Self-Energy of a Helical Dislocation*

ROLAND DE WIT†
University of Illinois, Urbana, Illinois
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Kröner's energy expression is used in this theoretical calculation. The helical dislocation is assumed to have a uniform shape with the Burgers vector along its axis. The axial length of the helix is large compared to its radius and the radius is large compared to the dislocation "cross section," which is of the order of a Burgers vector. For a helix of many turns and arbitrary pitch an expansion in a Fourier cosine series is used. The self energy is found in terms of elementary functions and Kapteyn series of Bessel functions. In the limiting cases of a tightly wound helix (small pitch) and a nearly straight helix (large pitch) simple expressions result, which have a plausible physical explanation. For a tightly wound helix the dominant term represents the contribution from the cylindrical part of the helix, the first-order terms represent the influence of the size of the dislocation cross section and the second order terms represent the effect of the axial component of the helix. For the nearly straight helix the dominant terms represent the contribution from the straight screw part and the second-order terms are taken to give the interaction between the turns of the helix. Finally the correction in the self-energy when a return loop is present is considered.

I. INTRODUCTION

THE theoretical possibility of a spiral prismatic dislocation growing from a screw dislocation was first suggested by Seitz.[1] Helical dislocations were first observed in synthetic calcium fluoride crystals by Bontinck and Amelinckx,[2] who pointed out that they were one species of the spiral prismatic dislocations. Amelinckx, Bontinck, Dekeyser, and Seitz[3] discussed a possible interpretation of the developments of these helices. They have since been observed by various methods in various substances by various investigators.[4] A number of results emerge consistently from most of these observations: (1) the axis of the helix is always in the direction of a possible Burgers vector, (2) the helix is usually very uniform, (3) the radius a and the pitch p (Fig. 1) of the helix are of the order of microns and (4) the pitch of various helices varies over a considerable range (almost from zero to infinity).

These results have been utilized in the subsequent calculation. The general uniformity is taken as a starting point, i.e., the dislocation is considered to be wrapped with a constant pitch around a right circular cylinder. Also this uniformity gives us some justification for the use of an isotropic theory. The third result above together with the knowledge that the Burgers vector b is of the order of angstrom units shows that $b \ll a$ or p. This allows us to ignore the atomic structure of the crystal and treat the medium as an elastic continuum in the present calculation.

Weertman[5] gave a theoretical contribution to the field of helical dislocations. He showed that the equilibrium form of a dislocation is a helix, when it is acted upon by an ordinary stress and a chemical stress produced by a deviation of the vacancy concentration from the equilibrium value. In his calculation he used for the line tension or the energy per unit length of the dislocation the simple and constant expression $\frac{1}{2}\mu b^2$. The present paper attempts to present a more refined expression for this quantity.

II. KRONER'S THEORY

A general expression for the interaction energy between two dislocations in an elastically isotropic infinite continuum has been derived by Kröner.[6] His expression consists of a double line integral along the two dislocation lines C and C', where the integrand is a function of the radius vector between the two line elements. It has been argued that the self-energy of a dislocation can be obtained by taking the curves C and C' separated by a distance r_0, corresponding roughly to the half-width of the dislocation, and inserting a factor $\frac{1}{2}$ in Kröner's expression.[7] A good estimate based on the Peierls model is that $r_0 \simeq \frac{1}{2}b$. A more accurate evaluation of the self energy will depend on a good theory of the dislocation core. However, since the final expressions

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† Now at the Department of Mineral Technology, University of California, Berkeley, California.

[1] F. Seitz, in *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1952), Vol. 1, p. 43ff. See especially p. 67.

[2] W. Bontinck and S. Amelinckx, Phil. Mag. **2**, 94 (1957).

[3] Amelinckx, Bontinck, Dekeyser, and Seitz, Phil. Mag. **2**, 355 (1957).

