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Disclination–dislocation model for the kink bands in polymers and fibre composites

N. A. PERTSEV, A. E. ROMANOV, V. I. VLADIMIROV
A.F. Ioffe Physico-Technical Institute, Academy of Sciences of the USSR, 194021 Leningrad, USSR

A disclination–dislocation model is proposed for the structure and movement of kink bands in oriented polymers and fibre composites, which describes bending and intermolecular slip inside the bands. It is shown that the band structure consists of special disclination–dislocation defects: slipped kinks. The mechanism of kink-band movement, based on the generation of such defects at the band front, is considered. The self elastic energy of slipped kinks is calculated and analysed in detail.

1. Introduction

In recent years many experimental data have been obtain on kink-band formation in different materials under plastic deformation. In crystals, kink bands arise under special conditions of loading only [1]; however, in oriented polymers and fibre composites they can be the dominant mode of plastic deformation. This behaviour results from the anisotropy of the plastic properties of the materials concerned.

Many authors have investigated kink bands in oriented polyethylene [2–6] and other polymers, for example, in polypropylene [2, 7] and nylon [7, 8]. Kink bands have also been studied in composites reinforced with glass or carbon fibres [9–11]. The kink bands are usually observed in materials under uniaxial compression [4–6, 8, 10], but in some cases their formation takes place under tension [5], shear deformation [2] and torsion [7]. From these works, it can be seen that, with respect to macroscopic plastic deformation, kink bands are equivalent to ordinary shear bands, but have a characteristic internal structure; where a change in orientation of the macromolecules of fibres takes place, the kink band is separated by plane boundaries (shown schematically in Fig. 1).

Most authors, when discussing the results obtained, believe [4, 8] that this change in orientation of the macromolecules is accompanied by intermolecular slip and it has been proposed [8] that the kink-band evolution could be interpreted in terms of dislocation motion. As in the case of crystals [1] it is supposed [12] that dislocation pairs of opposite sign appear inside the bands during the deformation process. These dislocations glide to the boundaries of the band forming rows of minimum stored elastic energy. The glide planes of dislocations are parallel to the macromolecular axes inside the band. We have been unable to find any attempt to provide a quantitative description of such a mechanism. Another approach, outlined in [13, 14], takes into consideration the bending

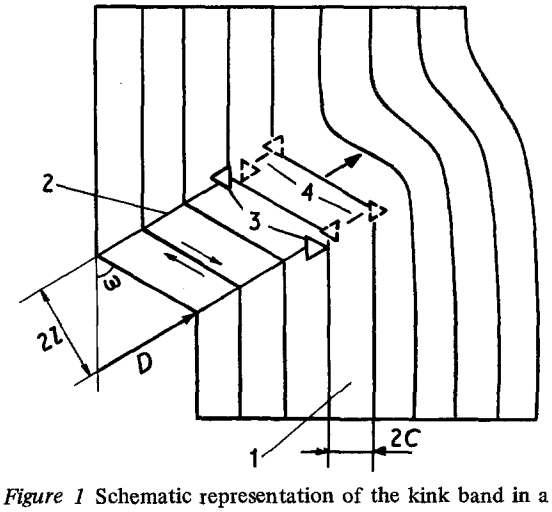

Figure 1 Schematic representation of the kink band in a non-homogeneous material. (1) macromolecules or fibres having a diameter = $2c$; (2) the plane boundary of the band; (3) wedge disclination dipole having strength ω; (4) disclination quadrupole being a structural unit under the elementary act of band propagation.

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of macromolecules, described in terms of wedge disclination-loop condensation. However, this description [13] gives no explanation of the macroscopic shear deformation connected with the kink bands.

Therefore, there is no successive theory able to explain the nucleation and development of kink bands in oriented polymers and fibre composites. In the present paper, a disclination–dislocation mechanism is proposed which takes into consideration the simultaneous chain or fibre bending and intermolecular slip in the band. It is shown that the inner structure of the band can be represented by a model involving special disclination–dislocation defects termed by us "slipped kinks". The self elastic energy of the slipped kink is also evaluated in the framework of linear isotropic elasticity.

