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Nonlocal theory of interaction between jogs and kinks

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THE PAPER deals with the problem of interaction of kinks and jogs within the framework of nonlocal continuum theory. The general formula in the integral form describing this interaction is derived. Then the detailed analysis of the simple case of the abrupt nonextendedd efects in the nondispersive medium is performed. The interaction is of the order r^{-3}, where r denotes the distance between defects. The neglected details of the structure of the defects and the material would give account to the terms of the order r^{-5} and lower. The obtained result shows that for small distances, and particularly in the creation processes, this kink-jog interaction contributoni is of the same order of magnitude as the nonlocal terms of kink-kink and jog-jog interaction.

Praca poświęcona jest problemowi oddziaływania przegięć z progami na podstawie nielokalnej teorii kontinuum. Otrzymano ogólne wyrażenie w postaci całkowej opisujące to oddziaływanie, a następnie przeprowadzono szczegółową analizę prostego przypadku skokowych nierozmytych defektów w ośrodku bezdyspersyjnym. Oddziaływanie jest rzędu r^{-3}, gdzie r oznacza odległość między defektami. Pominięte szczegóły struktury defektów i ośrodka dałyby wkład do członu rzędu r^{-5} i niższych. Otrzymany wynik wskazuje, że dla małych odległości a szczególnie w procesach kreacji wkład pochodzący od oddziaływania próg-przegięcie jest wielkością tego samego rzędu co i człony nielokalne oddziaływań przegięcie-przegięcie i próg-próg.

Работа посвящена проблеме взаимодействия перегибов с порогами, опираясь на нелокальную теорию континуум. Получено общее выражение в интегральном виде описывающее это взаимодействие и затем проведен подробный анализ простого случая скачкообразных неразмытых дефектов в бездисперсионной среде. Взаимодействие порядка r^3, где r обозначает расстояние между дефектами. Неучтенные подробности структуры дефектов и среды дали бы вклад в член порядка r^{-5} и в более низкие члены. Полученный результат показывает, что для малых расстояний, а особенно в процессах рождения, вклад происходящий от взаимодействия порог - перегиб является величиной того же самого порядка, что и нелокальные члены взаимодействия перегиб-перегиб и порог-порог.

1. Introduction

THE PROBLEMS of energy of kinks and jogs separately were studied in previous papers [1, 2, 3]. The considerations were based on the pseudocontinuum model introduced by ROGULA [4]; the details of the real crystal structure were taken into account and the interactions were assumed to be nonlocal in the sense of KROENER [5] and KUNIN [6].

We recall that the two straight-line segments of dislocations which are separated by a jog extend in different — most probably neighbouring — slip planes, whereas in the case of kinks the two segments extend in the same slip plane, along two different parallel lines of atoms.

The results obtained for the kink-kink and jog-jog interaction exhibit some common features: namely in the both cases the interaction energy can be written in the form of the infinite series

$$\frac{A}{r}+\frac{B}{r^3}+\frac{C}{r^5}\ldots, \tag{1.1}$$

where r denotes the distance between defects. The values of the constants $A, B, C\ldots$ depend on the case (kinks or jogs) and the details of the structure of the medium and the defect itself. The first terms of the order $1/r$ are identical with those obtained from the elasticity theory; the next ones take into account the shape of defects, their extent and the dispersion of the medium. The calculations were restricted to the first two terms. The next ones describe the finer structure of the properties mentioned above and would involve more parameters of the medium and the defects as well.

Within the framework of elastic continuum the jog-kink interaction equals zero because, roughly speaking, a kink and a jog are considered as two mutually perpendicular segments of dislocations. By means of the nonlocal theory it is possible to answer the question whether this interaction equals identically zero or not and, if not, what is the order of magnitude (in terms of the distance between defects) of the first nonvanishing term. It seems to be rather important to know that: if the first term would be, e.g., of the order of r^{-11} certainly we would not need to include this contribution to the energy of interacting defects; however if the first nonvanishing term is of the order r^{-3}, it should be taken into account when energy problems are considered (of course for distances of the order of interatomic distances).

