PHYSICAL REVIEW VOLUME 107, NUMBER 5 SEPTEMBER 1, 1957

# Helical Dislocations

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(Received May 16, 1957)

The equilibrium form of a dislocation line is shown to be a helix. If the helix is to contain many turns, its axis must be practically parallel to the Burgers vector. Pure screw dislocations can spontaneously assume the form of helices of many turns at large chemical stresses.

## INTRODUCTION

BONTINCK and Amelinckx[1] have observed helical dislocations in fluorite crystals. Amelinckx, Bontinck, Dekeyser, and Seitz[2] have given a detailed analysis of their creation. They have also pointed out their possible importance to whisker growth.

Although the formation of dislocation helices has been well analyzed, it is of interest to look at their creation from a somewhat different viewpoint. In this paper we show that the equilibrium form of a dislocation line acted on by an ordinary stress and a chemical stress produced by a deviation of the vacancy (or interstitial) concentration from the equilibrium value is indeed a helix. If the helix is to have many turns its axis must be practically parallel to the Burgers vector. Screw dislocations are shown to be unstable at large chemical stresses. They will spontaneously assume the form of helices of many turns.

## THEORY

Consider a dislocation line pinned at two points $A$ and $B$ (Fig. 1). Let $\mathbf{r}(\varphi)$ be a vector whose origin is midway between $A$ and $B$. By varying the parameter $\varphi$, let this vector sweep out the curve formed by the dislocation line. A unit tangent vector $\mathbf{t}$ to the curve is then given by $d\mathbf{r}/dr$. The radius of curvature vector $\mathbf{n}$ is equal to $d\mathbf{t}/dr$. The force per unit length acting on a dislocation element which is produced by curvature in the dislocation line is approximately equal to $\frac{1}{2}\mu b^2\mathbf{n}$, where $\mu$ is the shear modulus and $b$ is the length of the Burgers vector $\mathbf{b}$. This force must be balanced by that produced by the chemical stress and the ordinary stress to have equilibrium. It is easily shown from the work of Bardeen and Herring[3] that the force produced by the chemical stress is approximately $\pm(kT/b^3)[\ln(N/N_0)]\times(\mathbf{t}\times\mathbf{b})$, where $k$ is Boltzmann's constant, $T$ is the absolute temperature, $N$ is the actual concentration of vacancies, $N_0$ is the equilibrium concentration, and the plus or minus sign is used depending on the direction of $\mathbf{t}$. The force produced by the ordinary stress is simply $\mp(\mathbf{t}\times\mathbf{f})$ where $\mathbf{f}$ is a vector whose $i$th component is equal to

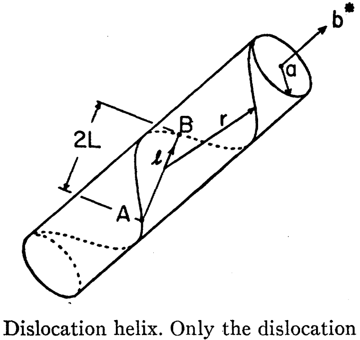

FIG. 1. Dislocation helix. Only the dislocation segment between $A$ and $B$ is considered in the text.

$$\sum_{j=1}^{3}\sigma_{ij}b_j,$$

$\sigma_{ij}$ being the usual stress component.[4] The equation of equilibrium is then equal to

$$\mathbf{n}=(\mathbf{t}\times\mathbf{b}^*), \tag{1}$$

where

$$\mathbf{b}^*=\pm\{(kT/b^3)[\ln(N/N_0)]\mathbf{b}-\mathbf{f}\}/\tfrac{1}{2}\mu b^2.$$

Since $\mathbf{n}\cdot\mathbf{b}^*=d(\mathbf{t}\cdot\mathbf{b}^*)/dr=0$, the angle that $\mathbf{t}$ makes with $\mathbf{b}^*$ must remain constant. From this fact it follows that the magnitude of $\mathbf{n}$ is also constant. Now the only curve whose radius of curvature is constant and whose tangent vector keeps a constant angle with a fixed direction in space is a helix.[5] Thus the equilibrium form of a dislocation line must be a helix.

