Archives of Mechanics ● Archiwum Mechaniki Stosowanej ● 25, 6, pp. 953–965, Warszawa 1973

# Self-energy and interaction of kinks

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THE SELF-ENERGY and interaction of two kinks with a dislocation is calculated. Our starting point is the general formula describing the energy of two kinks [1]. It is assumed that a kink is described by means of a linear function which depends on two parameters: the height of a kink $c$, and its width $\lambda$. The extended dislocation model in a weak-dispersion medium is studied. In particular, we have obtained results concerning abrupt kinks, the dispersion and extension being taken into account. Moreover, the expressions describing the dependence of energy on the width of a kink are given, together with the corresponding Tables and diagrams concerning the kinks on the edge and screw dislocations. The interaction energy up to the $1/r^3$-terms is found ($r$ is the distance between kinks). The problem of critical distance between kinks, at which the interaction energy would change its sign, is studied in detail.

Korzystając z ogólnego wyrażenia na energię [1] dwóch przegięć na dyslokacji, obliczono energię własną i oddziaływania dwóch przegięć. Zakłada się, że przegięcie jest opisane funkcją liniową zależną od parametrów $c$ i $\lambda$ — czyli wysokości i szerokości przegięcia. Rozważany jest model dyslokacji rozmytej w ośrodku słabodyspersyjnym. Otrzymano wyniki dla przegięcia skokowego z uwzględnieniem dyspersji i rozmycia. Podano także wyrażenie określające energię w zależności od szerokości przegięcia oraz odpowiednie tabele i wykresy dla przegięć na dyslokacji śrubowej oraz krawędziowej. Otrzymano także energię oddziaływania z dokładnością do członów rzędu $1/r^3$ ($r$ — odległość między przegięciami). Zbadano problem odległości krytycznej między przegięciami, przy której oddziaływanie zmieniałoby znak.

На основе общей формулы для энергии двух перегибов на дислокации [1] вычислены собственная энергия и энергия взаимодействия двух перегибов. Предполагается, что перегибы описываются линейными функциями, зависящими от параметров $c$ — высоты и $\lambda$ — ширины перегиба. Рассматривается модель размытой дислокации в слабодисперсной среде. Получены решения для скачкообразного перегиба, учитывающие дисперсию и размытие. Выведены также соотношения, определяющие энергию в зависимости от ширины перегиба. Приводятся таблицы и графики для перегибов на краевой и винтовой дислокациях. Вычисления энергии взаимодействия выполнены с точностью до членов порядка $1/r^3$, где $r$ обозначает расстояние между перегибами. Исследован вопрос о критическом расстоянии между перегибами, при котором меняется знак взаимодействия.

## Introduction

IN THE PREVIOUS paper [1], the general formula describing energy of two kinks on a dislocations was obtained. The energy depends on the radius of the Brillouin zone and the dispersion of a crystal. Moreover, it takes into account the inherent parameters of kinks.

Now, the results referred to will be applied to the study of self-energy and interaction of kinks.

The problem of self-energy has been studied by KROUPA, BROWN [2], BRAILSFORD [3], WALLACE and NUNES [4]. However, their results are not satisfactory. The energy calculated in [2 and 4] becomes negative for small kinks. Non-essential discrepancies between [2 and 4] are the result of different cut-off of a core. The expression obtained in [3] does not depend on the height of a kink, although the sign of energy depends on $\nu$. (In the case of screw dislocation, for example, the sign of energy changes at $\nu = 1/3$).

Furthermore, in all the papers indicated above, only abrupt kinks on dislocation lines in continuous media are studied.

In the present paper, we investigate the dependence of self-energy of such physical factors as the width and extension of a kink and the dispersion of a medium. The height of the kink is taken as one atomic distance.

The dependence of self-energy of the height of a kink will be given in a later paper.

## 1. The self-energy of a kink

The kink self-energy is given by:

$$W = \frac{1}{16\pi^3}\int d_3k\,[b_1^2 A_1(\mathbf{k}) + b_2^2 A_2(\mathbf{k})]\,\chi(\mathbf{k})\,\chi(-\mathbf{k}) \times \tag{1.1}$$
$$\times \int\int \vartheta_+(x)\vartheta_-(x')\cos k_1(x-x')\,dx\,dx',$$

where

$$A_1(\mathbf{k}) = 4\alpha(k)\frac{k_3^2}{k^4} - c_2^2(k)\frac{k_2^2}{k^2(k_2^2+k_3^2)},$$

$$A_2(\mathbf{k}) = c_2^2(k)\frac{1}{k^2} - 4\alpha(k)\frac{k_2^2k_3^2}{k^2(k_2^2+k_3^2)^2} - 4\alpha(k)\frac{k_2^2k_3^2}{k^4(k_2^2+k_3^2)},$$

$$\vartheta_\pm(x) = e^{\pm ik_2y(x)}y'(x), \qquad \alpha(k) = \frac{c_1^2(k)-c_2^2(k)}{c_1^2(k)}c_2^2(k),$$

$$\mathbf{b} = [b_1, b_2, 0] \quad \text{(Burgers vector)}$$

$y(x)$ is a function describing a shape of a kink, $c_{1,2}(k)$ — velocities of the transversal and longitudinal waves, respectively.