[4] S. Amelinckx in *Dislocations and Mechanical Properties of Crystals*, edited by J. C. Fisher *et al.* (John Wiley & Sons, New York, 1957), p. 40; Amelinckx, Bontinck, and Maenhout-Van der Vorst, Physica **23**, 270 (1957); W. Bontinck, Phil. Mag. **2**, 561 (1957); Barber, Harvey, and Mitchell, Phil. Mag. **2**, 704 (1957); S. Amelinckx and W. Bontinck, Acta Met. **5**, 345 (1957); Amelinckx, Bontinck, and Dekeyser, Phil. Mag. **2**, 1264 (1957); S. G. Ellis, Phil. Mag. **2**, 1285 (1957); D. A. Jones and J. W. Mitchell, Phil. Mag. **3**, 1 (1958); S. Amelinckx, Acta Met. **6**, 34 (1958); W. C. Dash, Bull. Am. Phys. Soc. Ser. II, **3**, 106 (1958); W. C. Dash, in *Growth and Perfection of Crystals*, edited by R. H. Doremus *et al.* (John Wiley & Sons, New York, 1958), p. 361; A. G. Tweet, J. Appl. Phys. **29**, 1520 (1958); W. C. Dash, Phys. Rev. Letters **1**, 400 (1958).

[5] J. Weertman, Phys. Rev. **107**, 1259 (1957).

[6] E. Kröner, Ergeb. angew. Math **5**, (1958). See especially p. 78.

[7] Roland de Wit, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1959), Vol. 10, p. 249.

of this paper depend only logarithmically on r_0, the uncertainty in this quantity is not very important.

For the present problem it is convenient to use a cylindrical coordinate system (ρ, ϕ, z) with the Burgers vector along the z direction. It has been shown that Kröner's expression then reduces to[8]

$$E_s=\frac{Gb^2}{8\pi}\oint_C\left[-\frac{m+1}{m-1}A_z dz+\frac{m}{m-1}\times(B_\rho d\rho+B_\phi\rho d\phi+B_z dz)\right], \quad (1)$$

$$A_z=\oint_{C'}\frac{dz'}{R}, \quad (2)$$

$$B_\rho=\oint_{C'}\left(\frac{1}{R}+\frac{Z^2}{R^3}\right)(\cos\Phi d\rho'+\sin\Phi\rho' d\phi'),$$

$$B_\phi=\oint_{C'}\left(\frac{1}{R}+\frac{Z^2}{R^3}\right)(-\sin\Phi d\rho'+\cos\Phi\rho' d\phi'), \quad (3)$$

$$B_z=\oint_{C'}\left(\frac{1}{R}+\frac{Z^2}{R^3}\right)dz',$$

$$R^2=\rho^2+\rho'^2-2\rho\rho'\cos\Phi+Z^2, \quad (4)$$

$$Z=z-z',\qquad \Phi=\phi-\phi'. \quad (5)$$

Here G is the modulus of rigidity and m is the reciprocal of Poisson's ratio. A_z is called the z component of the magnetic vector potential and the B's are called the dislocation potentials. It will be noticed that the above integrals are all closed. In the subsequent application to a finite length of helix, however, this condition is violated since the helix then has a beginning and an end. The result is therefore incomplete, but it can be completed by closing the dislocation with a return loop. This will be done at the end of this paper.

III. THE HELICAL GEOMETRY

For the calculation we consider two helices of the same pitch wound on two concentric cylinders of radii a and $(a+r_0)$ whose axes are along the z axis (Fig. 1). The equations of these two curves are given by

$$\rho'=a=\text{const},\qquad z'=p\phi',$$
$$\rho=a+r_0=\text{const},\qquad z=p\phi. \quad (6)$$

From (5) this also gives $Z=p\Phi$. For each turn of the helix we move in the z-direction by a distance $2\pi p$. If there are N turns, its total length L along the z-direction is

$$L=2\pi pN. \quad (7)$$

[8] See reference 7, Appendix.

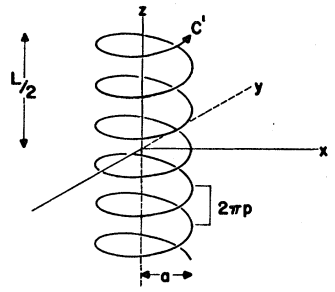

FIG. 1. The helical dislocation.