We wish next to look in more detail into the solution of Eq. (1). The general solution which gives a helix passing through the points $A$ and $B$ of Fig. 1 is

$$\mathbf{r}=a\left[\cos\varphi\,\mathbf{i}+(\sin\varphi-\sin\bar{\varphi})\mathbf{j}+\frac{Ll_2}{a}\left(\frac{\varphi-\frac{1}{2}m\pi}{\bar{\varphi}-\frac{1}{2}m\pi}\right)\mathbf{k}\right], \tag{2}$$

where $\mathbf{l}=l_1\mathbf{i}+l_2\mathbf{k}=$unit vector in direction $AB$, $2L$ =distance between $A$ and $B$, $a=$radius of cylinder tangent to helix, $\bar{\varphi}=\cos^{-1}(Ll_1/a)$, and $\bar{\varphi}\leq\varphi\leq m\pi-\bar{\varphi}$; $m=1, 3, 5, 7, \cdots$. The vector $\mathbf{k}$ is a unit vector in the direction of $\mathbf{b}^*$, $\mathbf{i}$ is a unit vector normal to $\mathbf{k}$ and in the plane formed by $\mathbf{k}$ and $\mathbf{l}$, and $\mathbf{j}$ is a unit vector

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

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

[3] J. Bardeen and C. Herring, in *Imperfections in Nearly Perfect Crystals*, edited by W. Shockley *et al.* (John Wiley and Sons, Inc., New York, 1952), p. 277.

[4] M. Peach and J. S. Koehler, Phys. Rev. 80, 436 (1950).

[5] Encyclopædia Britannica (Encyclopædia Britannica, Inc., London, 1953), Vol. 7, p. 365.

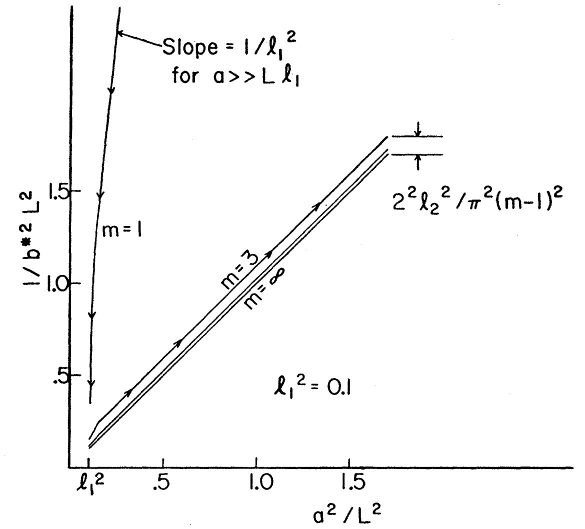

FIG. 2. Plot of $1/b^{*2}L^2$ *versus* $a^2/L^2$ for the case of $l_1^2=0.1$.

normal to both **i** and **k**. The relationship between $a$, $b^*$, and $m$ is

$$a^2=(1/b^{*2})-(Ll_2)^2/(\bar{\varphi}-\tfrac{1}{2}m\pi)^2. \qquad (3)$$

For $a \gg Ll_1$ this equation reduces to

$$a^2=(1/b^{*2})-[2Ll_2/(m-1)\pi]^2 \quad \text{for} \quad m>1,$$
$$a^2=(l_1/b^*)^2 \quad \text{for} \quad m=1.$$