To calculate the self-energy, we specify the functions occurring in the integral (1.1):

$$y(x) = c(1-x/\lambda), \qquad y'(x) = -c/\lambda. \tag{1.1'}$$

Hence the integration in the variables $x$, $x'$ can be carried out explicitly:

$$\Psi = \int_0^\lambda\int_0^\lambda \cos k_1(x-x')e^{ik_2[y(x)-y(x')]}y'(x)y'(x')\,dx\,dx' =$$
$$= \frac{c^2}{\lambda^2}\left[\frac{1-\cos(k_1\lambda+k_2c)}{\left(k_1+k_2\frac{c}{\lambda}\right)^2} + \frac{1-\cos(k_1\lambda-k_2c)}{\left(k_1-k_2\frac{c}{\lambda}\right)^2}\right], \tag{1.2}$$

$$\chi(\mathbf{k}) = \frac{\sin|k_2|\tilde{\zeta}}{|k_2|\tilde{\zeta}}, \tag{1.3}$$

$\tilde{\zeta}$ is an extension parameter of a dislocation line; it depends on the properties of the medium. The smallest physical values of $\tilde{\zeta}$ are of the order of a few Burgers vectors; the maximal ones are ten times larger. Obviously, $\chi(\mathbf{k}) = 1$ corresponds to the dislocation line without extension. But if we consider a dislocation in a crystal, it seems necessary

to take the extension into account [6, 7]. $\zeta$ depends on the medium properties. The experimental values of the parameters are given in [6] (Chapter 6, § 4, Table 8)

$$c_i^2(k) = c_i^2(0)\left[1-\frac{1}{24}\frac{\pi^2k^2}{k_m^2}\right], \tag{1.4}$$

where $k_m$ is a radius of the Brillouin zone.

Such a form of $c_i^2(k)$ describes weak-dispersion media. $c_i^2(k) = c_i^2(0)$ describes non-dispersion media. The general dispersion formula has the form:

$$c_i^2 = c_i^2(0)\frac{4k_m^2}{\pi^2k^2}\sin^2\frac{\pi^2\mathrm{k}^2}{4k_m^2}.$$

If we wish to consider weak-dispersion media, then formula (1.4) gives a satisfactory approximation. (Further, its form simplifies all the calculations). It is easily seen that the largest contributions to $W$ come from regions, where:

$$k_1\lambda+k_2c = 0, \quad \text{and} \quad k_1\lambda-k_2c = 0.$$

Let us investigate those two expressions separately. Making use of some transformations (rotations in a $0k_1k_2$ — plane), we obtain:

$$W = \frac{1}{16\pi^3}\int d_3\mathbf{k}\left[b_1^2\left(A_1^+(\mathbf{k})+A_1^-(\mathbf{k})\right)+b_2^2\left(A_2^+(k)+A_2^-(\mathbf{k})\right)\right],$$

$$\chi^2(k) = \frac{c^2}{c^2+\lambda^2}\,\frac{1-\cos k_1\sqrt{c^2+\lambda^2}}{k_1^2},$$

$$A_1^{\pm} = 4\alpha(k)\,\frac{k_3^2}{k^4}-c_2^2(k)\,\frac{k_1^2c^2+k_2^2\lambda^2\pm 2k_1k_2\lambda c}{k^2[k_3^2(c^2+\lambda^2)+k_1^2c^2+k_2^2\lambda^2\pm 2k_1k_2\lambda c]}, \tag{1.5}$$

$$A_2^{\pm} = c_2^2(k)\,\frac{1}{k^2}-4\alpha(k)\,\frac{k_3^2(k_1^2c^2+k_2^2\lambda^2\pm 2k_1k_2\lambda c)}{k^4[k_3^2(c^2+\lambda^2)+k_1^2c^2+k_2^2\lambda^2\pm 2k_1k_2\lambda c]}-$$

$$-4\alpha(k)\,\frac{k_3^2(k_1^2c^2+k_2^2\lambda^2\pm 2k_1k_2\lambda c)}{k^2[k_3^2(c^2+\lambda^2)+k_1^2c^2+k_2^2\lambda^2\pm 2k_1k_2\lambda c]^2}.$$

In what follows, we discuss the dependence of $W$ on the dispersion and extension parameters. Let us put $\lambda = 0$, which corresponds to the abrupt kink:

$$W = \frac{1}{8\pi^3}\int d_3k\,\chi^2(k_1)\left[b_1^2\left(4\alpha(k)\frac{k_3^2}{k^4}-c_2^2(k)\,\frac{k_1^2}{k^2(k_1^2+k_3^2)}\right)\right. \tag{1.6}$$

$$\left.+b_2^2\left(c_2^2(k)\frac{1}{k^2}-4\alpha(k)\frac{k_1^2k_3^2}{k^2(k_1^2+k_3^2)^2}-4\alpha(k)\,\frac{k_1^2k_3^2}{k^4(k_1^2+k_3^2)}\right)\right]\frac{1-\cos k_1c}{k_1^2}.$$