The above relations (6) give for Eqs. (1), (2), (3), and (4)

$$E_s=\frac{Gb^2}{8\pi}\int_{-\frac{1}{2}L}^{\frac{1}{2}L}\left[-\frac{m+1}{m-1}A_z+\frac{m}{m-1}\left(B_\phi\frac{\rho}{p}+B_z\right)\right]dz, \quad (8)$$

$$A_z=\int_{-\pi N}^{\pi N}\frac{p d\phi'}{R}, \quad (9)$$

$$B_\phi=\int_{-\pi N}^{\pi N}\left(\frac{1}{R}+\frac{p^2\Phi^2}{R^3}\right)\cos\Phi a d\phi',$$
$$B_z=\int_{-\pi N}^{\pi N}\left(\frac{1}{R}+\frac{p^2\Phi^2}{R^3}\right)p d\phi', \quad (10)$$

$$R^2=a^2+\rho^2-2a\rho\cos\Phi+p^2\Phi^2. \quad (11)$$

The integrals (9) and (10) are difficult to perform because the variable of integration ϕ' appears in the integrand under the radical R both as an algebraic function in Φ^2 and as the argument of a trigonometric function in $\cos\Phi$. For their evaluation a hint is taken from the work of Snow[9] who calculated the inductance of a tightly wound helical wire by using the trick of writing the reciprocal radius R^{-1} in his integrals as an integral over a Fourier-Bessel series. For our purposes it is sufficient to look at his expansion as a Fourier series.

The basic idea is that since R in (4) is an even function of Φ, its reciprocal can be expanded in a Fourier cosine series. The Fourier coefficients, which are given in terms of integrals over R^{-1} by Fourier theory, can be inserted in this series, so that we obtain

$$\frac{1}{R}=\frac{2}{\pi}\sum_{n=0}^{\infty}\epsilon_n\int_0^\pi\frac{d\psi\cos n\psi\cos n\Phi}{(\rho^2+\rho'^2-2\rho\rho'\cos\psi+Z^2)^{\frac{1}{2}}},$$

where $\epsilon_0=\frac{1}{2}$ and $\epsilon_n=1$ for $n\geq 1$. Finally the relations (6) can be inserted giving us

$$\frac{1}{R}=\frac{2}{\pi}\sum_{n=0}^{\infty}\epsilon_n\int_0^\pi\frac{d\psi\cos n\psi\cos n\Phi}{Q}, \quad (12)$$

$$Q^2=P^2+p^2\Phi^2,$$
$$P^2=a^2+\rho^2-2a\rho\cos\psi. \quad (13)$$

[9] C. Snow, Bur. Standards Sci. Papers **21**, 431 (1926–27); Bur. Standards J. Research **9**, 419 (1932).

It is seen that this expansion removes from under the radical the trigonometric function of Φ and leaves only an algebraic function, which makes the integrations in (9) and (10) much simpler. This is done, however, at the expense of an additional sum and integral.

IV. EVALUATION OF THE POTENTIAL FUNCTIONS

A. The Vector Potential

If we substitute (12) in (9) and make a slight change of variable we have

$$A_z=\frac{2p}{\pi}\sum_{n=0}^{\infty}\epsilon_n\int_0^{\pi}d\psi\cos n\psi\int_{\phi-\pi N}^{\phi+\pi N}\frac{d\Phi\cos n\Phi}{Q}.$$

We now introduce the first approximation, that there are many turns:

$$N\gg 1. \tag{14}$$

The case where the helix has less than one turn can be treated as a perturbation of a straight line. Under the above approximation it will be seen that the cosine in the denominator of the last integrand will go through many oscillations while the numerator decreases steadily with increasing Φ. Therefore it will be permissible to let the limits of integration go to infinity, except for the first term in the sum which lacks a cosine term. If this is done and the integrals performed we have

$$A_z=\frac{1}{\pi}\int_0^{\pi}d\psi\Big[\ln(p\Phi+Q)\Big]_{\phi-\pi N}^{\phi+\pi N}+\frac{4}{\pi}\sum_{n=1}^{\infty}\int_0^{\pi}d\psi\cos n\psi K_0(nP/p),$$

where K_0 is the modified Bessel function of the second kind and of order zero.