2. Kink-band structure and mechanism of movement

2.1. Wedge disclination description of kink bands

The kink band is a zone where the material is tilted relative to the surrounding volume at a certain angle, ω. In contrast, in crystal twins this angle is not unambiguously defined by the solid structure symmetry. The shear of material is realized along the plane boundaries of the band. The magnitude of shear is $D = 4l \tan(\omega/2)$, where $2l$ is the thickness of the band (see Fig. 1). In the case of an infinite range of band plane boundaries being perpendicular to the vector D, kink-band propagation is equivalent to wedge partial-disclination dipole motion. This dipole is shown in Fig. 1. The mechanism of movement of such a dipole in crystals has been considered [15, 16] in detail: the band motion is dictated by dislocation structure evolution. In turn, in polymers and composites such kink-band movement is determined by peculiarities of internal structure, i.e. in polymers by macromolecular diameter and by forces of intermolecular interaction and in composites by fibre diameter and strength, and by fibre spacing, as well as by properties of matrix–fibre interlayer. Under these conditions the elementary act of dipole (kink-band front) motion is its translation by a distance of one diameter of macromolecule or fibre. Therefore the kink band moves through the potential relief with a characteristic period.

One can think that the process of motion develops in the following manner. At first the disclination quadrupole is generated near the wedge disclination dipole at the front of the kink band. The one arm of the quadrupole is equal to the band thickness $2l$, the other is equal to the diameter of the macromolecule or fibre. Then the annihilation between the initial dipole and the pair of opposite-sign disclinations in quadrupole takes place (Fig. 1). This process is equivalent to the passing of the band front to the next well of the potential relief. However, the disclination dipole does not overcome the potential barrier at once, but ejects (as a dislocation) a double kink, which broadens along the dipole axes.

2.2. "Finite" analogue of the disclination quadrupole

To ascertain the structure of such disclination dipole ejection it is necessary to construct the quadrupole analogue having a finite length in the direction of the Frank vector $\boldsymbol{\omega}$. For this purpose let us consider a specific transformation of an initial quadrupole, shown schematically in Fig. 2. Under this transformation two bi-axial disclination dipoles convert into mono-axial disclination dipoles of opposite signs and produce two dislocation dipoles. In such an interpretation, disclination dipoles model the macromolecular or fibre bending whereas dislocation dipoles permit consideration of the intermolecular slip or shift in the matrix–fibre boundary. Now one can close the ends of dislocation and disclination lines as shown in Fig. 3. Thus, the "finite" analogue of the quadrupole so obtained consists of

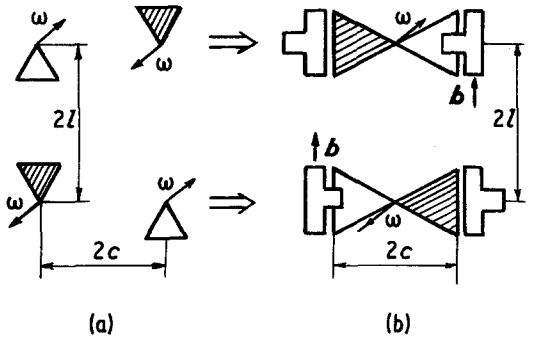

Figure 2 Transformation of disclination quadrupole into a disclination–dislocation defect by means of the displacement of the initial axes of rotation. (a) The initial quadrupole having arms $2l$ and $2c$ and angle of rotation, ω. (b) Final state of the defect. Bi-axial disclination dipoles are replaced by mono-axial ones and additional edge dislocations with Burgers vector $b = 2c \tan(\omega/2)$. The zones are dashed where the wedges are inserted into the body when disclinations are created.

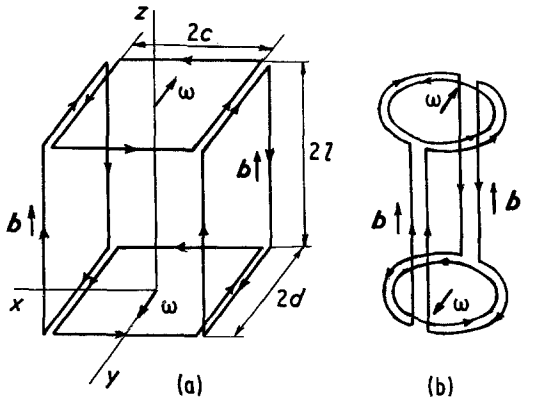

Figure 3 Structure of slipped kinks in fibres of (a) rectangular and (b) circular cross-sections. The case in (a) also corresponds to a kink covering several macromolecules in the direction of vector $\boldsymbol{\omega}$.

