-monotonous profile of the strain rate (see Fig. 4). This result resembles the experimental data observed during dynamic deformation processes.

In conclusion we wish to emphasize that our method is different from the generally accepted ones. In the latter, the one-dimensional equations for deformations and stresses are closed by the one-dimensional constitutive equation which is expressed via dislocation dynamics (as in the case of the Gillman–Johnston equation). Our approach permits the use of the well-known three-dimensional formulation in the mechanics of fluids.

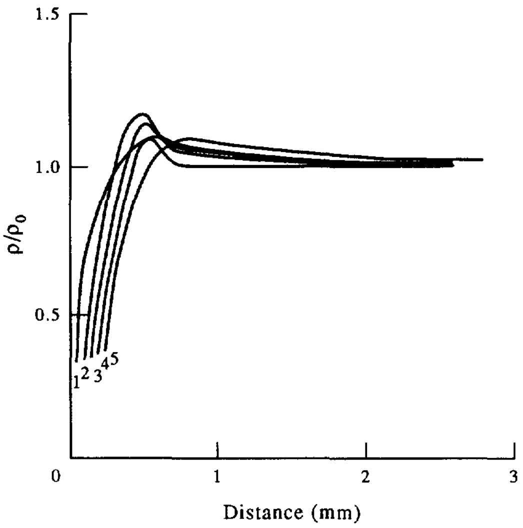

Fig. 1. Dependence of the normalized dislocation density on the distance from the load boundary for drag coefficient $B = 3 \times 10^{-4}$ ps and different moments after beginning the loading. 1—τ_1 = 45 ns, 2—τ_2 = 60 ns, 3—τ_3 = 90 ns.

7. CONCLUSIONS

(1) The kinetic approach is developed taking into account the dislocation distribution in the velocity space, long-range mutual interaction and inertial effects. The procedure employed here is similar to that used in the kinetic theory of fluids and gases. The mean dynamic variables, such as the density dislocation tensor, velocity tensor, etc. are introduced as different order moments of the dislocation velocity distribution function. These values are chosen to coincide with the well-known dynamic variables of the classical continuous dislocation theory.

(2) An example of the application of the kinetic approach to compressive pulse propagation is given on the basis of an explicit form of the kinetic equation of relaxation type. Decay decrement appears to be directly dependent on the collective oscillation frequency of the dislocation structure and on the diffusive dislocation velocity.

(3) The transport equations as different order moments of the kinetic equation are subsequently derived by using a standard procedure of averaging. In the absence of sources

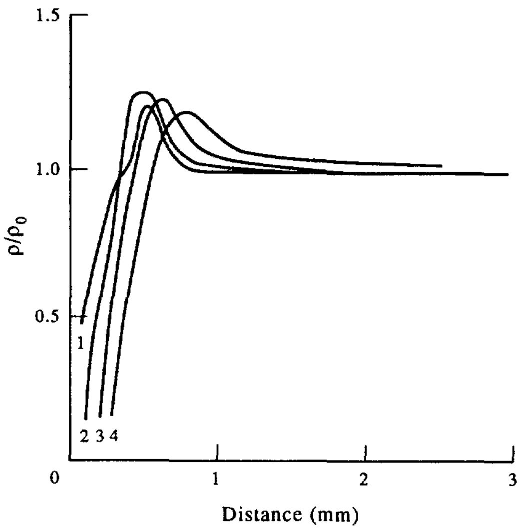

Fig. 2. As Fig. 1. for $B = 10^{-4}$ ps.

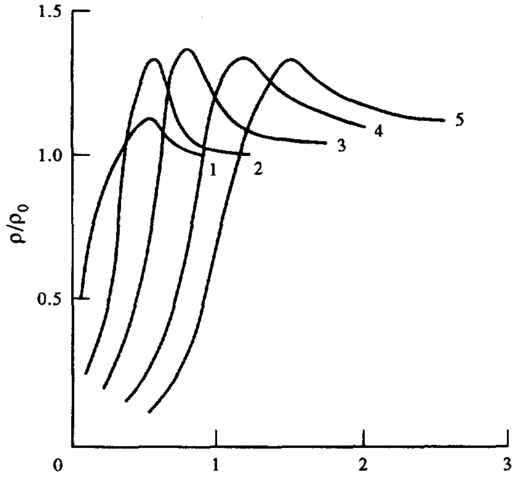

Fig. 3. As Figs 1 and 2 for $B = 10^{-5}$ ps.