For $a=Ll_1$ there is the relation

$$a^2=(1/b^*)^2-(2Ll_2/m\pi)^2.$$

From Fig. 1 it can be seen that no solution can exist for $a$ less than $Ll_1$. In Fig. 2 we have plotted curves of $1/L^2b^{*2}$ *versus* $a^2/L^2$ for different values of $m$ for the case where $l_1^2$ is equal to 0.1. Only the curve for $m$ equal to one gives stable equilibrium. The curves for higher values of $m$ are all positions of unstable equilibrium. However, since the motion of a dislocation line at high temperatures will in general involve climb and thus proceed at a finite speed, it should be possible to catch a dislocation, as Bontinck and Amelinckx have done, in the position of a helix of more than one turn. To see this, consider a partly edge and partly screw dislocation which has had the following history. Let the ordinary stress be equal to zero; let the dislocation line be in a small crystal to which we can add or remove vacancies at will; and let the original concentration of vacancies be the equilibrium concentration. If vacancies are now added to the crystal the value of $b^*$ will increase and the curve of $m=1$ will be followed as indicated by the arrows in Fig. 2. When $a$ becomes equal to $Ll_1$ an unstable situation exists. Turns can now be put into the helix in the manner envisaged by Bontinck and Amelinckx. The maximum number of turns can be estimated if dislocation interaction between neighboring turns is taken into account. It is reasonable to expect that no more turns can be put into a helix when the interaction force becomes greater than the force due to the curvature of the dislocation line. Therefore the distance between turns should be greater than the radius of the cylinder tangent to the helix. The maximum number of turns is thus of the order of $1/l_1$. If ten turns are to be obtained, the angle between **l** and **b** must be less than 6°. Thus, only dislocations which are practically pure screw can give rise to helices of many turns. Once a helix with many turns is formed it is unstable. If vacancies are consumed, the value of $b^*$ can be lowered and the value of $a$ will increase. The path indicated for $m=3$ in Fig. 2 may finally be followed, since as $a$ is increased the number of turns must decrease.

In Fig. 3 we have plotted curves of $1/L^2b^{*2}$ *versus* $a^2/L^2$ for various values of $m$ for a pure screw dislocation which is acted upon only by a chemical stress. A straight screw dislocation is always in an equilibrium position. However, from Fig. 3 it can be seen that for large enough chemical stresses the perfectly straight position is an unstable one. Therefore if a large enough chemical stress is suddenly applied to a crystal, say by quenching from a higher to a lower temperature, all the screw dislocations will spontaneously grow into helices. No prior climb is required of the dislocation as was the case of a mixed dislocation. The number of turns initially induced in a screw dislocation can be related to the chemical stress by the following formula [obtained from Eq. (3)]:

$$\text{number of turns} \approx (kTL/\pi\mu b^4)\ln(N/N_0). \qquad (4)$$

In order to have ten turns in the helix, it is necessary only that

$$|N-N_0|/N_0 \sim 0.05.$$

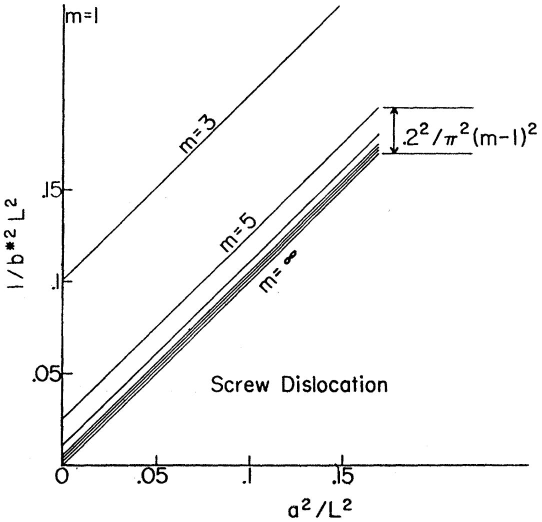

FIG. 3. Plot of $1/b^{*2}L^2$ *versus* $a^2/L^2$ for the case of a pure screw dislocation with $l_1=0$.

Helices of many turns can be put into pure screw dislocations through the application of tensile or compressive stresses parallel to the Burgers vector of the dislocation. For this situation the vector **f** of Eq. (1) is parallel to the Burgers vector. The number of turns that can be created is of the order of

$$\text{number of turns} \approx 2\sigma L/\mu\pi b, \qquad (5)$$

where $\sigma$ is the applied stress.