two glide dislocation loops and two symmetrical wedge disclination loops of opposite signs. This arrangement forms a special defect termed by us a "slipped kink". It is important that this defect is not merely a composition of disclinations and dislocations but one new quantity, since the Burgers vector, $\boldsymbol{b}$, of dislocation loops is unequivocally connected with the strength ω of disclination ones by relation $\boldsymbol{b} = \omega c$.

During the formation of slipped kinks in front of the kink band, both the bending and slipping of macromolecules is effected. This behaviour is in qualitative agreement with experimental data. After slipped-kink broadening takes place along the whole length of the band boundary, the configuration becomes again equivalent to the considered disclination quadrupole; this indicates that band propagation into the next potential well has taken place. Consequently, the double kinks of the disclination dipole formed during its movement can be modelled by slipped kinks covering a limited number of macromolecules or fibres (Fig. 4).

2.3. Properties of slipped kinks in the kink bands

In oriented polymers the kink-band nucleation can be described as follows: first a group of slipped kinks in several neighbouring macromolecules forms and then the group boundary propagates by means of joining new slipped kinks. Accordingly, the disclination–dislocation structure of kink bands contains slipped kinks in all the macromolecules within it, as shown in Fig. 5. The kinks in rows of macromolecules arranged in

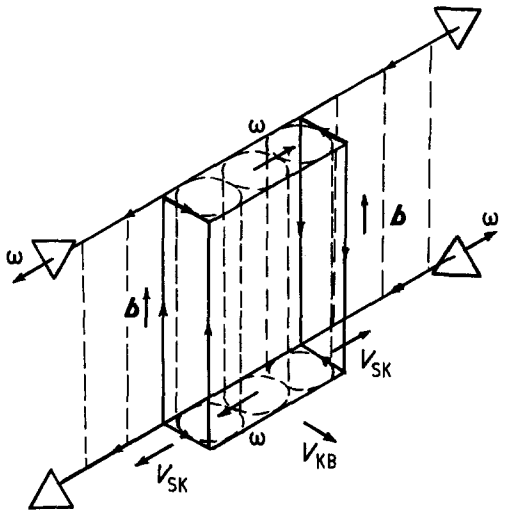

Figure 4 The mechanism of kink-band front movement. V_{KB} = the velocity of the band front; V_{SK} = the velocity of slipped kink broadening.

the direction of Frank vector $\boldsymbol{\omega}$ unite forming rectangular-shaped defects.

Special defects are also necessary to describe the plastic deformation of composite materials having a plastic matrix and undeformable fibres. In the matrix the dipole motion can be effected in the usual way [16], but by virtue of compatibility conditions the special defects must form around the fibres. They are also the slipped kinks.

Finally, some principal properties of slipped kinks are noted. The presence of symmetrical disclination loops points to the influence on slipped kink formation of non-uniform external and internal elastic fields. This can lead to the preferential nucleation of kink bands near the sources of such non-uniform fields. In turn, the

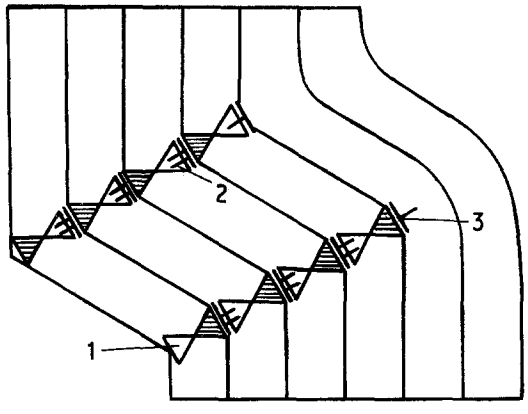

Figure 5 Disclination–dislocation structure of the kink-band. (1) Symmetrical disclination loops (or mono-axial dipoles); (2) dislocations with Burgers vector $2\boldsymbol{b}$; (3) dislocations with Burgers vector $\boldsymbol{b}$.

dislocation part of the defect provides the shear required. The work done by the applied stress is also connected with dislocations and has the magnitude (when a single defect is created) of

$$A = \tau_{xz} b 2S_b, \tag{1}$$

where τ_{xz} is the applied uniform shear stress, $2S_b$ denotes the total dislocation loop area and b is Burgers vector.