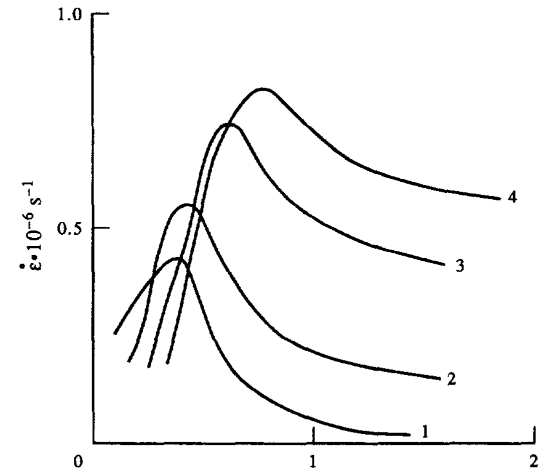

Fig. 4. Dependence of the strain rate on the distance from the load boundary $x = 0$ for drag coefficient $B = 10^{-4}$ ps and different moments after beginning the loading.

and sinks of dislocations, the zero moment equation appears to coincide with the corresponding "Burgers vector conservation" equation in a continuous theory of dislocations.

(4) The step-like stress pulse propagation is investigated as a simulating task of interest. To close the derived system of transport equations, a constitutive equation in the Cauchy form is used, which makes it possible to account for a non-local dislocation interaction.

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APPENDIX

The second moment of the kinetic equation for dislocations can be obtained by multiplying the kinetic equation by $\vec{v}$ and integrating in the velocity space

$$\int \vec{v}\times\left(\vec{v}\times\frac{\partial \hat{f}}{\partial t}\right)\mathrm{d}\vec{v} = \frac{\partial}{\partial t}\int \vec{v}\times(\vec{v}\times\hat{f})\,\mathrm{d}\vec{v} - \int \vec{v}\times(\dot{\vec{v}}\times\hat{f})\,\mathrm{d}\vec{v} - \int \dot{\vec{v}}\times(\vec{v}\times\hat{f})\,\mathrm{d}\vec{v}$$

$$= \frac{\partial}{\partial t}\int(\vec{c}+\vec{u})\times[(\vec{c}+\vec{u})\times\hat{f}]\,\mathrm{d}\vec{v} - \frac{1}{m}\int \vec{v}\,(\sigma\times\hat{f})\,\mathrm{d}\vec{v} - \frac{1}{m}\int \hat{\sigma}\times(\vec{v}\times\hat{f})\,\mathrm{d}\vec{v} + \frac{2B}{m}\int \vec{v}\times(\vec{v})\,\mathrm{d}\vec{v}$$

$$= \left(\frac{\partial}{\partial t}+\frac{2B}{m}\right)[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})] - \frac{1}{m}\vec{u}\times(\hat{\sigma}\times\hat{\rho}) - \frac{1}{m}\hat{\sigma}\times(\vec{u}\times\hat{\rho}).$$

Here

$$\hat{S} = \int(\vec{c}\times(\vec{c}\times\hat{f}))\,\mathrm{d}\vec{v}$$

$$\int \vec{v}\times(\vec{v}\times(\nabla_v\times(\vec{v}\times\hat{f})))\,\mathrm{d}\vec{v} = \int \vec{v}\times(\vec{v}\times\nabla_v\times\hat{A})\,\mathrm{d}\vec{v}, \quad A = \vec{v}\times\hat{f}.$$

In component form we have:

$$e_{ijk}v_k e_{jlm}v_m e_{lpq}\frac{\partial}{\partial v_q}A_{pn} = e_{ijk}e_{jlm}e_{lpq}\left[\frac{\partial}{\partial v_q}(v_k v_m A_{pn} - \delta_{kq}v_m A_{pn} - v_k\delta_{mq}A_{pn}\right].$$

The first integral equals zero since the distribution function equals zero at the ends of the integration interval. The other two terms give:

$$-e_{ijk}e_{jmn}e_{lpq}[\delta_{kq}v_m A_{pn} + v_k\delta_{mn}A_{pq}] = (\delta_{il}\delta_{km} - \delta_{im}\delta_{kl})[e_{lpk}v_m A_{np} + e_{lpk}v_k A_{pn}] = 2\,e_{ipk}v_k A_{pn} + e_{kpi}v_k A_{pn} = 3(\vec{v}\times\hat{A})_{in}.$$

So

$$\int \vec{v}\times(\vec{v}(\nabla_v\times(\vec{v}\times(\vec{v}\times\hat{f})))\,\mathrm{d}\vec{v} = 3\int \vec{v}\times(\dot{\vec{v}}\times\hat{f})\,\mathrm{d}\vec{v} = \frac{3}{m}\int \vec{v}\times(\hat{\sigma}\times\hat{f})\,\mathrm{d}\vec{v}$$

$$-\frac{3B}{m}\int \vec{v}\times(\vec{v}\times\hat{f})\,\mathrm{d}\vec{v} = \frac{3}{m}\vec{u}\times(\hat{\sigma}\times\hat{\rho}) - \frac{3B}{m}[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})].$$