We now introduce the second approximation, that the length of the cylinder on which the helix is wound is much larger than its radius:

$$L\gg a, \tag{15}$$

or by (7) and (13) that $2\pi pN\gg P$. This allows us to evaluate the first integral in A_z above in an approximate way, for the integrand then reduces to

$$\ln[(2\pi pN+2p\phi)(2\pi pN-2p\phi)]-\ln(P^2).$$

To evaluate the series of integrals we use Gegenbauer's addition theorem,[10] which states that

$$K_0[(z^2+Z^2-2zZ\cos\phi)^{\frac{1}{2}}]=2\sum\epsilon_n I_n(z)K_n(Z)\cos n\phi,$$

if $z<Z$, where the sum extends from zero to infinity. I_n and K_n are the modified Bessel functions of the first and second kind. It follows from this expression by integrating and making the appropriate substitutions, using (13) and the relation $a<a+r_0=\rho$, that

$$\frac{1}{\pi}\int_0^{\pi}d\psi\cos m\psi K_0(nP/p)=I_m(na/p)K_m(n\rho/p).$$

So we finally obtain for A_z, after making use of (6) and (7) in the first term,

$$A_z=\frac{1}{\pi}\int_0^{\pi}d\psi\{\ln[(L+2z)(L-2z)]-\ln(P^2)\}+4\sum_{n=1}^{\infty}I_n(na/p)K_n(n\rho/p)$$
$$=\ln[(L+2z)(L-2z)]-2\ln\rho+4S, \tag{16}$$

where we have defined

$$S=\sum_{n=1}^{\infty}I_n(na/p)K_n(n\rho/p). \tag{17}$$

B. The Dislocation Potentials

With the help of the magnetic vector potential A_z found above, it is now relatively easy to evaluate the dislocation potentials B_z by a simple trick. Since from (11) we can write

$$p\frac{\partial}{\partial p}\left(\frac{1}{R}\right)=-\frac{p^2\Phi^2}{R^3},$$

it follows from (9) and (10) that we have between B_z and A_z the relation

$$B_z=2A_z-p\partial A_z/\partial p.$$

If we use (16) in this expression, taking into account the dependence of the first term on p through (6) and (7), we obtain

$$B_z=2\ln[(L+2z)(L-2z)]-4\ln\rho+8S-2-4p\partial S/\partial p. \tag{18}$$

It is possible to evaluate the dislocation potential B_ϕ in (10) by an entirely analogous procedure. The result is

$$B_\phi=\frac{2a^2}{p\rho}+4\frac{p^2}{\rho}\frac{\partial S}{\partial p}-8\frac{a}{p}T+4a\frac{\partial T}{\partial p}, \tag{19}$$

where we have defined

$$T=\sum_{n=1}^{\infty}I_n'(na/p)K_n'(n\rho/p). \tag{20}$$

The I_n' and K_n' represent the derivatives of the Bessel functions with respect to their arguments.

[10] A. Erdélyi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 44.

V. THE SELF-ENERGY OF THE HELIX

A. General Expression

If we substitute (16), (18), and (19) in (8) the integration is elementary and we have the result

$$E_s=L\frac{Gb^2}{4\pi}\left\{\frac{m}{m-1}\left[\frac{a^2}{p^2}+2a\rho p\frac{\partial}{\partial p}\left(\frac{T}{p^2}\right)-1\right]+\ln\frac{2L}{\rho}-1+2S\right\}. \quad (21)$$

This is the self-energy of a helical dislocation. In this expression S and T are given by (17) and (20) and $\rho=a+r_0$; p is the pitch of the helix as illustrated in Fig. 1, a and L are the radius and length of the cylinder on which it is wound, and G and m are the modulus of rigidity and the reciprocal of Poisson's ratio. The approximations used are that there are many turns ($N\gg1$) and that the cylinder is long ($L\gg a$).

B. The Tightly Wound Helix

If we set $p\ll a$, then the helix is tightly wound, in other words the turns are close together. It is then possible to evaluate S and T more explicitly by using the following asymptotic expansions of the Bessel functions as $x\rightarrow\infty$:

$$I_n(x)\rightarrow(2\pi x)^{-\frac{1}{2}}e^x,$$
$$K_n(x)\rightarrow(2\pi^{-1}x)^{-\frac{1}{2}}e^{-x}.$$

If we substitute these in (17) we have to first order in p/a, using $r_0=\rho-a$,

$$S\rightarrow\sum\tfrac{1}{2}p(a\rho)^{-\frac{1}{2}}n^{-1}e^{-nr_0/p}=-\tfrac{1}{2}p(a\rho)^{-\frac{1}{2}}\ln(1-e^{-r_0/p}).$$

A further simplification in this expression can be made. Since r_0 represents the half-width of the dislocation and $2\pi p$ the separation between two consecutive turns along the axial direction, it is reasonable to expect that $r_0<2\pi p$. Actually, as we saw at the beginning of this paper, we have in many cases that

$$r_0\simeq\tfrac{1}{2}b\ll p,$$

i.e., the turns are separated by a distance much larger than the dislocation cross section. Therefore we can write

$$S\simeq-\tfrac{1}{2}p(a\rho)^{-\frac{1}{2}}\ln(r_0/p).$$

If we are calculating E_s in (21) only to second order, i.e., only to terms of order a^2/p^2, a/p, and 1, then S is negligible since it is of order p/a.