Therefore, using the special defects, the so-called slipped kinks, makes it possible to give an adequate description of the structure and movement of kink bands in oriented polymers and fibre-composites.

3. Strain energy of slipped kinks

The kink-band motion is a process of energy barriers overcoming the applied stress, with the aid of thermal agitation. The barrier height is the most essential characteristic of this motion. Therefore, if the band movement is determined by the ejection of slipped kinks, one must know the self energy of such disclination–dislocation defects.

3.1. Method of energy evaluation

We shall calculate the strain energy of a slipped kink consisting of a rectangular disclination and dislocation loops (Fig. 3). Such a form of defect permits consideration of its asymmetry. Rectangular defects are very useful for describing kink-band motion by means of the generation of slipped kinks of various lengths. Finally, such an approach permits the slipped-kink critical size to be obtained.

One can be convinced that the energy of the slipped kink, W, can be written in a general form as

$$W = 2W^{s}_{\omega} + W^{i}_{\omega} + 2W^{s}_{b} + W^{i}_{b} + 4W^{i}_{b\omega}, \tag{2}$$

where W^{s}_{ω} and W^{i}_{ω} are respectively the self and interaction energies of the disclination loops, W^{s}_{b} and W^{i}_{b} are the self and interaction energies of the glide dislocation loops and $W^{i}_{b\omega}$ is the interaction energy between dislocation and disclination loops.

The interaction of slipped-kink components in the framework of linear isotropic elasticity will be described in the same way as has been done for disclination loops in polymers [13]. The self energies of the loops may be evaluated when the work necessary for loop plastic-distortion creation is calculated. The interaction energies are determined from calculating the additional work done to create one loop in the stress field of another.

3.2. Elastic properties of rectangular wedge disclination loop

The component σ^{ω}_{zz} of the stress tensor of a rectangular wedge disclination loop is responsible for self and interaction energies in the given formulation. The stress tensor of arbitrarily-shaped disclination loops (including rectangular-shaped ones) may be obtained using the following method, similar to that proposed for dislocation loops [17, 18].

Let a disclination loop having an area, S, and Frank vector, Ω, lie in the plane $z = 0$. One can represent this loop in the form of a union of infinitesimal disclination loops dS_0 with the same vector of rotation. Each loop dS_0 is equivalent to the symmetrical disclination loop (with the axis of rotation Ω' in the centre of the loop) and dislocation loop with Burgers vector $b = \Omega \times R_0$, where $R_0 = x_0 e_x + y_0 e_y$ is a vector being drawn from the application point of Ω to the common centre of the disclination and dislocation loops. The pure infinitesimal disclination loops give no contribution to elastic fields [19]. Therefore, for stress tensor calculation we shall only take into consideration the stresses of infinitesimal dislocation loops $\sigma^{b}_{km} = b^{j} g^{j}_{km}$, whose representation may be found, for example, in [20]. Then, the following expression is obtained for stress tensor, σ^{Ω}_{km}, of an arbitrarily-shaped disclination loop lying in the plane $z = 0$:

$$\sigma^{\Omega}_{km}(x, y, z) = \iint_{S} e_{jlt} \Omega_l R_{0_t} g^{j}_{km} \times [(x - x_0), (y - y_0), z] \, dx_0 \, dy_0, \tag{3}$$

where e_{jlt} are the Levi–Chivita tensor components; Einstein's rule of summarizing is used, and integration is carried out over the area S. Hence, the expression for the σ^{ω}_{zz} component of the stress tensor of rectangular wedge disclination loop is obtained (the loop plane is $z = 0$ and its vector of rotation is $\Omega = \omega e_y$, Fig. 3a):

