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On static helical instabilities of screw dislocations in a SmA phase and on their consequence on plasticity

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Abstract. — The stability of a screw dislocation in a SmA phase submitted to a dilative or compressive strain normal to the layers is investigated. It is shown that the screw line transforms to a helical line, whose handedness depends on the signs of the Burgers' vector and of the strain. For small strains the process necessitates some activation energy; there is a critical strain above which it is spontaneous. Some consequences are proposed, like: a) the nucleation of edge dislocation lines in the so-called undulation instability, and b) the easy crossing without pinning of edge and screw dislocation lines. The analysis stays entirely in the limit of linear elasticity, and it is proposed that interesting non-linear phenomena should appear for high strain values.

1. Introduction. — This note is devoted to the study of the static instability of a screw dislocation in a SmA phase, when the layers that this dislocation traverses are submitted to a constant tension or compression $\gamma = \frac{\partial u}{\partial z} (u(z) \text{ is the displacement function of the layer at level } z)$. Situations with a quasi-constant tension or compression have already been studied:

a) A perfect homeotropic SmA sample in tension displays the so-called undulation instability [1]; what will be the role of screw dislocations which can be thought of as being extremely numerous, since their line energy is so small [2].

b) It can be shown theoretically [3] and it has been observed experimentally [4] that in a wedge of layered matter, edge dislocations form a stable tilt wall in the middle plane of the wedge. These dislocations are surrounded by zones alternatively in tension and compression; which shape will the neighbouring screw lines take, and how will they interact with the edge lines? Some recent observations by one of us (L.B.) seem to indicate that edge dislocation lines can move in the middle plane (under the influence of a thermal gradient; this motion is a climb) without changing shape (they remain straight although they cross a presumably large number of screw dislocations), which fact seems to demonstrate a weak interaction between screw and edge lines.

Let us depict briefly the situation we are going to study and the results we shall obtain: one considers a specimen (thickness $d$) bounded by parallel rigid
walls with strong anchoring homeotropic conditions (Fig. 1). Let us call $a$ the algebraic displacement of the walls ($d \to d + a$) corresponding to an homogeneous dilatation $\gamma = \partial u/\partial z = a/d$. Let us assume that the screw dislocation, which is supposed to be strongly pinned to the rigid walls, changes its shape under the effect of $\gamma$. We shall assume that such a change in shape can be analysed as a linear superposition of helices $z = b_3 z/2$, where $b_3$, the algebraic pitch of the helix, takes any value $d/p$ ($p$ positive : right-handed helix ; $p$ negative : left-handed helix). Then it can be shown that the variation in energy of the screw line contains three contributions :

- two positive contributions due to the increase in length of the line

$$d \to l = d \left(1 + \frac{4 \pi^2 r^2}{b_3^2}\right)^{1/2} \approx d \left(1 + \frac{2 \pi^2 r^2 p^2}{d^2} + \cdots\right)$$

($r$ is the radius (small compared to $b_3 = d/p$) of the helix), viz. : a contribution $W_1$ related to the long distance distortions of the edge and screw components of the line, and a supplementary core contribution $\Delta W_c$ proportional to $2 \pi^2 r^2 p^2 / d^2$ in a first approximation ;

- a contribution $W_2$ due to the interaction with the rigid boundaries (more precisely, the work on the cut surface of the helical line done by the stresses induced by the boundary displacement $a$).

The complete calculation of $W_1$, $W_2$ and $\Delta W_c$ is given below (paragraphs 2 and 3). Line tension of a screw line is calculated and nucleation of helices in relationship with points a) and b) mentioned above is discussed in paragraph 4. All the calculations assume linear elasticity. Note that the transformation of screw lines to helices and the formation of edge dislocation loops is well known in solid crystals [5]. Conclusions are drawn in paragraph 5.