Let us integrate the second item of the equation

$$\int \vec{v}\times\{\vec{v}\times[\nabla_r\times(\vec{v}\times\hat{f})]\}\,\mathrm{d}\vec{v} = \nabla_r\cdot\int \vec{v}[(\vec{v}\times(\vec{v}\times\hat{f})]\,\mathrm{d}\vec{v} = \nabla_r\cdot\hat{U}$$

where

$$\hat{U} = \int \vec{c}[\vec{c}\times(\vec{c}\times\hat{f})]\,\mathrm{d}\vec{v} + \int \vec{c}[\vec{c}\times(\vec{u}\times\hat{f})]\,\mathrm{d}\vec{v} + \int \vec{c}[\vec{u}\times(\vec{c}\times\hat{f})]\,\mathrm{d}\vec{v}$$

$$+\vec{u}\int \vec{c}\times(\vec{c}\times\hat{f})\,\mathrm{d}\vec{v} + \vec{u}\left[\vec{u}\times\left(\vec{u}\times\int \hat{f}\,\mathrm{d}\vec{v}\right)\right] = \hat{Q} + \vec{u}[\vec{u}\times(\vec{u}\times\hat{\rho})] + \vec{u}\cdot\hat{S} + \vec{c}[\vec{u}\times(\vec{c}\times\hat{f})]\,\mathrm{d}\vec{v} + \int \vec{c}[\vec{c}\times(\vec{u}\times\hat{f})]\,\mathrm{d}\vec{v}.$$

Let us now combine the last two integrals into a common term P_1. Then the second term of the desired equation has the form:

$$\int \vec{v}\times\{\vec{v}\times[\nabla_r\times(\vec{v}\times\hat{f})]\}\,\mathrm{d}v = \nabla_r\{\hat{Q}+\vec{u}\cdot[S+\vec{u}\times(\vec{u}\times\hat{\rho})]+\hat{P}_1\} = J_{\mathrm{coll}}.$$

For the interaction part of the transport equation we have:

$$\alpha\int \vec{v}\times(\vec{v}\times\hat{f})\,\mathrm{d}\vec{v} = \alpha\vec{u}\times(\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho}))+\alpha\hat{T}+\alpha\hat{P}_2,$$

where

$$\hat{T} = \int \vec{c}\times[\vec{c}\times(\vec{c}\times\hat{f})]\,\mathrm{d}\vec{v}$$

and

$$\hat{P}_2 = \int \vec{c}\times[\vec{u}\times(\vec{c}\times\hat{f})+\vec{c}\times(\vec{u}\times\hat{f})]\,\mathrm{d}\vec{v}.$$

If we take into account that dislocations cannot move along on their own, then

$$\hat{P}_2 = -2\vec{u}\hat{P}+\vec{u}\times\int\vec{c}(\vec{c}\cdot\hat{f})\,\mathrm{d}\vec{v} = -2\vec{u}\cdot\hat{P}.$$

Multiplying the second term of the right hand side of the kinetic equation by $\vec{v}$ and integrating over the velocity space we obtain:

$$-\beta\int \vec{v}\times(\vec{v}\times\hat{f})\,\mathrm{d}\vec{v}\cdot\hat{\rho} = -\beta[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]\cdot\hat{\rho}.$$

So, the right hand side of the second moment of the kinetic equation has the form:

$$J_{\mathrm{coll}} = \alpha[\vec{u}\times[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]+\hat{T}-2\vec{u}\cdot\hat{P}]-\beta[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]\cdot\hat{\rho}.$$

Now we can write the complete transport equation:

$$\left(\frac{\partial}{\partial t}-\frac{B}{m}\right)\cdot[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]+\frac{2}{m}\vec{v}\times(\hat{\sigma}\times\hat{\rho})-\frac{1}{m}\hat{\sigma}\times(\vec{u}\times\hat{\rho})$$
$$+\nabla_r(\hat{Q}+\vec{u}[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]+\hat{P}_1) = \alpha[\vec{u}\times[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]+\hat{T}-2\vec{u}\cdot\hat{P}]-\beta[\hat{S}+\vec{u}\times(\vec{u}\times\hat{\rho})]\cdot\hat{\rho}.$$

Let us show that this equation is analogous to the equation of energy conservation. Simplifying the equation for the one-dimensional case when sources and channels are absent, we obtain:

$$\left(\frac{\partial}{\partial t}-\frac{B}{m}\right)(S+u^2\rho)+\frac{1}{m}\sigma bu\rho+\nabla\cdot[Q+u(S+u^2\rho)+P_1] = 0$$

or

$$\frac{\partial}{\partial t}(S+u^2\rho)+\frac{1}{m}\sigma b\rho u-\frac{B}{m}(S+u^2\rho)+\nabla[Q+u(S+u^2\rho)+P_1] = 0.$$

The term $(S+u^2\rho)$ can be identified with the total energy of dislocation motion where S is analogous to the chaotic motion energy and $u^2\rho$ is the kinetic energy of that motion with a mean velocity u. The equation just obtained shows that the energy of moving dislocations appears to be spent on the work against external forces, viscosity damping of dislocations in the medium, the work against internal stresses due to dislocation interactions and for heat transport. The right hand side of the equation is the energy for source activation and annihilation of dislocations during their interaction.