$$\sigma^{\omega}_{zz} = -\frac{G\omega}{4\pi(1-\nu)} \left[\frac{1}{2} \ln \left| \frac{R - v}{R + v} \right| - \frac{vz^2(2u^5 + 2xu^4 - z^2u^3 + xz^4)}{u^3 R (u^2 + z^2)^2} - \frac{z^4 v^3 (u + x)}{u R^3 (u^2 + z^2)^2} + \frac{xvR(z^4 + z^2v^2 - v^2u^2 - 3z^2u^2)}{u^3(z^2 + v^2)^2} \right]_{(-c-x)}^{c-x} \Bigg|_{(-d-y)}^{d-y}, \tag{4}$$

where $R^2 = u^2 + v^2 + z^2$, G is the shear modulus and ν is Poisson's ratio. Substituting this component into the well-known integral expression for the self energy of a disclination loop [13], and after integration, the energy W^s_ω, in the case of rectangular wedge loop in the following form, becomes

$$W^s_\omega = \frac{G\omega^2}{\pi(1-\nu)}\left[c^2 d \ln\frac{4cd}{r_0[d+\sqrt{(c^2+d^2)}]} - \frac{c^3}{3}\ln\frac{r_0[c+\sqrt{(c^2+d^2)}]}{4cd} + \frac{2}{9}(5c^2-d^2)\sqrt{(c^2+d^2)} - \frac{2}{9}(5c^3-d^3) - 2c^2 d\right], \quad (5)$$

where r_0 is the disclination line core radius. The same method can be applied for the calculation of the interaction energy, W^i_ω, between considered disclination loops. This energy will be equal to

$$W^i_\omega = \frac{G\omega^2}{\pi(1-\nu)}\left[2d(2l^2-c^2) \times \ln\frac{[d+(d^2+l^2)^{\frac{1}{2}}](d^2+l^2)^{\frac{1}{2}}}{l[d+(c^2+d^2+l^2)^{\frac{1}{2}}]} - \frac{2}{3}c^3\ln\frac{[c+(c^2+l^2)^{\frac{1}{2}}](d^2+l^2)^{\frac{1}{2}}}{l[c+(c^2+d^2+l^2)^{\frac{1}{2}}]} - 2(c^2+l^2)^{\frac{1}{2}}\left(-\frac{7}{9}c^2+\frac{32}{9}l^2-\frac{c^2l^2}{c^2+l^2}\right) - 2(d^2+l^2)^{\frac{1}{2}}\left(-c^2+\frac{2}{9}d^2+\frac{32}{9}l^2+\frac{c^2l^2}{d^2+l^2}\right) + 2(c^2+d^2+l^2)^{\frac{1}{2}}\left(-\frac{10}{9}c^2+\frac{2}{9}d^2+\frac{32}{9}l^2 - \frac{c^2l^2}{c^2+l^2}+\frac{c^2l^2}{3(d^2+l^2)}\right)+\frac{64}{9}l^3\right]. \quad (6)$$

In these formulae, $2c$ and $2d$ are the disclination loop sizes and $2l$ is the distance between two loops (see Fig. 3a).

3.3. Elastic properties of a rectangular glide dislocation loop and its interaction with a disclination loop

The remaining terms in Equation 2 can be determined if the stress tensor of a dislocation line segment [21] is used. The interaction energy between the rectangular glide dislocation loops W^i_b and their self energies W^s_b are determined by the total stress σ^b_{xz} of the four dislocation segments of each dislocation loop. Evaluating the work done in creating the plastic distortions connected with dislocation loops under this stress σ^b_{xz} we obtain the energies W^s_b and W^i_b as follows:

$$W^s_b = \frac{Gb^2}{\pi(1-\nu)}\left[(d^2+l^2)^{\frac{1}{2}} - l - d - d \times \ln\frac{d+(d^2+l^2)^{\frac{1}{2}}}{l} + d\ln\frac{4d}{r_0}\right] + \frac{Gb^2}{\pi}\left[(d^2+l^2)^{\frac{1}{2}} - l - d - l \times \ln\frac{l+(d^2+l^2)^{\frac{1}{2}}}{d} + l\ln\frac{4l}{r_0}\right]; \quad (7)$$