2. The method of calculation. — The method of calculation for $W_1$ and $W_2$ has been introduced by Kléman [2].

Let us briefly recall the method : we first consider a medium submitted at point $r$ to an unit force directed along the $z$ direction. This force gives rise at any point $r'$ to a displacement field $U(r/r')$ which satisfies the equation :

$$- K \Delta^2 U(r/r') + B \frac{\partial^2}{\partial z^2} U(r/r') - \delta(r - r') = 0$$

where

$$\Delta^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)^2$$

and where $K$ and $B$ are the elastic constants of the smectic A phase.

In a finite sample with homogeneous boundary conditions, $U(r/r') = 0$ for $z = \pm d/2$, and the solution of equation (1) can be written

$$U(r/r') = \frac{1}{(2\pi)^3} \sum d \sum \exp(-iq(r - r')) \times$$

$$Kq^4 + B \frac{\pi^2 n^2}{d}$$

$$\times \left[\cos \frac{m\pi}{d}(z - z') - (-1)^p \cos \frac{m\pi}{d}(z + z')\right] d^2 q$$

$$\text{where} \quad r = (x, y, 0) \quad \text{and} \quad q = (q_x, q_y, 0)$$

$U(r/r')$ is a typical even Green function of $(r - r')$.

Any quantity relative to a dislocation in a sample can be derived from the above expression. Especially, the total energy of the configuration can be written under the form

$$W_s = -\frac{\varepsilon}{2} \int \left[d(r) d(r') \Sigma_{13} \Sigma_{13}' U(r/r') dS_i dS'_j\right]$$

(3)

where $\Sigma_{13}$ and $\Sigma_{13}'$ are some differential operators

$$\Sigma_{13} = -K \frac{\partial}{\partial x} A$$

$$\Sigma_{23} = -K \frac{\partial}{\partial y} A$$

$$\Sigma_{33} = B \frac{\partial}{\partial z}$$

$$\Sigma_{13}' = -K \frac{\partial}{\partial x} A' \text{ etc...}$$

The integrations take place over the surfaces on which the imposed displacement is different from zero, viz. :

- the cut surface bounded by the screw line on which $d(r) = d(r') = b$ ; $\varepsilon = 1$ ;
- the rigid boundaries on which $d(r) = d(r') = \pm a/2$ for $z = \pm d/2$ ; $\varepsilon = 2$ (Fig. 1).

After development, equation (3) appears to be a sum of three characteristic integrals $W_1$, $W_2$, $W_3$. $W_1$ is a twofold integration over the cut surface, and can be transformed into a double line integral :

$$W_1 = -\frac{b^2 K B}{2} \int \int \Delta U(r/r') (dx dx' + dy dy')$$

(4)

which is the self-energy of the helical line in the limited sample with fixed boundary conditions [2]. The integration is made twice along the dislocation line,

$$W_2 = -\frac{ab}{2} \int \int \Sigma_{33} \Sigma_{13}' U(r/r') dx dy dS'_i$$

(5)
where \( \Sigma \) is the boundary (displaced by an amount \( a/2 \)) and \( \Sigma' \) the cut surface.

\( W_2 \) can anyway be easily calculated since it is simply the work done on the cut surface of the helical line by the stresses induced by the displacement at the boundary; it can be expressed as a simple surface integral:

\[
W_2 = \frac{Bab}{d} \int dx \, dy
\]

where the integration is done on the oriented projection in the horizontal plane of the cut surface of the helical line; it is always possible, whatever might be the signs of \( a \) and \( b \) (\( b \): Burgers' vector) to choose the chirality of the helix in such a way that \( W_2 \) is negative

\[
W_2 = -p \pi a^2 \frac{B}{d} |ab|
\]

and one can show that this result is obtained when the dislocation line spirals with the same helicity as the layers around the screw dislocation line when \( a \) is negative (in compression), and with the opposite helicity when \( a \) is positive (in tension). This is easy to understand: when \( a \) is negative, a spiralling of the dislocation line with the same helicity as the layers pushes the extralayer outside the cylindrical domain limited by the helical line, and vice versa:

\[
W_3 = \pm a^2 \int \Sigma_{33} \Sigma'_{33} U(r') \, dx' \, dy' \quad (7)
\]

is the work of the applied stress which displaces the boundary. This quantity does not depend on the dislocation's configuration and we need not to calculate it.