2. The energy of the dislocation line with two defects

In the paper [1] the general expression for the energy of a single dislocation of any shape in the framework of isotropic pseudocontinuum model was given:

$$W = \frac{1}{16\pi^3}\int_B d^3k A_{abil}(\mathbf{k}) b_i b_l \chi(\mathbf{k})\chi(-\mathbf{k})\psi_{ab}(\mathbf{k}), \tag{2.1}$$

where

$$A_{abil} = c_{nklm}(k)c_{rwip}(k)G_{nr}(\mathbf{k})\epsilon_{pka}\epsilon_{smb}\frac{k_w k_s}{k^2}, \tag{2.2}$$

$$\psi_{ab} = \int_L e^{-i\mathbf{k}\cdot\mathbf{x}}dx_a \int_L e^{i\mathbf{k}\cdot\mathbf{x}'}dx'_b, \tag{2.3}$$

L denotes the dislocation line and $\chi(\mathbf{k})$ describes the structure of the line. G_{nr} and c_{ijkl} are the Fourier components of the Green tensor function of the isotropic pseudocontinuum and the tensor function describing elastic properties of the pseudocontinuum, respectively

$$G_{ij}(k) = \frac{1}{\varrho k^2}\left\{\frac{\delta_{ij}}{c_2^2(k)} + \frac{k_i k_j}{k^2}\left[\frac{1}{c_1^2(k)} - \frac{1}{c_2^2(k)}\right]\right\}, \tag{2.4}$$

$$c_{ijkl}(k) = \varrho\{[c_1^2(k) - c_2^2(k)]\delta_{ij}\delta_{kl} + c_2^2(k)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\}, \tag{2.5}$$

$k = |\mathbf{k}|$, ϱ is the mass density; c_1 and c_2 are the velocities of the longitudinal and transversal waves, respectively. The integration extends over the first Brillouin zone. The derivation of the formula (2.1) and all the details concerning the forms of the dislocation density tensor etc. are given in the papers [1] and [2].

We choose the Cartesian coordinates system $x = x_1, y = x_2, z = x_3$ with origin at 0. To calculate the kink-jog interaction we consider the dislocation line to be extended along the OX axis, with a double defect "king-jog" sloped at some angle θ to the slip plane. The Burgers vector $\mathbf{b}$ has only the single b_2 component. The case $\theta = 0$ corresponds then to two kinks, while $\theta = \pi/2$ describes the two jogs situation. For the cases of our interest we could restrict ourselves to the following range of values of θ:

$$0 < \theta < \pi/2.$$

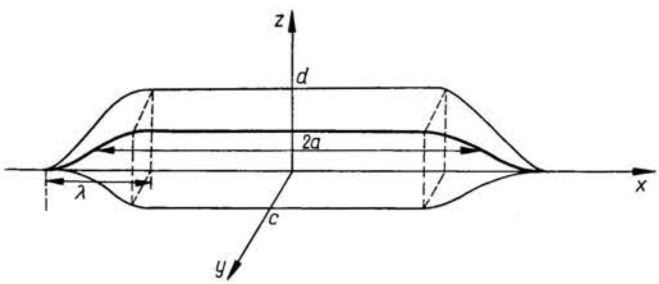

FIG. 1.

The projection of the line onto OXY-plane describes the situation of two kinks on the edge dislocation, of the height c, length λ and separated by the distance $2a$; we can call it the "kink component" of the defect; the similar projection onto OXZ-plane describes the dislocation line with two jogs of the height d and length λ, separated by the same distance $2a$; it correponds to the "jog component" of the defect. Speaking about the distance between defects we will always mean the distance measured along the OX axis, i.e. $2a$. Assuming such a system of coordinates and the Burgers vector $\mathbf{b} = [0, b, 0]$, we can rewrite the formula (2.1) in the form

$$W = \frac{b^2}{16\pi^3} \int_B d^3k A_{ab22}(\mathbf{k}) \psi_{ab}(\mathbf{k}) \chi(\mathbf{k}) \chi(-\mathbf{k}). \tag{2.6}$$

Further on we will omit the indices 22 in the expressions A_{ab22}. Function $\chi(\mathbf{k})$ depends on k_2 and k_3 only, what is of considerable importance for the further considerations.