We start with the simplest case: non-dispersion medium and non-extended line of a kink, e.g., $\chi^2(k_1) = 1$, $c_i^2(k) = c_i^2(0)$.

$$W_1^0 = \frac{c\mu b_1^2}{8\pi}\left[\frac{1.361}{1-\nu}-1.011\right], \qquad W_1^0 = \frac{c\mu b_2^2}{8\pi}\left[2.112-\frac{0.908}{1-\nu}\right]. \tag{1.7}$$

If we take into account a dispersion, we obtain additional terms:

$$\Delta W_1 = -\frac{c\mu b_1^2}{8\pi}\left[\frac{0.129}{1-\nu}-0.055\right], \quad \Delta W_2 = -\frac{c\mu b_2^2}{8\pi}\left[0.204-\frac{0.087}{1-\nu}\right]. \tag{1.8}$$

Numerical data are as follows (energy is given in $\frac{c\mu b^2}{8\pi}$ – units):

| $\nu$ | 0 | 1/3 | | $\nu$ | 0 | 1/3 | 1/2 |
|---|---|---|---|---|---|---|---|
| $W_1^0$ | 0.350 | 1.030 | 1.711 | $W_2^0$ | 1.304 | 0.750 | 0.296 |
| $\Delta W_1$ | −0.074 | −0.137 | −0.403 | $\Delta W_2$ | −0.117 | −0.074 | −0.032 |
| $W_1^0+\Delta W_1$ | 0.276 | 0.893 | 1.308 | $W_2^0+\Delta W_2$ | 1.187 | 0.676 | 0.264 |

It is seen that the dispersion diminishes the values of self-energy. Putting $\nu = 1/3$, which corresponds to typical crystals, we obtain: $\Delta W/W_0 \approx 10\%$.

If we did not restrict ourselves to weak-dispersion crystals, the effect indicated might be much more apparent.

Now, let us turn to the extension dependence. The following approximate formula is valid for the values of the extension parameter which are of physical significance:

$$\begin{aligned} W_1^\zeta &= W_1^0 \cdot R_\zeta + \frac{c\mu b_1^2}{8\pi}(1-R_\zeta)\left\{\left[\frac{\ln(4\zeta^2+1)}{2\zeta}+\frac{1}{2\zeta}\right]\frac{1}{1-\nu}-\frac{1}{\zeta}\right\}, \\ W_1^\zeta &= W_2^0 \cdot R_\zeta + \frac{c\mu b_2^2}{8\pi}(1-R_\zeta)\left\{\left[\frac{\ln(4\zeta^2+1)}{2\zeta}+\frac{1}{2\zeta}\right]-\frac{\pi^2}{96\zeta}-\frac{1}{1-\nu}\cdot\frac{1}{\zeta}\right\}, \end{aligned} \tag{1.9}$$

where $R_\zeta = 1/2\zeta$, $\zeta = \tilde{\zeta}/c$.

We do not insert a graphical picture of $W(\zeta)$, because $\zeta$, like $\mu$ and $\nu$, is a medium-dependent quantity. To calulate $W$ for a given $\zeta$, we have to put appropriate values of $\mu$ and $\nu$ in the energy expression instantaneously. However, it is possible to compare the energy values of the extended and non-extended dislocation, in the same medium. For example, we have:

$$\begin{aligned} &\text{for Cu:} \quad W_1^\zeta = 0.096\ \text{eV} \quad \text{and} \quad W_1 = 0.161\ \text{eV}, \\ &\text{for Al:} \quad W_1^\zeta = 0.140\ \text{eV} \quad \text{and} \quad W_1 = 0.158\ \text{eV}. \end{aligned}$$

It is seen that the self-energy depends markedly on the extension. It can be disregarded only when $\tilde{\zeta} < b$; that is the case, for example, for Fe and Si. For most crystals, the parameter $\tilde{\zeta}$ is much larger than $b$, and the extension has to be taken into account, even in an abrupt kink model. The values of self-energy calculated from the formula (1.9) are larger than experimental data. This discrepancy is due to the width of a kink having been overlooked.

Let us put $\lambda > c$. We obtain the following expressions for the self-energy of a kink on the screw ($W_1$) and edge ($W_2$) dislocations, respectively:

$$\begin{aligned} W_1^\lambda &= \frac{c\mu b_1^2}{8\pi}\left\{R_\lambda\left[\frac{1.488}{1-\nu}-1.131\right]+(1-R_\lambda)\left[\frac{\ln(4n^2+1)}{(1-\nu)2n}-\frac{\ln(4n^2+1)+2}{4n}\right]\right\}, \\ W_2^\lambda &= \frac{c\mu b_2^2}{8\pi}\left\{R_\lambda\left[2.263-\frac{0.935}{1-\nu}\right]+(1-R_\lambda)\left[\frac{\ln(4n^2+1)+2}{2n}-\frac{2\ln(4n^2+1)+3}{(1-\nu)8n}\right]\right\}, \end{aligned} \tag{1.10}$$