However, the contribution of T is significant. We find, similarly, from (20) that $T\rightarrow-S$. If we use this result in (21), we have to second order in p/a

$$E_s=L\frac{Gb^2}{4\pi}\left\{\frac{m}{m-1}\left[\frac{a^2}{p^2}-\frac{(a\rho)^{\frac{1}{2}}}{p}\left(\ln\frac{r_0}{p}+1\right)-1\right]+\ln\frac{2L}{\rho}-1\right\}. \quad (22)$$

More terms can be obtained in this expansion by taking more terms in the asymptotic expansions of the Bessel functions.

The energy expression can also be written in terms of the number of turns per unit length of the helix, which is defined by $\nu=N/L$. From (7) we find the relation $2\pi p\nu=1$. If we substitute p from this in (22), we have

$$E_s=LGb^2\frac{m}{m-1}\{\nu^2\pi a^2-\tfrac{1}{2}\nu(a\rho)^{\frac{1}{2}}[\ln(2\pi\nu r_0)+1]\}+L\frac{Gb^2}{4\pi}\left[\ln\frac{2L}{\rho}-\frac{2m-1}{m-1}\right]. \quad (23)$$

This expression allows us to make a plausible physical interpretation of the result. The dominant term represents the contribution to the helix of a cylindrical dislocation, i.e., a stack of closely packed circular dislocations.[11] It can also be argued that the first-order term containing r_0 represents the influence of the size of the dislocation cross section; this is the term that can be improved by a better core calculation. Finally, the second order terms give the effect of the axial component of the helix. The self-energy of a straight screw dislocation is given by[12]

$$E_s{}^s=L\frac{Gb^2}{4\pi}\left[\ln\frac{2L}{r_0}-\frac{2m-1}{m-1}\right]. \quad (24)$$

We see that the second-order terms in (23) represent a screw of half-width $\rho\simeq a$ rather than r_0.

C. The Nearly Straight Helix

If we set $a\ll p$, then the helix will be stretched out, in other words it will be almost straight. It is now possible to evaluate S and T more explicitly by using the expansions of the Bessel functions for small arguments. We find that

$$S\rightarrow-\tfrac{1}{2}\ln(r_0/p)+\tfrac{1}{4}a\rho p^{-2}[\gamma+\ln(r_0/2p)-\tfrac{1}{2}],$$
$$T\rightarrow-\tfrac{1}{2}p^2(a\rho)^{-1}\ln(r_0/p)+\tfrac{1}{4}[\gamma+\ln(r_0/2p)+\tfrac{1}{2}+a/\rho],$$

where $\gamma=0.577$ is Euler's constant. If we use these results in (21), we have to second order in a/p

$$E_s=L\frac{Gb^2}{4\pi}\left\{\ln\frac{2L}{r_0}-\frac{2m-1}{m-1}-\frac{a\rho}{4p^2}\times\left[2\frac{m+1}{m-1}\left(\gamma+\ln\frac{r_0}{2p}\right)+\frac{5m-1}{m-1}\right]\right\}. \quad (25)$$

We see that here the dominant terms represent the contribution to the helix of the straight screw dislocation, Eq. (24). The second order terms can be said

[11] Reference 7, Eq. (19.4).
[12] Reference 7, Eq. (17.4).

to give the effect of the interaction between turns of the helix.