$$W^i_b = \frac{2Gb^2}{\pi(1-\nu)}\left[2c - \frac{l^2+2c^2}{\sqrt{(l^2+c^2)}} - 2(c^2+d^2)^{\frac{1}{2}} + \frac{l^2+2c^2}{l^2+c^2}(c^2+d^2+l^2)^{\frac{1}{2}} + d\ln\frac{d+(c^2+d^2)^{\frac{1}{2}}}{c} - d\ln\frac{d+(c^2+d^2+l^2)^{\frac{1}{2}}}{(c^2+l^2)^{\frac{1}{2}}}\right] + 2\frac{Gb^2}{\pi}\left[l\ln\frac{l+(c^2+l^2)^{\frac{1}{2}}}{c} - l\ln\frac{l+(c^2+d^2+l^2)^{\frac{1}{2}}}{(c^2+d^2)^{\frac{1}{2}}} + c - (c^2+d^2)^{\frac{1}{2}} - (c^2+l^2)^{\frac{1}{2}} + (c^2+d^2+l^2)^{\frac{1}{2}}\right], \quad (8)$$

where the core radius of the dislocation line, r_0, will now be equal to the core radius of the disclination line, and b is the magnitude of the dislocation loop Burgers vector.

The evaluation of the interaction energy, $W^i_{b\omega}$, is based on the work of the dislocation loop stress σ^b_{zz} when the wedge disclination loop is created:

$$W^i_{b\omega} = \frac{Gb\omega}{\pi(1-\nu)}\left[cd + d^2\ln\frac{c+(c^2+d^2)^{\frac{1}{2}}}{d} + cd\ln\frac{[d+(c^2+d^2)^{\frac{1}{2}}]r_0}{4cd} + cd\ln\frac{d+(d^2+l^2)^{\frac{1}{2}}}{l}\right]$$

$$
\begin{aligned}
&- cd \ln \frac{d + (c^2 + d^2 + l^2)^{\frac{1}{2}}}{(c^2 + l^2)^{\frac{1}{2}}} \\
&- (c^2 + l^2)^{\frac{1}{2}} \frac{cl^2}{c^2 + l^2} \\
&+ l^2 \ln \frac{c + (c^2 + l^2)^{\frac{1}{2}}}{l} \\
&- (d^2 + l^2) \ln \frac{c + (c^2 + d^2 + l^2)^{\frac{1}{2}}}{(d^2 + l^2)^{\frac{1}{2}}} \\
&+ \frac{cl^2}{c^2 + l^2} (c^2 + d^2 + l^2)^{\frac{1}{2}} \Bigg] . \qquad (9)
\end{aligned}
$$

3.4. Analysis of slipped kink self energy

Substituting the calculated energies into Equation 2 and summarizing, allowing for $b = \omega c$, gives the elastic energy, W, of the slipped kink. The full expression for W is not derived here, as it is extremely cumbersome. When $d \gg_{\max} \{c, l\}$ this energy becomes:

$$
W = \frac{G\omega^2 2d}{\pi(1-\nu)} \left[c^2 \ln \frac{c^2 + l^2}{c^2} + l^2 \ln \frac{c^2 + l^2}{l^2} + c^2 \right] \qquad (10)
$$

which is equivalent to the wedge disclination quadrupole energy with an accuracy of c^2. The appearance of this term is caused by the method of assigning the defect.

If the length of slipped kink along the z-axis is much greater than the other defect dimensions ($l \gg_{\max} \{c, d\}$) then the following approximate expression can be used:

$$
W = \frac{G\omega^2 c^2 2l}{\pi} \ln \frac{2d(c^2 + d^2)^{\frac{1}{2}}}{cr_0} . \qquad (11)
$$

Equation 11 corresponds to the energy of the slipped kink having appeared at the single fibre or macromolecule, when this defect is elongated in the direction of the fibre axis. In turn, if the size of the defect along the Frank vector is comparable to its size along the z-axis and both these sizes are much greater than the defect size along the third axis ($_{\min} \{d, l\} \gg c$), then the energy of the slipped kink may be written as:

$$
\begin{aligned}
W = {} & \frac{4G\omega^2 c^2}{\pi(1-\nu)} \\
& \times \Bigg[(1-\nu) l \ln \frac{4dl}{[l + (d^2 + l^2)^{\frac{1}{2}}](2cr_0)^{\frac{1}{2}}} \\
& - \frac{4l^2}{3(d^2 + l^2)^{\frac{1}{2}}} + d \ln \frac{2dl}{c[d + (c^2 + d^2)^{\frac{1}{2}}]} \\
& + \left(\frac{13}{9} - \nu \right) (d^2 + l^2)^{\frac{1}{2}} \\
& + \left(\nu - \frac{17}{18} \right) d + \left(\nu - \frac{10}{9} \right) l \Bigg] . \qquad (12)
\end{aligned}
$$

The given asymptotes are the best for analysis of the energy balance of kink-band motion.