$$
\begin{aligned}
\Delta W_\lambda^1 &= -\frac{c\mu b_1^2}{8\pi}\left\{R_\lambda\left[\frac{0.254}{1-\nu}-0.205\right]+(1-R_\lambda)\left[\frac{\pi^2}{48n}\cdot\frac{1}{1-\nu}-\frac{\pi^2}{96n}\right]\right\},\\
\Delta W_\lambda^2 &= -\frac{c\mu b_2^2}{8\pi}\left\{R_\lambda\left[0.411-\frac{0.334}{1-\nu}\right]+(1-R_\lambda)\left[\frac{\pi^2}{48n}-\frac{1}{1-\nu}\frac{\pi^2}{864n}\right]\right\},
\end{aligned}
\tag{1.11}
$$

where $n = \lambda/c$ and $\Delta W$ denote additional dispersion-terms. The $n$-dependence of $W_1$ and $W_2$ is visualized in Tables 1, 2 and in diagrams 1, 2.

**Table1**

| $n$ | $W_1(\nu)$ | $W_1$ | | |
|---|---|---|---|---|
| | | $\nu = 0$ | $\nu = \frac{1}{3}$ | $\nu = \frac{1}{2}$ |
| 10 | $\frac{0.394}{1-\nu}-0.250$ | 0.144 | 0.341 | 0.538 |
| 15 | $\frac{0.301}{1-\nu}-0.184$ | 0.117 | 0.266 | 0.420 |
| 20 | $\frac{0.243}{1-\nu}-0.146$ | 0.097 | 0.220 | 0.340 |
| 25 | $\frac{0.206}{1-\nu}-0.121$ | 0.085 | 0.188 | 0.291 |
| 30 | $\frac{0.177}{1-\nu}-0.104$ | 0.073 | 0.161 | 0.250 |
| 35 | $\frac{0.157}{1-\nu}-0.091$ | 0.066 | 0.144 | 0.223 |
| 40 | $\frac{0.141}{1-\nu}-0.081$ | 0.060 | 0.130 | 0.201 |
| 50 | $\frac{0.117}{1-\nu}-0.067$ | 0.050 | 0.108 | 0.167 |
| 60 | $\frac{0.100}{1-\nu}-0.058$ | 0.042 | 0.092 | 0.142 |
| 70 | $\frac{0.088}{1-\nu}-0.050$ | 0.038 | 0.078 | 0.126 |
| 80 | $\frac{0.077}{1-\nu}-0.045$ | 0.033 | 00.070 | 0.109 |
| 90 | $\frac{0.071}{1-\nu}-0.040$ | 0.030 | 0.066 | 0.101 |
| 100 | $\frac{0.065}{1-\nu}-0.037$ | 0.028 | 0.060 | 0.093 |

**Table 2**

| $n$ | $W_2(\nu)$ | $W_2$ | | |
|---|---|---|---|---|
| | | $\nu = 0$ | $\nu = \frac{1}{3}$ | $\nu = \frac{1}{2}$ |
| 10 | $0.498 - \frac{0.226}{1-\nu}$ | 0.272 | 0.159 | 0.046 |
| 15 | $0.371 - \frac{0.170}{1-\nu}$ | 0.201 | 0.116 | 0.031 |
| 20 | $0.292 - \frac{0.134}{1-\nu}$ | 0.158 | 0.091 | 0.024 |
| 25 | $0.242 - \frac{0.112}{1-\nu}$ | 0.132 | 0.074 | 0.018 |
| 30 | $0.208 - \frac{0.096}{1-\nu}$ | 0.112 | 0.064 | 0.016 |
| 35 | $0.182 - \frac{0.085}{1-\nu}$ | 0.097 | 0.056 | 0.012 |
| 40 | $0.163 - \frac{0.076}{1-\nu}$ | 0.087 | 0.049 | 0.011 |
| 50 | $0.134 - \frac{0.062}{1-\nu}$ | 0.072 | 0.041 | 0.010 |
| 60 | $0.115 - \frac{0.054}{1-\nu}$ | 0.061 | 0.034 | 0.008 |
| 70 | $0.101 - \frac{0.047}{1-\nu}$ | 0.054 | 0.030 | 0.007 |
| 80 | $0.090 - \frac{0.042}{1-\nu}$ | 0.048 | 0.027 | 0.006 |
| 90 | $0.081 - \frac{0.038}{1-\nu}$ | 0.043 | 0.024 | 0.005 |
| 100 | $0.074 - \frac{0.035}{1-\nu}$ | 0.039 | 0.022 | 0.004 |

If we have experimental values of self-energy and the coefficients $\mu, \nu$ for a given medium, then the Table above enables us to determine the width of a kink in an arbitrary crystal. Then, we can find the full energy of interactions between kinks in any material (the dependence of interaction energy of the kink width will be discussed in the next chapter).