We have also to add to \( W_5 \) the variation of the core energy \( \Delta W_c \) between the helix and the straight screw dislocation.

This energy is not known precisely. Since we are dealing with a liquid phase, it is difficult to imagine a hollow core in the screw dislocation. The centre of the dislocation can be full of matter. The core energy per unit length of dislocation \( \varepsilon \) is given by:

\[
w_c = F \pi r_e^2
\]

\( F \) being an energy per unit volume and \( r_e \) the core radius.

For example, if the core is isotropic:

\[
F = k_n \Delta T_c \frac{1}{v}
\]

\( v \) being the molecular volume.

\( \Delta T_c \) is the difference of temperature from that of the transition Sm \( \rightarrow \) I.

Thus, for the increase in the core energy of the line, one obtains, for \( r \ll d \):

\[
\Delta W_c = 8 \pi^4 2 \pi^2 r_e^2 p^2 \frac{d}{d}
\]

The total energy of the line is then given by:

\[
W_T = W_1 + W_2 + \Delta W_c.
\]

3. Results of calculations. — The energy \( W_1 \) given by equation (4) can be transformed to the following non-dimensional expression (see Appendix):

\[
W_1' = \frac{W_1}{b^2 K \lambda} = \frac{r'^2}{4} \int_0^\infty dk' \int_0^{\infty} du \frac{\cos 2pu}{\sinh k' \pi} \times
\]

\[
\times \int_0^{2k'/\pi} \left( u \cosh k' u - \frac{\sinh k' u}{k'} \right) \quad (9)
\]

with \( \lambda = \sqrt{K/B} \).

\( r' \) and \( k' \) being dimensionless parameters given by

\[
r' = r \quad (10)
\]

\[
k' = d \lambda q^2/\pi \quad (11)
\]

where \( q \) is the reciprocal of a length in a plane perpendicular to the screw dislocation line. A cut-off value \( k'_c \) has to replace the infinite value in the integration range of \( k' \) because the integral diverges:

\[
k'_c = 4 \pi d \lambda r_e^2
\]

where \( r_e \) is the core radius introduced above.

An upper limit of \( W_1' \) can be found by using the inequality

\[
0 < \frac{1}{\sinh k' \pi} \left( u \cosh k' u - \frac{\sinh k' u}{k'} \right) < \pi
\]

which leads to

\[
W_1' < \pi^2 r^2 \int_0^{q_c} J_1^2(qr) \, q \, dq.
\]

The right-hand side for \( p = 1 \) is the elastic energy of a loop in an infinite sample [2].

The energy \( W_1' \) was calculated numerically as a function of \( r' \); the integration was performed on the interval 0.01 < \( k' < k'_c \) for \( p = 1 \) and \( p = 2 \).

Since \( \Delta W_c \) depends on \( k'_c \), we take for \( k'_c \) the value which minimizes the sum \( W_1' + \Delta W_c \).

\[
\Delta W_c = 8 \pi^4 p^2 \left( \frac{F \lambda^2 d}{Kb^2} \right) r_e^2 k'_c.
\]

In practice, we find that \( k'_c \) is independent of \( p \) and depends linearly on \( d \) (we need to know more precisely \( F \) in order to give the proportionality coefficient), which means that the core radius \( r_e \) is practically independent of the sample thickness (eq. (12)). This is a very satisfying result.
Universal curves, independent of the sample thickness, can be obtained when plotting $W_1'$ and $W_1' + \Delta W_c'$ against $r'$ for different values of the parameters $k_c'$ and $p$ (Fig. 2).

3.1 VARIOUS REGIMES OF THE SCREW DISLOCATION.

The dependence of $W_T' = W_1' + W_2' + \Delta W_c'$ on $r'$ for a given value of $k_c'$ and $p$ drastically varies with $a/b$ (Fig. 3).

One can define three behaviours of $W_T'(r')$ depending on $a$:

1) $0 < a < a_c$.