3. The energy of the two kink-jog defects

The defect described in the preceding section, possessing the kink and jog components, will be called the kink-jog defect. We assume that the dislocation line with a double kink-jog can be described in a parametric way

$$x_1 = x, \quad x_2 = y(x), \quad x_3 = z(x), \tag{3.1}$$

and the functions $y(x)$ and $z(x)$ are differentiable for any $x \in R$. Then we can rewrite ψ_{ab} in the form

$$\psi_{ab} = f_a^- f_b^+, \tag{3.2}$$

where

$$f_1^{\pm} = \int\limits_L \exp[\pm i(k_1x+k_2y+k_3z)]dx$$

$$= 2\pi\delta(k_1)+2\int\limits_0^\infty \cos k_1x\{\exp[\pm i(k_2y+k_3z)]-1\}dx,$$

(3.3)

$$f_2^{\pm} = \int\limits_L \exp[\pm i(k_1x+k_2y+k_3z)]dy = \pm 2i\int\limits_0^\infty \sin k_1x\cdot y'(x)\exp[\pm i(k_2y+k_3z)]dx,$$

$$f_3^{\pm} = \int\limits_L \exp[\pm i(k_1x+k_2y+k_3z)]dz = \pm 2i\int\limits_0^\infty \sin k_1x\cdot z'(x)\exp[\pm i(k_2y+k_3z)]dx.$$

The energy of the two defects is defined as the difference of the expressions (1.1) for the dislocation line with the defects and the straight line dislocation, when the distance between defects tends to infinity, what in our description corresponds to the displacements

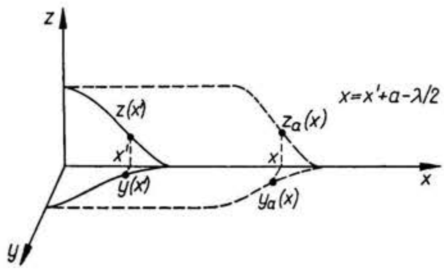

FIG. 2.

of the functions $y(x)$ and $z(x)$ by $a-\lambda/2$ (see Fig. 2). The displaced functions are denoted $y_a(x)$ and $z_a(x)$. Then the behaviour of the energy expression for $a\to\infty$ is studied. From the formulas (3.3), for $a\to\infty$ we obtain

$$f_1^{\pm} = 2A_{\pm}\frac{\sin k_1(a-\lambda/2)}{k_1}+2\int\limits_0^\infty \cos k_1X\varphi_{\pm}(x)dx,$$

(3.4)

$$f_2^{\pm} = \pm 2i\int\limits_0^\infty \sin k_1X\vartheta_{\pm}(x)dx,$$

$$f_3^{\pm} = \pm 2i\int\limits_0^\infty \sin k_1X\eta_{\pm}(x)dx,$$

where the following notations were introduced:

(3.5) $$A_{\pm} = \exp[\pm i(k_2c+k_3d)]-1,$$

(3.6) $$\varphi_{\pm}(x) = \exp[\pm(k_2y+k_3z)]-1,$$

(3.7) $$\vartheta_{\pm}(x) = y'(x)\exp[\pm i(k_2y+k_3z)],$$

(3.8) $$\eta_{\pm}(x) = z'(x)\exp[\pm i(k_2y+k_3z)],$$

(3.9) $$X = x+a-\lambda/2,\quad X' = x'+a-\lambda/2.$$

To obtain the appropriate expressions ψ_{ab} for double defect we have to multiply the functions f_a^+ and subtract the corresponding expressions for the straight line dislocation (the functions A_{ab} depend on the properties of the medium only). The latter procedure will change the form of ψ_{11} only, so this term will be treated seperately. The terms ψ_{22}, ψ_{23}, ψ_{32} and ψ_{33} can be written down directly from the formulae (3.4), without any additional operations. As far as the remaining terms (except ψ_{11}) are concerned, first we can notice that the following terms can be disregarded:

$$2\pi\delta(k_1)2i\int \vartheta_\pm(x)\sin k_1 X dx,$$

$$2\pi\delta(k_1)2i\int \eta_\pm(x)\sin k_1 X dx,$$

since after integration they yield zero contributions. The second parts of the functions $\psi_{12}, \psi_{21}, \psi_{13}, \psi_{31}$ can be integrated by parts and finally we obtain