The self-energy values calculated above are positive in the regions of physical significance of all parameters appearing in the energy expression. Let us observe that the maximum of the energy corresponds to the abrupt-kink model. This special case has been studied by several authors. If the extension of a line is taken into account, the energy values decrease. If $\lambda \to \infty$, then $W \to 0$. This is one more reason not to treat kinks as segments of a straight dislocation line: if we had done so, then we would have obtained $W \to \infty$, when $\lambda \to \infty$.

$W_1$ and $W_2$ depend on $\nu$ in a different fashion: $W_1$ is an increasing function of $\nu$, and $W_2$ — a decreasing one. This reflects the fact that kinks are "fastened" to straight-line segments of dislocations.

Let us consider now the expression $W_1^0$ [cf. (1.7)] which describes the energy of a kink on a screw, dislocation. The second term corresponds precisely to the "fastening" effect. It does not depend on $\nu$, in the same manner as the energy of screw dislocations does not depend on $\nu$. When $\nu$ increases, then the first term increases as well and the second one remains constant; in consequence, $W_1^0$ is an increasing function of $\nu$.

The expression $W_2$ [cf. formulae (1.7)] describes the energy of a kink on an edge-dislocation. In $W_2$ only the second term depends on $\nu$. The first term is constant (it describes the behaviour of a kink as a piece of a screw dislocation line). Thus, the second term is responsible for the "fastening", effect. In fact, the kink is then fastened to the edge dislocation, the energy of which depends on $\nu$ (it increases with increasing $\nu$). The second increasing term is subtracted from the constant first term, and finally, $W_2^0$ is a decreasing function of $\nu$. It is very essential that $W_2^0$ depends in some way on $\nu$. A consequence of this dependence is that it is impossible to treat a kink as a segment of a straight dislocation line.

$W_1$ and $W_2$ depend markedly on $\nu$. Hence it is impossible to state in general which of these quantities is larger (as a matter of fact they are almost equal). Hence, in typical crystals, the self-energy values of kinks on screw and edge dislocations, differ by about 10%.

## 2. The interaction energy of two kinks

Let us investigate now the interaction, energy. It is given by:

$$(2.1)\qquad W = \frac{1}{4\pi^3}\int d_3\mathbf{k}\,\chi^2(k^2)[b_1^2 A_1(\mathbf{k}) + b_2^2 A_2(\mathbf{k})]\int\int e^{ik_2[y(x)-y(x')]}y'(x)y'(x')\times$$
$$\times[\sin 2k_1 a \sin k_1(x+x'-\lambda) - \cos 2k_1 a \cos k_1(x+x'-\lambda)]\,dx\,dx'.$$

Now, we represent this expression as a one-dimensional Fourier transform of some function of $k_1$:

$$W = W(a) = \int [f_1(k_1)\sin 2k_1 a + f_2(k_1)\cos 2k_1 a]\,dk_1.$$

Let us change the integration variables. In spherical coordinates we have:

$$k_1 = k\cos\theta, \quad k_2 = k\sin\theta\cos\varphi, \quad k_3 = k\sin\theta\sin\varphi$$
$$dk_1\,dk_2\,dk_3 = k^2\sin\theta\,dk\,d\theta\,d\varphi$$

and a is the first component of the vector $\mathbf{a} = [a, 0, 0]$. In such a coordinate system, $\cos 2k_1 a$ depends on $k$ and $\theta$ only, and is evidently independent of $\varphi$. Substituting $A_1$ and $A_2$ as in 1.1 and expanding the integrand of (2.1) nearly $k = 0$, we obtain an expression which can be explicitly integrated in the variables $\theta$ and $\varphi$. The integrand depends then on $k$ only and the whole integral becomes the one-dimensional Fourier transform $W(a)$:

$$W(a) = \int [\sin 2ka f_1(k) + \cos 2ka f_2(k)]\,dk.$$

The point $k = 0$ is the only singularity of the integrand; this justifies our expansion nearly $k = 0$. To calculate $W(a)$ we shall make use of the following Lighthill theorem (1962) [5]: Let us assume that:

— a distribution $f(x)$ possesses a finite number of singularities $x_1, \ldots, x_M$;

— for arbitrary $m$, the $N$-th derivative of $f(x)-F_m(x)$ is absolutely integrable in any interval containing $x_m$; $F_m$ is a linear combination of distributions: $|x-x_m|^\beta$, $|x-x_m|^\beta \times \operatorname{sgn}(x-x_m)$, $|x-x_m|^\beta \log|(x-x_m)|$, $|x-x_m|^\beta \log(x-x_m)\operatorname{sgn}(x-x_m)$ and $\delta^{(p)}(x-x_m)$ for some values of $\beta$ and $p$;

— $f^N(x)$ is good-behaving at infinity.

Then:

The Fourier transform of $f(x)$ satisfies the following equation:

$$g(y) = \sum_{m=1}^{M} G_m(y) + o(|y|^{-N}), \quad \text{when} \quad |y| \to \infty.$$

In the above equation, $g(y)$ is a Fourier transform of $f(x)$ and $G_m(y)$ are Fourier transforms of $F_m(x)$.