VI. CORRECTION FOR A RETURN LOOP

As mentioned before the above expressions for the self energy are incomplete since the helix is not a closed line. The addition of a return loop will remedy the situation (Fig. 2). It can be shown that the total energy for the helix and its return loop can be written

$$E_s = E_s^A + E_s^B + E_I^{AB}.$$

Here E_s^A is the self-energy of the helix found above in Eq. (21). If the return loop is a straight line of length L running parallel to the helix from $z=\frac{1}{2}L$ to $z=-\frac{1}{2}L$, then E_s^B is the self energy of a straight screw given by (24). The quantity E_I^{AB} is the interaction energy between the helix A and the return loop B. It is found by setting

$$\rho' = a = \text{const}, \quad z' = p\phi',$$
$$\rho = h = \text{const}, \quad \phi = 0,$$

where h is the distance between the return loop and the center of the helix. These relations can be substituted in the expressions (1), (2), (3), (4), and (5) and the calculation carried out, remembering that the result must be multiplied by the factor 2 for the interaction energy. We assume that $L \gg h \gtrsim a$, so that the return loop is close to the helix but not inside it. If we also use the previous approximations that $N \gg 1$ and $L \gg a$ we find that

$$E_I^{AB} = -L\frac{Gb^2}{2\pi}\left[\ln\frac{2L}{h} - \frac{2m-1}{m-1}\right].$$

Finally, if we substitute these results in the above expression for the total energy we have

$$E_s = L\frac{Gb^2}{4\pi}\left\{\frac{m}{m-1}\left[\frac{a^2}{p^2} + 2a\rho p\frac{\partial}{\partial p}\left(\frac{T}{p^2}\right)\right] + \ln\frac{h^2}{\rho r_0} + 2S\right\}. \quad (26)$$

For the case where $h \lesssim a$, i.e., when the return loop is inside the cylinder, we obtain the same expression with h replaced by a.

For $p \ll a$ the above expression reduces in second order to

$$E_s = L\frac{Gb^2}{4\pi}\left\{\frac{m}{m-1}\left[\frac{a^2}{p^2} - \frac{(a\rho)^{\frac{1}{2}}}{p}\left(\ln\frac{r_0}{p} + 1\right)\right] + \ln\frac{h^2}{\rho r_0}\right\},$$

and for $a \ll p$ to

$$E_s = L\frac{Gb^2}{4\pi}\left\{\ln\frac{h^2}{r_0^2} - \frac{a\rho}{4p^2}\left[2\frac{m+1}{m-1}\left(\gamma + \ln\frac{r_0}{2p}\right) + \frac{5m-1}{m-1}\right]\right\}.$$

The dominant term in the last expression,

$$L\frac{Gb^2}{2\pi}\ln\frac{h}{r_0},$$

gives the self and interaction energies of two straight screw dislocations separated by a distance h.

VII. CONCLUSION

If we let a and N be constant but vary p, which is proportional to L by (7), then we keep the projected area $\pi a^2 N$ of the helix constant, while its length varies; in other words we let the helix change its shape by glide but not by climb. It is then seen from the above expressions that the total self energy E_s for the case $p \ll a$ will decrease with increasing p, while for the case $a \ll p$ it will increase with increasing p. That is a tightly wound helix will try to extend itself while a nearly straight helix will try to compress itself. An equilibrium position must exist for some intermediate value of p, found by minimizing E_s. This position will readily be assumed when glide is easy.

Now consider the case where we let L and $\pi a^2 N$ be constant but vary N, and consequently also a and p; in other words we are considering a dislocation segment between two points separated by a distance L, at which a certain number of vacancies (proportional to $\pi a^2 N$) have condensed or evaporated. The final result can be a helix with few turns of large radius or with many turns of small radius. A rough calculation using the above expressions shows that the total self energy E_s increases with increasing N. On energy grounds then we would expect helices of few and large turns. However, helices of many turns seem to be the experimental rule; this could be the result if vacancy redistribution along the dislocation is slower than in the lattice.

It is seen in this paper that a rather general expression can be derived for the self-energy of a helical dislocation without too much difficulty. The result, Eq. (21), involves the little known functions S and T, Eqs. (17) and (20). However, these functions can be evaluated to arbitrary precision in terms of elementary functions in the two limiting cases of small and large pitch. We find that this leads to physically meaningful results for the self-energy. The dislocation core is treated roughly and taken into account by the single parameter r_0. This is a consequence of using continuum theory and of our ignorance of the core structure. Two further

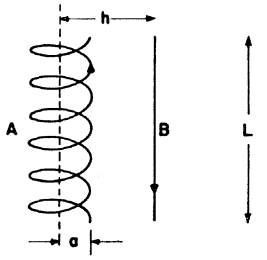

FIG. 2. The helix with a return loop.

limitations on the result of this paper are that we use isotropic theory and an infinite medium. The mathematical complexities of the theory would be multiplied considerably if both these simplifications were not made. Finally, since the general formulas require closed dislocation loops, we close the helix with a return loop. This eliminates spurious and possibly misleading terms.