$$\psi_{12} = -\frac{4}{k_1}\iint \sin k_1 X \sin k_1 X' [k_2\vartheta_+(x)\vartheta_-(x') + k_3\eta_-(x)\vartheta_+(x')]dxdx', \tag{3.10}$$

$$\psi_{21} = -\frac{4}{k_1}\iint \sin k_1 X \sin k_1 X' [k_2\vartheta_+(x)\vartheta_-(x') + k_3\eta_+(x)\vartheta_-(x')]dxdx', \tag{3.11}$$

$$\psi_{13} = -\frac{4}{k_1}\iint \sin k_1 X \sin k_1 X' [k_3\eta_+(x)\eta_-(x') + k_2\vartheta_-(x)\eta_+(x')]dxdx', \tag{3.12}$$

$$\psi_{31} = -\frac{4}{k_1}\iint \sin k_1 X \sin k_1 X' [k_3\eta_+(x)\eta_-(x') + k_2\vartheta_+(x)\eta_-(x')]dxdx', \tag{3.13}$$

$$\psi_{22} = 4\iint \sin k_1 X \sin k_1 X' \vartheta_+(x)\vartheta_-(x')dxdx', \tag{3.14}$$

$$\psi_{23} = 4\iint \sin k_1 X \sin k_1 X' \vartheta_-(x)\eta_+(x')dxdx', \tag{3.15}$$

$$\psi_{32} = 4\iint \sin k_1 X \sin k_1 X' \vartheta_+(x)\eta_-(x')dxdx', \tag{3.16}$$

$$\psi_{33} = 4\iint \sin k_1 X \sin k_1 X' \eta_+(x)\eta_-(x')dxdx'. \tag{3.17}$$

It would be very convenient to reduce ψ_{11} to the form similar to the others ψ_{ab}. Integration by parts yields

$$\begin{aligned}\psi_{11} = {} & 4\pi i\delta(k_1)\int \frac{\sin k_1 X}{k_1}[k_2(\vartheta_-(x) - \vartheta_+(x)) + k_3(\eta_-(x) - \eta_+(x))]dx \\ & + \frac{4}{k_1^2}\iint \sin k_1 X \sin k_1 X' [k_2\vartheta_+(x) + k_3\eta_+(x)][k_2\vartheta_-(x') + k_3\eta_-(x')]dxdx'.\end{aligned} \tag{3.18}$$

To get rid off the term proportional to a, which appears in ψ_{11}, after integration over k_1, we have to add and subtract the second part of ψ_{11} multiplied by $A_{11}^0 (A_{11}^0 = A_{11}(k_1 = 0))$. Then for large values of a:

$$a/c \gg 1, \quad a/d \gg 1, \quad a/\lambda \gg 1$$

and after integration over k_1 the first term in ψ_{11} is cancelled by the second one (multiplied by A^0_{11}), so that the energy can be written in the form

$$W = \frac{b^2}{16\pi^3}\int [A_{ab}(\mathbf{k})\psi_{ab}(\mathbf{k}) - A^0_{11}(\mathbf{k})\psi_{11}(\mathbf{k})]\chi(\mathbf{k})\chi(-\mathbf{k})d^3k. \tag{3.19}$$

Here ψ_{11} is redefined and given by

$$\psi_{11} = \frac{4}{k_1^2}\int\int \sin k_1 X \sin k_1 X' [k_2\vartheta_+(x) + k_3\eta_+(x)][k_2\vartheta_-(x') + k_3\eta_-(x')]dxdx'. \tag{3.20}$$

4. The general formula for the kink-jog interaction energy

Expression (3.19) describes the whole energy of two kink-jogs. We would like to isolate the part corresponding to the kink-jog interaction. For this purpose we will rewrite the formula (3.19) in a more explicit form