All the values of integrals appearing in the interaction energy expression are collected in the Table below. The integrands are written in the first column. The subsequent columns contain three-dimensional integrals of these functions — i.e. the angular integrals followed by $k$-integrals. Their values are as Table 3.

**Table 3**

| $f(\mathbf{k})$ | $\int f(\mathbf{k})d_3\mathbf{k}$ | $\int f(\mathbf{k})k^2 d_3\mathbf{k}$ | $\int f(\mathbf{k})k_1^2 d_3\mathbf{k}$ | $\int f(\mathbf{k})k_2^2 d_3\mathbf{k}$ |
|---|---|---|---|---|
| $\frac{1}{k^2}\cos 2k_1 a$ | $\frac{\pi^2}{a}$ | 0 | $-\frac{\pi^2}{2a^3}$ | $\frac{\pi^2}{4a^3}$ |
| $\frac{k_3^2}{k^4}\cos 2k_1 a$ | $\frac{\pi^2}{2a}$ | $\frac{\pi^2}{4a^3}$ | $-\frac{\pi^2}{4a^3}$ | $\frac{\pi^2}{8a^3}$ |
| $\frac{k_2^2\cos 2k_1 a}{k^2(k_2^2+k_3^2)}$ | $\frac{\pi^2}{2a}$ | 0 | $-\frac{\pi^2}{4a^3}$ | $\frac{3\pi^2}{8a^3}$ |
| $\frac{k_2^2 k_3^2\cos 2k_1 a}{k^2(k_2^2+k_3^2)^2}$ | $\frac{\pi^2}{8a}$ | 0 | $-\frac{\pi^2}{16a^3}$ | $\frac{\pi^2}{32a^3}$ |
| $\frac{k_2^2 k_3^2\cos 2k_1 a}{k^4(k_2^2+k_3^2)}$ | $\frac{\pi^2}{8a}$ | $\frac{\pi^2}{16a^3}$ | $-\frac{\pi^2}{16a^3}$ | $\frac{\pi^2}{16a^3}$ |

More strictly, all expressions in the Table above should be multiplied by $\operatorname{sgn} a$. However, we restrict ourselves to positive values of a only; hence there is no need to insert this factor.

The full interaction energy (up to $1/a^3$ — terms) is as follows:

$$W = -\frac{c^2\mu}{8\pi(1-\nu)}\frac{1}{2a}[b_1^2(1+\nu)+b_2^2(1-2\nu)] + \frac{c^4\mu}{96\pi(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2(3\nu-1) + b_2^2\frac{1}{2}(1-4\nu)\Big] + \frac{c^2\lambda^2\mu}{12\pi(1-\nu)}[b_1^2(1+\nu)+b_2^2(1-2\nu)]\frac{1}{(2a)^3} + \frac{c^4\mu}{48\pi(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2-\frac{1}{4}b_2^2\Big] + \frac{c^4\zeta^2\mu}{24\pi(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2(3\nu-1)+\frac{1}{2}b_2^2(1-4\nu)\Big]. \tag{2.2}$$

Restricting ourselves to $1/2a$ — terms only, we obtain:

$$W_0 = -\frac{c^2\mu}{8\pi(1-\nu)}\frac{1}{2a}[b_1^2(1+\nu)+b_2^2(1-2\nu)] \tag{2.3}$$

(in the first-order of approximation).

Let us classify separately terms occurring in (13) as regards their physical meaning: The characteristic abrupt-kink term:

$$W_k = \frac{c^4\mu}{96\pi(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2(3\nu-1)+\frac{1}{2}b_2^2(1-4\nu)\Big]. \tag{2.4}$$

The term which takes into account the finite width of a kink:

$$W_\lambda = \frac{c^2\lambda^2\mu}{12\pi(1-\nu)}\frac{1}{(2a)^3}[b_1^2(1+\nu)+b_2^2(1-2\nu)]. \tag{2.5}$$

The dispersion term:

$$W_d = \frac{c^4\mu}{48\pi(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2-\frac{1}{4}b_2^2\Big] \tag{2.6}$$

More generally, $W_d$ has the form:

$$W_d = -\frac{c^2\mu\alpha''(0)}{4\pi(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2-\frac{1}{4}b_2^2\Big]. \tag{2.6}$$

The extension of line-term:

$$W_r = \frac{c^4\zeta^2\mu}{24(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2(3\nu-1)+b_2^2\frac{1}{2}(1-4\nu)\Big]. \tag{2.7}$$

The term $W_\lambda$ in the Eq. (2.5) has been calculated for a kink which was described by a linear function: $y(x) = c(1-x/\lambda)$. When the shape of a kink is given by the arbitrary function $y(x)$, then:

$$W_\lambda = \frac{\mu C_\lambda}{2\pi(1-\nu)}\frac{1}{(2a)^3}\Big[b_1^2(1+\nu)+b_2^2(1-2\nu)\Big], \tag{2.8}$$

where:

$$C_\lambda = \int_{-\infty}^{\infty}\int \eta'(x)\eta'(x')\,(x+x')^2\,dx\,dx', \qquad \eta'\Big(x-\frac{\lambda}{2}\Big) \overset{\text{df}}{=} y'(x).$$