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Optical Absorption in Pure Single Crystal InSb at 298° and 78°K*

S. W. KURNICK† AND JOHN M. POWELL‡
Chicago Midway Laboratories, University of Chicago, Chicago, Illinois
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The absorption spectra of single crystal homogeneous InSb were measured in the spectral range 5 to 10 microns at temperatures of 78°K and 298°K. Primary emphasis was placed on the precise determination of absorption coefficients less than 400 cm^{-1}. Absorption spectra were measured in many samples over the following range of impurity concentrations. Net impurity concentrations, expressed in atoms cm^{-3}, ranged from 5×10^{15} to 9.5×10^{16} in p-type samples, and from 2×10^{15} to 3×10^{17} in n-type samples, as determined from Hall coefficients measured at 78°K.

In general, the spectral range covered included regions where the absorption was dominated by either free-carrier absorption or valence-conduction band transitions. Free-carrier absorption in p-type InSb indicates a simple valence-band structure about $\mathbf{k}=0$, consisting of light and heavy hole bands. Free carrier cross sections at 298°K are $\sigma_p=8.65\times10^{-16}$ cm^2 per hole and $\sigma_n=0.23\times10^{-16}$ cm^2 per electron (at 9 μ). Whereas the free hole absorption coefficient is roughly independent of wavelength, the free electron absorption σ_n varies as λ^2 and agrees well with the classical Zener-Drude model.

The main absorption edge at both temperatures may be extended to lower absorption coefficients α by subtracting the extrapolated free carrier absorption coefficients α_c. The resultant band edge $\ln(\alpha-\alpha_c)$ values when plotted against the photoenergy ($\hbar\omega$) fits a straight line. The slopes of these band edges increase at the lower temperature and decrease (either at 78° or 298°K) as the acceptor concentration in the optical sample increases. Various models previously proposed are compared with the experimental results.

I. INTRODUCTION

THE measurement of infrared absorption is a standard procedure in studying certain properties of semiconductors. When applied to InSb, these measurements have yielded a reasonably clear picture of band structure and effective masses, free carrier absorption, and lattice vibrations.[1–6] In addition, many attempts were made to interpret the shape of the band edge,[7–9] and more recent studies have been made on the interaction of impurities (donors or acceptors) with the band structure itself.[10,11]

The purpose of our measurements was to evaluate the edge absorption and the free carrier absorption of InSb with more than ordinary emphasis upon the precise evaluation of absorption coefficients and the quality control of the semiconductor material. This detailed data on the absorption edge shape, as well as the shift in its effective cutoff, will be used to compare the various band edge interpretations.

II. EXPERIMENTAL DETAILS

A. InSb Samples

A summary of the InSb material used is shown in Table I. The samples were cut from large single crystals

TABLE I. InSb samples.

Specimen (see Figs. 3 and 4)	Net impurity concentration[a] (cm^{-3})	Mobility (cm^2/volt-sec)[b]	Total impurity concentration[c] (cm^{-3})
a	$2.07\times10^{17}n$	43 600	$2.1\times10^{17}n$
A	$2.95\times10^{17}n$	38 500	$3.0\times10^{17}n$
b, B	$2\times10^{15}n$	192 000	$4\times10^{15}n$
c	$2.75\times10^{16}p$	2900	$2.7\times10^{16}p$
C	$2.52\times10^{16}p$	3060	$2.5\times10^{16}p$
d, D	$9.5\times10^{16}p$	1650	$9.5\times10^{16}p$
E	$6.6\times10^{15}p$	4550	···

[a] Concentrations determined from Hall coefficient measurements at 78°K and defined as $1/eR_H$.
[b] Mobility determined from $R_H\sigma=\mu B$ at 78°K.
[c] Reference 12.

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† Present address: John Jay Hopkins Laboratory for Pure and Applied Science, General Atomic Division of General Dynamics Corporation, San Diego, California.

‡ Now at Raulind Corporation, Chicago, Illinois.

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