For very small values of $a$, $W_T'$ increases indefinitely with $r'$ and the screw line remains straight; there is a first threshold $a_c$ for which an inflexion point appears on the curve for a given $r'$ (We do not reach these values with our computations, and anyhow we would have to take into account another expression of the core energy valid for large $r'$ for which the dislocation is mostly of edge character.)

2) $a_c < a < a_v$.

$W_T'(r')$ has a maximum $W_{max}$ for $r' = r_0$.

$W_{max}$ is clearly an activation energy for the transformation to the helical shape. This is a regime of nucleation (and ulterior growth). For given values of $k_c'$ and $p$, $W_{max}$ and $r_0$ decrease when $a$ increases. One can define a critical value of $a$, noted $a_c$ for which $W_{max} = 0$.

3) $a > a_c$.

$W_T'$ decreases continuously with $r'$. This is a regime of instability of the screw dislocation.

The final description of the nucleation process cannot be given without comparing the activation times with the characteristic time of the experiment, which will be discussed in the next paragraph.

4. Discussion.

4.1 LINE TENSION OF A SCREW DISLOCATION.

The self-energy $W_1$ of a straight screw line is zero in the approximation we use [2], apart from a core energy term. But the line tension $\tau$ is non-vanishing. It is defined by $(dW_1/dr)_{r=r_0}$, where $l$ is the length of the line of helical shape. The value of $W_1$ for $r$ vanishingly small is easily obtained from equation (9). One gets:

$$W_1 \simeq \frac{2b}{\ln \frac{2\pi \lambda}{pr}}$$

this quantity goes to zero with $r$, as expected.
Now we have
\[ \frac{dl}{dr} = 4 \pi^2 p^2 r \]
hence
\[ \tau = \frac{B b^2}{8} \ln \frac{2 \pi d \lambda}{\rho r_c}. \]

The logarithmic factor appears as a small correction; \( \tau \) has the same form as for a dislocation in a solid [6]; although \( W_t = 0 \), the line tension is large.

One can infer from this expression a natural frequency of vibration of a line oscillating with wavelength \( d \). Similarly to the case of solids, let us attach an effective mass \( m_0 \) to the moving line; this mass, on dimensional arguments, is proportional to \( \rho b^2 \) per unit length. If we now balance the line tension with the forces of inertia, we obtain
\[ \omega \sim c_i/d \]
where \( c_i = \sqrt{B/\rho} \) is the second sound velocity [7]. A typical value of \( \omega \) for \( d = 10 \mu m \) is \( 10^8 \) s\(^{-1} \).

Let us stress that our estimation of \( \omega \) relies on the hypothesis that the vibrational movement of the dislocation line is related to a movement of matter which can be Fourier-analysed in second sound oscillations (transverse acoustical waves). There are also non-dissipative (first sound) longitudinal oscillations in a SmA phase, which have the advantage of being much less anisotropic (\( c_i \) depends in fact drastically on the wave vector) and more rapid. It appears here that a complete knowledge of the vibrational state of the screw dislocation would require to solve the hydrodynamical equations in the absence of dissipation. However, the spectrum will necessarily include the highest frequencies hereabove obtained and probably some corresponding to first sound waves. Note that \( \omega \) is much larger than any frequency related to the relaxation of dissipative modes, like layer undulations \( (\omega_1 \sim K_1/d^2 \sim 10^2 \) s\(^{-1} \)) or permeation \( (\omega_2 \sim B\rho/b^2 \sim 10^{-1} \) s\(^{-1} \)), so that there cannot be any interference between these modes.

We can therefore adopt \( \omega \sim c/d \) as the natural frequency of the line with some confidence, where \( c \) is at least of the order of the maximum velocity of second sound waves.

4.2 NUCLEATION OF HELICES. — The nucleation process requires an activation energy. If we assume that the thermally activated process developed for dislocations in solids [6] is still valid, each screw dislocation, under tension or compression, has a probability to spiral given by:
\[ P_t = \frac{c}{a} \exp \left( -\frac{W_{\text{max}}}{k_B T} \right) \]
where \( k_B \) is Boltzmann's constant.