We did not insert into the Table above, the function integrated with $\sin 2k_1 a$, because in a linear approximation we have:

$$\int\int y'(x)y'(x')e^{ik_2[y(x)y(x')]}\sin k_1(x+x'-\lambda)dx\,dx' = 0.$$

More generally, for arbitrary symmetric kink i.e. such that

$$\int_0^{\lambda/2} y(x)dx = \int_{-\lambda/2}^{0} y(x)dx),$$

the integral referred to also vanishes. One can expect that "sinusoidal" terms give rise to the interaction energy of non-symmetric kinks. However, the lowest order of approximation sensitive to these corrections is $a^{-4}$. That is why we disregard them.

Obviously, the term $W_0$, proportional to $a^{-1}$, makes the main contribution to the interaction energy. Let us bear in mind that our investigation applies to great distances only — i.e. to large values of $a$. Nevertheless, let us estimate the critical value of $a$, at which $2a^{-3}$ — term become equal to $a^{-1}$ — term. Let us start with the simplest case of abrupt-kink a non-dispersive medium (i.e. we neglect terms $W_d$, $W_r$, $W_\lambda$)

$$W_1 = -\frac{c^2\mu b_1^2}{8\pi}\frac{1}{2a}\frac{1+\nu}{1-\nu} + \frac{c^4\mu b_1^2}{96\pi}\frac{1}{(2a)^3}\frac{3\nu-1}{1-\nu},$$

(2.9)

$$W_2 = -\frac{c^2\mu b_2^2}{8\pi}\frac{1}{2a}\frac{1-2\nu}{1-\nu} + \frac{c^4\mu b_2^2}{192\pi}\frac{1}{(2a)^3}\frac{1-4\nu}{1-\nu};$$

$W_1$ and $W_2$ correspond to the screw and edge dislocations, respectively. It is seen that, as in the case of self-energies, $W_1$ is an increasing function of $\nu$, and $W_2$ — a descreasing one (it decreases to zero when $\nu = 1/2$). This last phenomenon is well known in the theory of elasticity. An abrupt-kink is then described as a segment of a straight-line screw dislocation, whose Burgers vector is $\mathbf{b}_2$. Consequently, $W_2$ then describes an interaction of two segments of parallel screw dislocations. The critical values of a distance between kinks are then as follows:

$$2a_1 = \frac{c}{2}\sqrt{\frac{3\nu-1}{3(1+\nu)}}, \qquad 2a_2 = \frac{c}{2}\sqrt{\frac{1-4\nu}{6(1+\nu)}}.$$

The maximal values of $2a_1$ and $2a_2$ are equal to $c/6$ and $c/2\sqrt{6}$, respectively. Both of them are situated far below the limits of applicability of our approximation: $a/c \gg 1$. It is of interest that both the terms of $W_1$ have the same sign for $\nu < 1/3$. Similarly, $W_2$ behaves in such a way when $\nu > 1/4$. Obviously, when we consider the case of large $a$, the phenomenon referred to is not very important because in $W_1$ and $W_2$ the second terms are much smaller than the first ones. Consequently, an interaction of abrupt kinks in non-dispersive medium is described by (2.3). This expression agrees with the results of BRAILSFORD [3] and that of KROUPA and BROWN [2]. Their approach was based on the elastic medium theory.

Let us investigate now an extended kink of width $\lambda$, on a dislocation line in non-dispersive medium:

$$W = -\frac{c^2\mu}{8\pi(1-\nu)}\frac{1}{2a}[b_1^2(1+\nu)+b_2^2(1-2\nu)]+\frac{c^2\lambda^2\mu}{12\pi(1-\nu)}\frac{1}{(2a)^3}[b_1^2(1+\nu)+b_2^2(1-2\nu)].$$

The critical distance for the screw and edge dislocations is $2a = \lambda\sqrt{2/3}$. But the definition of distance between kinks implies that $2a > \lambda$. Consequently, that result is outside the physical interest. Nevertheless, it does not seem justified to omit the second term, especially, when it is desired to be precise. In fact, if $\lambda/c \gg 1$, then the second term at distances of a few $\lambda$ diminishes the interaction energy by 10–20 per cent.

The dispersion does not modify anything significantly; the critical value of $a$ is situated below the limit of applicability of our approximation. It is of interest, however, that $W_{2a}$ is negative, and, consequently, it is added to $W_0$. Therefore, there is no critical distance at all and the kinks always attract one another.

Now, let us take into account the extension of dislocation. In the interest of simplicity we investigate the abrupt-kink a non-dispersive medium.