Equations 10 to 12 correspond to the cases when the slipped kink can be represented by a surface or linear defect. Under this condition two groups can be singled out from defect dimensions $2c$, $2d$ and $2l$: one is characterized by length h and the other one by length L (where $L \gg h$). Here L is the characteristic size of the surface or the length of the line. Upon analysing Equations 10 to 12 it is convincing that the slipped kink energy may be estimated as $W \sim G\omega^2 h^2 L$. The form of the given dependence permits a comparison of this energy with the energy of the dislocation line in a linear approximation $W_L \sim Gb^2 L$, where $\boldsymbol{b}$ is the Burgers vector of dislocation and L is its length.

If ωh is of the order of $\boldsymbol{b}$, the energy behaviour of the slipped kinks is similar to that of a dislocation. This case is realized in polymers, where $\omega \sim 1$ [2–4] and h is of the order of the macromolecular diameter. In fibre composites the condition $\omega h \gg \boldsymbol{b}$ holds, since the fibre diameter is much larger than the interatomic distance. This leads to conditions favourable for the formation of cracks in the tilted fibres rather than for the nucleation of slipped kinks. Such cracks were observed when kink-band evolution was investigated in fibre composites [11].

The total free Helmholtz energy of the slipped kink consists of the calculated elastic energy together with the entropy associated with the defect and the energies of the disclination and dislocation cores. There are good reasons to believe [13] that the elastic energy represents the main part of the total energy, so that the other terms may be ignored when the energetics of processes due to the slipped kinks are considered.

4. Conclusions

(1) A disclination–dislocation model has been proposed for the structure of kink bands in

oriented polymers and fibre composites. The proposed model is able to describe both simultaneous chain or fibre bending and intermolecular slip in the band.

(2) The mechanism has been considered for kink-band evolution by means of a wedge disclination dipole movement. It has been shown that kink-band (dipole) motion is effected by ejecting special disclination–dislocation defects, the so-called slipped kinks.

(3) The geometrical properties of a slipped kink have been studied. It has been discovered that such a defect consists of two opposite-sign wedge disclination loops and two glide dislocation loops. Thus, characteristics of disclination and dislocation loops in the defect are unequivocally linked with one another.

(4) The elastic energy of a slipped kink has been calculated on the basis of the self and interaction energies of its components. The various limit cases of kink energy with varying defect dimensions have been investigated.

In addition, kink-band evolution in fibre composites can be accompanied by fibre fracture. This process takes place if it is energetically favourable to form a pair of cracks in the fibre rather than to form a slipped kink.

The disclination–dislocation model for kink-band structure and motion proposed in the present work suggests the possibility of the theoretical description of the deformation behaviour of plastically non-homogeneous materials. The main characteristics of the deformation processes under investigation are: the critical applied stress, τ_c, of the kink-band nucleation and motion, the velocity, V_{KB}, of kink-band propagation through the material as a function of the applied stress τ and the tempeature T. It is obvious that the relations between these characteristics and the structural properties of the material are of great value. For example, the critical applied stress, τ_c, is determined by the number of slipped kinks in the band formation from which kink-band development becomes energetically favourable. Likewise, the velocity, V_{KB}, depends on the critical length, $2d_c$, of the slipped kink ejected by a disclination dipole (Fig. 4). For this to be achieved, the interaction between the slipped kink and the disclination dipole must be taken into consideration. The dependence of the direction of the band motion on the structural and external parameters is also of great interest. This direction is again determined from the standpoint of the best energy balance for kink-band formation and propagation.

All these questions and a comparison of this model with the experimental data will be presented in a subsequent publication.

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