The time necessary to create an helix (and by the way to relax the local stress by this process) can be estimated as \( t \sim 1/P_t \).

4.3 COMPARISON WITH THE NUCLEATION OF EDGE DISLOCATION LOOPS IN THE ABSENCE OF SCREW DISLOCATION LINES. — The nucleation of edge dislocation loops has been described as a slow process [8]. It would be interesting to compare both processes which have in common the advantage of relaxing plastically stresses applied normally to the layers.

The energy associated with one loop of radius \( r \) is given by:
\[ E = 2 \pi r K_1 - \pi r^2 B \frac{a}{d} b \]
where \( K_1 \) is an energy per unit length of line comparable to a Frank constant \( K \sim 10^{-6} \) dyne.

The energy is maximum for
\[ r^* = \frac{\lambda}{\sqrt{d}} \frac{d}{ba} \]
which corresponds to an activation energy \( E^* \) given by:
\[ E^* = \pi \frac{\lambda^3}{b^4} \frac{d}{a} \cdot \left( \frac{b}{a} \right). \]

Let us study for example both activation energies for a given sample of CBOOA of thickness \( d = 140 \mu m \) under a strain \( a/b = 3 \). For this compound, \( b = 35 \AA \) and \( \lambda = 22 \AA \) at 351 K [9].

The activation energy \( W_{\text{max}} \) for nucleation of an helix is of the order of 0.18. This value is the maximum of the curve \( W_{\text{max}}(r') \) for \( a/b = 3 \) and \( k_c = 3.17 \times 10^4 \) calculated with a core radius \( r_c \) equal to the Burgers' vector \( b \). The activation time is then \( t \sim 10^{-6} \) s, which is very short, while the dimensionless energy \( E^* \) necessary to nucleate a loop is very large, of the order of \( 10^6 \), which corresponds to an infinite activation time. Therefore, the nucleation of an helix is much shorter and can play a role in experiments, if the associated activation times are of the order of the experimental times corresponding to a local relaxation of the stress.

4.4 UNDULATION INSTABILITY [1]. — This mechanical instability is obtained when an homeotropic sample is dilated by a amount \( a \) larger than a critical displacement \( \delta_c = 2 \pi \lambda \). Parallel undulations appear above \( \delta_c \) with a wave number \( q_c = (2 \pi/d\lambda)^{-1} \). They can be imaged directly, or by light scattering; in that case, one can follow the relaxation of the undulations (when the dilative strain is removed) by observing the time of decay of the photosignals. The relaxation time \( \tau \) is of the order of 5 to 10 ms for \( a \sim \delta_c \) and increases linearly in a range of dilation not exceeding a few units of \( \delta_c \) (up to 100 ms) then a new regime of
linear increase appears with a larger slope \( \frac{\partial \gamma}{\partial \alpha} \), corresponding to the appearance of a second series of cross undulations and/or non-linear phenomena [9]. These various relaxation processes are explained in terms of climb of edge dislocations according to [9]. These dislocations are in the form of dipoles elongated along the undulations; they provide the extralayers necessary to relax the stresses created by the undulations.

The existence of screw dislocations and the related helices explains why edge dislocations form so easily. Let us calculate some typical figures related to the experimental results of [9].

i) Let us assume that the nucleation time of an edge dislocation is as high as 100 ms in an undulation instability experiment. According to equation (14) this requires that thermal fluctuations overcome an activation energy \( E^* \) of the order of 2. But the activation energies calculated above for the nucleation of edge loops \textit{ex-nihilo} are much larger (\( \sim 10^4 \)). Therefore the dislocations which relax the undulations cannot nucleate \textit{ex-nihilo} in the short time allowed in this kind of experiment (much shorter than 100 ms, anyway).

ii) Let us take \( a/b \approx 3 \), a value corresponding to a nucleation time for helices of \( \sim 10^{-6} \) s for a sample of thickness \( d \sim 120 \mu m \). This value \( a/b \) is smaller than \( \delta_s \) for the case of CBOOA \( (\delta_s/b = 3.9) \) and HOBHA \( (\delta_s/b = 15.9) \). Therefore lines with edge components exist below \( \delta_s \).

iii) In fact, one reaches the instability of the screw lines \( (a > a_s) \) even before reaching the threshold \( a = \delta_s \) since \( a_s/b = 3.18 \).