In the case of screw dislocation, we have:

$$W_1 = -\frac{c^2\mu b_1^2}{8\pi}\frac{1}{2a}\frac{1+\nu}{1-\nu}+\frac{c^4\zeta^2\mu b_1^2}{24\pi}\frac{1}{(2a)^3}\frac{3\nu-1}{1-\nu}.$$

The critical distance does exist provided $\nu > 1/3$, and equals:

$$2a_1 = \tilde{\zeta}\sqrt{\frac{3\nu-1}{3(1+\nu)}}.$$

Hence it is very small in typical, real media — in the case Ag, for example, it equals $1.2c$ (It happens that $\nu < 1/3$ in crystals with large values of $\tilde{\zeta}$, of order 40b).
The energy of edge dislocation is as follows:

$$W_2 = -\frac{c^2\mu b_2^2}{8\pi}\frac{1}{2a}\frac{1-2\nu}{1-\nu}+\frac{c^4\zeta^2\mu b_2^2}{48\pi}\frac{1}{(2a)^3}\frac{1-4\nu}{1-\nu}.$$

The critical value does exist, provided $\nu < 1/4$, and is equal to:

$$2a_2 = \tilde{\zeta}\sqrt{\frac{1-4\nu}{6(1+\nu)}}.$$

In the case of Cu, we have, for example: $2a_2 = 23c$ [6]. When we pass over to the general dislocation, the situation becomes much more complicated. Although there exists a critical distance for the term proportional to $b_1^2$, this is not the case for term proportional to $b_2^2$. If $\nu < 1/4$ or $\nu > 1/3$, then the very existence of critical distance depends markedly on the relative direction od **b** with respect to the dislocation line.

If $1/4 < \nu < 1/3$, then the critical distance does not exist at all. Consequently, the interaction energy increases when the line-extension is taken into account. In the screw and edge cases the $\nu$-dependence of energy is different: the interaction energy of screw dislocations is an increasing function of $\nu$, and that of edge dislocations — a decreasing one.

In the limit-case, when $\nu = 1/2$, the first term, proportional to $(2a)^{-1}$, vanishes, and the energy of edge dislocation is as follows:

$$W_2 = -\frac{c^4\zeta^2\mu b_2^2}{24\pi}\frac{1}{(2a)^3} - \frac{c^4\mu b_2^2}{96\pi}\frac{1}{(2a)^3} - \frac{c^4\mu b_2^2}{96\pi}\frac{1}{(2a)^3} = W_r + W_d + W_k.$$

However, this possibility is somewhat abstract and academic, because our model is applicable to crystals only, where $0.2 < \nu < 0.4$

Finally, at large distances, we have the following estimation of the interaction energy as Eq. (2.3).

The expression (2.3) depends on the height of a kink and on elastic material constants only. For small distances, the shape parameters of a kink and the material parameters should be taken into account, because they may modify the energy significantly. It is known that the most probable distance at which double kinks are created equal 20b [7]. The continuation of the process depends precisely on the interaction energy of kinks. At such small distances the formula (2.3) is useless; rather the general formula (2.4) should be used.

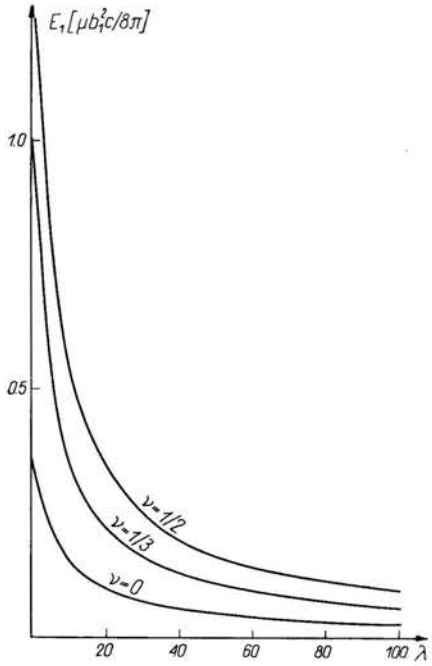


FIG. 1.

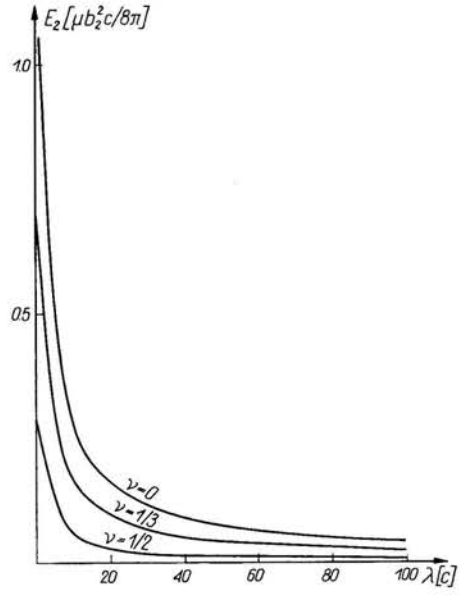


FIG. 2.

**Acknowledgement**

The author is greatly indebted to Dr. D. ROGULA for his encouragement in this work, valuable critical suggestions and many fruitful discussions.

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*Received January* 29, 1973.