From the foregoing analysis we might reasonably ascribe the helices observed by Bontinck and Amelinckx to pure screw dislocations on two scores. The first is that a dislocation line must be practically pure screw anyway to obtain a large number of turns in a helix. The second is that only a modest excess or deficiency of vacancies is required to spontaneously change a perfectly straight screw dislocation into a helix of many turns.

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PHYSICAL REVIEW VOLUME 107, NUMBER 5 SEPTEMBER 1, 1957

# Fundamental Absorption of Barium Oxide from Its Reflectivity Spectrum*

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(Received May 20, 1957)

The reflectivity spectrum of single crystals of barium oxide, cleaved in vacuum, was measured as a function of temperature. The Kramers-Kronig integral relation was applied to derive the spectral dependence of both the absorption constant and index of refraction in the fundamental absorption region. The absorption compares favorably with results of previous thin-film transmission measurements and confirms the intrinsic nature of the multiple structure, recently explained by Overhauser as resulting from spin-orbit interaction in exciton creation. Large time-dependent changes of the reflectivity spectrum were observed even in a vacuum of $10^{-7}$ mm Hg at liquid-nitrogen temperature and are interpreted as interference effects from a growing surface layer of $Ba(OH)_2$, formed with a diffusion-limited rate of growth.

## I. INTRODUCTION

It is the purpose of this paper to present experimental results for the fundamental absorption of barium oxide and to call attention to the seldom used analytical method by which these results were obtained from specular-reflectivity measurements on single crystals. Furthermore, since barium oxide represents an extreme case for rapidity of surface contamination, because of the ease of hydroxide formation, a vacuum cleaving technique had to be adopted. The description of both this technique and the surface-contamination effects observed may be of general interest.[1]

## II. THEORY

The absorption constant in the fundamental region is most easily obtained from transmission measurements on appropriately thin films. This has been done for barium oxide by Zollweg.[2] However, there are difficulties associated with both accurate film-thickness measurements and the corrections for reflectivity losses. Also, there often remains uncertainty about the degree of lattice perfection of the films, the film stoichiometry, and the amount of surface contamination.[3] For these reasons, it is highly desirable to make a second and independent determination of the absorption from reflectivity measurements.[4]

The Fresnel equations (one for each component of polarization) for the reflection of radiation from an absorbing medium involve both the real and imaginary parts of the complex index of refraction. The imaginary part is simply related to the absorption constant. Since both the real and imaginary parts are usually unknown quantities, the commonly used reflectivity methods require two measurements, either at two different angles if the amount of polarization is known, or separately for both components of polarization at one non-normal incident angle. Because of the complexity of the Fresnel equations at non-normal incidence, one generally resorts to graphical methods of solution.[5] Normal-incidence measurements, as used in the method described in the remainder of this section[6] have the advantage that the analysis is based on the much simpler single Fresnel equation for this case. Also, for near normal incidence there is only a small variation of reflectivity with in-

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* Based on a Ph.D. thesis submitted to Cornell University.

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[1] Dr. L. Apker of the General Electric Company, Schenectady, New York, has suggested the applicability of this technique to the deliquescent lithium halide salts.

[2] R. J. Zollweg, Phys. Rev. **97**, 288 (1955).

[3] See, for example, O. S. Heavens, *Optical Properties of Thin Solid Films* (Academic Press, Inc., New York, 1955).

[4] There is a qualitative resemblance between reflectivity and absorption spectra. This resemblance gives one the approximate positions of the absorptions directly from the reflectivity spectrum. See Hartman, Nelson, and Siegfried, Phys. Rev. **105**, 123 (1957).

[5] I. Simon, J. Opt. Soc. Am. **41**, 336 (1951); D. G. Avery, Proc. Phys. Soc. (London) **B65**, 425 (1952).

[6] T. S. Robinson, Proc. Phys. Soc. (London) **B65**, 910 (1952).