4.5 A MECHANISM OF INTERACTION BETWEEN SCREW AND EDGE IN SmA. — The experiment which is related in point b paragraph 1 is made by decreasing the temperature of the specimen. The total effect is that the layer thickness slightly decreases and the edge dislocations move off the edge of the wedge, under the action of a force per unit length \( F = Bb \frac{a}{d} \).

where \( a \) is the displacement of the boundaries equivalent to the layer thickness decrease, \( d \) the specimen thickness. One can relate this force to the velocity \( V \) of the dislocations

\[
F = Bb \frac{a}{d} = \eta \kappa bV
\]

(17)

where \( \eta \) is a viscosity coefficient, \( \kappa \) the inverse of a length of the order of a molecular length [10]. A typical observed velocity is \( V = 50 \mu m/s \), which yields, for a specimen of thickness \( d \sim 100 \mu m \), a value \( a/b \approx 20 \). Other mechanisms than the temperature decrease can induce a movement of the dislocations, and they can also be characterized by a displacement of the boundaries.

The value \( a/b \) is large enough to cause a spontaneous helical instability of the screw dislocations. Let us show that this instability favours an easy crossing of edge and screw dislocations. Assume \( a < 0 \). The helix into which the screw line transforms is equivalent to an edge loop with one layer removed in its interior. Therefore it attracts those edge dislocation lines which are between the screw line and the edge of the wedge, and pushes apart those which are on the other side. This process is probably very effective, because the helix is certainly a little bit flattened in the centre plane of the wedge, due to the image forces which repel edge dislocation segments. Therefore the moving edge dislocation encounters what is more like a small edge loop than a homogeneously twisted helix. We can imagine that this small edge loop is absorbed by the attracted edge dislocation line and detached from the screw line when the interaction changes sign. After the edge dislocation line has passed, a new edge loop nucleates immediately on the screw dislocation line. The whole process favours easy crossing and could be called, as suggested by F. C. Frank, antipinning. Clearly the same effect occurs, with signs reversed for the interactions, when \( a > 0 \). Notice that there is no dependence on the sign of the screw dislocation line considered.

It is interesting to compare this behaviour, characteristic of a SmA phase, with that in the SmC phase. Observations have been made in the same material, the same sample, possessing the two phases (AMC 11) [11]. It is remarkable that the edge lines are strongly pinned on screw lines in the SmC phase. The Young modulus of the SmC phase is practically 100 times smaller than in the SmA phase [12], because of the easy possibility of changing the angle of tilt of the molecules in any deformation involving dilatation or compression of the layers. This effect leads to an effective penetration length \( \lambda_s \) which is practically 10 times larger than in the SmA phase. Therefore the radius \( r^* \) of nucleation of an edge loop \textit{ex-nihilo} is more than 20 times larger than in the SmA phase, which suggests that the nucleation time of an helix from the screw line is extremely long, in other words that this process is not effective in the mutual crossing of the two lines.

5. Conclusion. — The analysis that we have done stays entirely in the limits of the assumption of linear elasticity; moreover even in these limits we neglected the effect of image forces on the helix, by assuming a regular helix. It is easy to see that rigid boundaries are repulsive. Therefore the spiraling elements tend to accumulate in the middle of the specimen and, by a non-linear process that we do not describe, form edge loops. This is certainly not in contradiction with the analysis of crossing we have done above or the analysis of the plastic relaxation of the undulation instability; in that case spirals of quasi-edge character (small pitch) would more easily fill the
troughs of the undulations than spirals whose pitch is comparable to the specimen thickness.

Also, in some circumstances, the edge loops may give rise to small cofocal domains, if they detach from the father-line, and if the strain which has led to the formation of such loops is removed. This may be perhaps more easily seen in well-controlled experiments in compression, during which no undulation instabilities form.