$$\begin{aligned} W = \frac{b^2}{4\pi^3}\int d^3k\,\chi(\mathbf{k})\chi(-\mathbf{k})\int\int \sin k_1 X \sin k_1 X' \Big\{\vartheta_+(x)\vartheta_-(x')\Big[A_{22} \\ -\frac{k_2}{k_1}(A_{12}+A_{21}) + \frac{k_2^2}{k_1^2}(A_{11}-A^0_{11})\Big] + \eta_+(x)\eta_-(x')\Big[A_{33} - \frac{k_3}{k_1}(A_{13}+A_{31}) \\ +\frac{k_3^2}{k_1^2}(A_{11}-A^0_{11})\Big] + \vartheta_+(x)\eta_-(x')\Big[A_{32} - \frac{k_2}{k_1}A_{31} - \frac{k_3}{k_1}A_{12} + \frac{k_2k_3}{k_1^2}(A_{11}-A^0_{11})\Big] \\ +\vartheta_-(x)\eta_+(x')\Big[A_{23} - \frac{k_2}{k_1}A_{13} - \frac{k_3}{k_1}A_{21} + \frac{k_2k_3}{k_1^2}(A_{11}-A^0_{11})\Big]\Big\}dxdx'. \end{aligned} \tag{4.1}$$

From the formulae (2.2), (2.4) and (2.5) we can calculate now the values of functions A_{ab}

$$\begin{aligned} A_{11} &= 2\varrho\alpha\left[\frac{2k_3^2}{k^4} + \frac{k_1^2k_2^2}{k^6}\right], \\ A_{22} &= c_2^2\varrho\frac{k_1^2+k_3^2}{k^4} - 2\alpha\varrho\frac{k_2^2(k_1^2+k_3^2)}{k^6}, \\ A_{33} &= 2\varrho\alpha\left[\frac{2k_1^2}{k^4} + \frac{k_2^2k_3^2}{k^6}\right], \\ A_{12} &= -2\varrho\alpha\frac{k_1k_2}{k^6}[k^2-k_2^2], \\ A_{21} &= -\varrho c_2^2\frac{k_1k_2}{k^6}[k^2-2\beta k_2^2], \\ A_{13} &= -2\varrho\alpha\frac{k_1k_3}{k^6}[2k^2-k_2^2], \\ A_{31} &= -2\varrho\alpha\frac{k_1k_3}{k^6}[2k^2-k_2^2], \\ A_{23} &= -\varrho c_2^2\frac{k_2k_3}{k^6}[k^2-2\beta^2k_2^2], \\ A_{32} &= -2\varrho\alpha\frac{k_2k_3}{k^6}[k^2-k_2^2], \end{aligned} \tag{4.2}$$

where

$$\alpha(k) = c_2^2(k)\beta(k) = c_2^2(k)\frac{c_1^2(k)-c_2^2(k)}{c_1^2(k)}. \tag{4.3}$$

If we insert the expressions (4.2) into (4.1) and take into account the symmetry of the isotropic Brillouin zone, we can easily find out that the first two terms in the expression (4.1), proportional to $\vartheta_+\vartheta_-$ and $\eta_+\eta_-$, describe the energy of the kink and jog component seperately; we will not obtain terms proportional to the products $c^n d^m$ but only to c^n and d^m. The kink-jog ineraction can be included in the last two terms only. The careful analysis of the symmetries of the corresponding expressions appearing there shows that those two terms do not contain the self-energy contributions, independent on a, and the kink-jog interaction energy is given by

$$\begin{aligned} W_{j-k} = & -\frac{b^2\varrho}{4\pi^3}\int d^3k\alpha(k)\times k_2k_3\times\chi(\mathbf{k})\chi(-\mathbf{k}) \\ & \times\left[\frac{1}{k^4}-\frac{k_3^2}{k^4(k_2^2+k_3^2)}-\frac{k_3^2}{k^2(k_2^2+k_3^2)^2}\right]\times\iint[\vartheta_+(x)\eta_-(x')+\vartheta_-(x)\eta_+(x')] \\ & \times[\cos 2k_1a\cdot\cos k_1(x+x'-\lambda)-\sin 2k_1a\cdot\sin k_1(x+x'-\lambda)]\,dx\,dx'. \end{aligned} \tag{4.4}$$

More precisely, the expression $\sin k_1X\cdot\sin k_1X'$ is equivalent to

$$\frac{1}{2}[\cos k_1(x-x')-\cos 2k_1a\cdot\cos k_1(x+x'-\lambda)+\sin 2k_1a\cdot\sin k_1(x+x'-\lambda)].$$

The term proportional to $\cos k_1(x-x')$ which being independent of a would correspond to the self-energy contribution does not appear in the formula (4.4) because of the symmetries of the Brillouin zone. The functions A_{ij} contained in the brackets in the last two terms of the expression (4.1) are odd functions of k_2 and k_3, therefore the integral is equal to zero.