Finally other possibilities might be imagined like

the role of these instabilities in dynamic experiments in alternating strains, in which an effective decrease of the bulk Young modulus is observed, depending on the frequency and particularly visible in low frequencies [13]. This possibility, as well as those which can be imagined coming from non-linear processes, remain to be studied in more detail.

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APPENDIX

The evaluation of the energy $W_1$. — The transformation of the energy $W_1$ which leads from expression (4) to expression (9) consists of the following steps. First, the evaluation of $\Delta U(r/r')$ by using (2) gives

$$- \Delta U(r/r') = \frac{1}{(2\pi)^2} \int \frac{d^2q}{Bn^2} \left[ \frac{q^2 e^{-iqr}}{d^2 [n^2 + k^2]} \left( \cos \frac{n\pi}{d} (z - z') - (1)^r \cos \frac{n\pi}{d} (z + z') \right) \right]. \quad (A.1)$$

The equations of the helical line are

$$x = r \cos \theta, \quad y = r \sin \theta, \quad z = \frac{d}{2p} \frac{\theta}{p} \pi \quad \text{for} \quad -pn < \theta < pn.$$

Using the parameters $\alpha = \frac{\psi}{2p} = \frac{\theta - \theta'}{2p}$ and $\beta = \frac{\varphi}{2p} = \frac{\theta + \theta'}{2p}$ the quantity

$$\sum \frac{\cos \frac{n\pi}{d} (z - z') - (1)^r \cos \frac{n\pi}{d} (z + z')}{Bn^2 \left( n^2 + k^2 \right)}$$

is transformed to [14]:

$$\frac{d^2}{Bn^2} \sum \frac{\cos n\alpha - (1)^r \cos n\beta}{n^2 + k^2} = \frac{d^2}{2Bn\kappa} \frac{\cosh k'(\pi - \alpha) - \cosh k' \beta}{\sinh k' \pi}, \quad k' = \frac{d\lambda q^2}{\pi}. \quad (A.2)$$

The element $dx \, dx' + dy \, dy'$ can be rewritten by using $\varphi$ and $\psi$ as

$$dx \, dx' + dy \, dy' = -\frac{1}{2} \cos \psi \, d\psi \, d\varphi.$$

The limits of integration for $\varphi$ are

$$-\frac{\psi}{2p} + \pi > \frac{\psi}{2p} > -\frac{\psi}{2p} + \pi \quad \text{for} \psi \text{ fixed}.$$

Then the integration over $\psi$ takes place in the interval $0 < \psi < 2 \pi n$. By using (A.1) and (A.2) the energy $W_1$ takes form

$$W_1 = -\frac{Kr^2 b^2 d}{q(2\pi)^3} \int q^3 dq' \, d\theta_\psi \cos \left( 2qr \sin \frac{\psi}{2} \sin \theta_\psi \right) \frac{\cosh k'(\pi - \alpha) - \cosh k' \beta}{\sinh k' \pi} \frac{\cosh k'(\pi - \alpha) - \cosh k' \beta}{\sinh k' \pi} \cos \psi \, d\psi \, d\varphi. \quad (A.3)$$

Integration over $\varphi$ in (A.3) with the relation

$$\frac{1}{2\pi} \int_0^{2\pi} \cos \left( 2qr \sin \frac{\psi}{2} \sin \theta_\psi \right) d\theta_\psi = J_0(2qr \sin \frac{\psi}{2})$$
gives
\[
W_1 = \frac{Kb^2}{8} \frac{r^2}{d^2} p \int \frac{dk'}{\sinh k' \pi} J_0 \left( \frac{2 qr \sin \frac{\psi}{2}}{k'} \right) \left[ (\pi - \alpha) \cosh k' (\pi - \alpha) - \frac{1}{k'} \sinh k' (\pi - \alpha) \right] d\psi \quad (A.4)
\]
with \( q dq = \frac{\pi}{2} \frac{dk'}{\lambda d} \). The substitution \( \pi - \alpha = u \) in (A.4) leads to the expression (9).

References