5. Explicit formula for interaction between abrupt nonextended jogs and kinks in nondispersive medium

The formula (4.4) is a general one and involves all the parameters describing the defects and the properties of the medium. To find the kink-jog interaction in an explicit form we have to determine the functions $c_i(k)$ and $\chi(\mathbf{k})$ and to choose the shape of the defects. We consider the simple case of a nondispersive medium, or, in other words, the case when velocities of waves do not depend on the wave vector $\mathbf{k}$:

$$c_i(k) = c_i(0), \quad i = 1, 2, \quad \alpha(k) = \alpha(0). \tag{5.1}$$

The defects are supposed to be nonextended what corresponds to the fact that function $\chi(\mathbf{k})$ is constant:

$$\chi(\mathbf{k}) = 1. \tag{5.2}$$

We assume the linear models of defects:

$$\begin{aligned} y(x) &= c(1-x/\lambda), \\ z(x) &= d(1-x/\lambda), \end{aligned} \quad x\in[0,\lambda]. \tag{5.3}$$

With those assumptions we can now perform the integrations over x and x'. Recall that

$$\int_0^\lambda\int_0^\lambda \sin k_1(x+x'-\lambda)\,[\vartheta_+(x)\eta_-(x')+\vartheta_-(x)\eta_+(x')]\,dx\,dx' = 0$$

therefore in the case of linear defects there are no terms proportional to $\sin 2k_1 a$. The same fact appeared also in the discussion of kinks and jogs [2, 3].

We are interested in the case of abrupt defects, when $\lambda = 0$. So after integration we will find an approximate expression for $c/\lambda \gg 1$ and $d/\lambda \gg 1$. The energy expression depends on a and is of the form of a one-dimensional Fourier transform but the Cartesian coordinate system is not suitable for further calculations. We change variables to the spherical ones:

$$k_1 = k\cos\theta,\quad k_2 = k\sin\theta\cos\varphi,\quad k_3 = k\sin\theta\sin\varphi. \tag{5.4}$$

After the integration over the angles θ and φ, the energy is given in the form

$$W_{j-k}(a) = \int [f_1(k)\sin 2ka + f_2(k)\cos 2ka]\,dk$$

and the only singularity of the functions f_1 and f_2 is at $k = 0$; *m* order to find the values of $W_{j-k}(a)$ for $|a| \to \infty$ we have to expand the functions at $k = 0$ and to find the corresponding Fourier transforms. Finally

$$W_{j-k} = \frac{b^2c^2d^2\mu}{96\pi(1-\nu)}\frac{1}{r^3}, \quad r = 2a. \tag{5.5}$$

6. Conclusions and remarks

The expression obtained (5.5) indicates that the kink-jog interaction is not identically zero. It could be written in the form of an infinite series

$$\sum_{n=1}^{\infty}\frac{A_n}{r^{2n+1}}.$$

In the simplest case of abrupt nonextended defects in the nondispersive medium this series is reduced to the first term. The higher order terms would appear if we took into account details of the structure of the medium and more sophisticated models of the defect. It does not seem to be well-advised, however, because if we study the problem of interaction of kinks and jogs we must remember that jog-jog contributions and kink-kink ones as well start from the terms of the order $1/r$, and the terms $1/r^3$ are the additional nonlocal ones. For the distances at which those additional terms in jog-jog and kink-kink interactions are important, the term given by the formula (5.5) must not be neglected: it is of the same order as the term $1/r^3$ in the jog-jog interaction (putting $c = d$) for the abrupt nonextended jog, when the medium is nondispersive [3]. The additional result of the paper is that the self-energy of the kink-jog defect does not contain interfering terms: it is the sum of selfenergies of the kink and jog components. The nonlocality of interactions does not change this important property of the energy. The result is valid for any dislocation line, not only for the defects of the line, because in the paper no restrictions on the height of the defects were imposed and very high jogs or kinks become the segments of the straight line dislocations, edge and screw dislocations, respectively.

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