Dislocation Contribution to the Elastic Constants of Body-Centered Cubic Crystals

BAL KRISHNA AGRAWAL AND G. S. VERMA
Department of Physics, University of Allahabad, Allahabad, India
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Expressions for dislocation contribution to the elastic constants of bcc crystals are obtained and applied to lithium. The contribution comes out to be less than 1% for screw dislocations. For edge dislocations, the contribution is about 1.3%. Edge dislocations are found to make a contribution about seven times larger than that of a similar density of screw dislocations.

RECENTLY Koehler and deWit[1] have calculated the dislocation contribution to the elastic constants of fcc crystals. For Cu and Pb, the contribution can amount to a few percent in a pure annealed crystal. In the present paper we have obtained expressions for the dislocation contribution to the elastic constants of bcc crystals, and the results of the calculation are given for lithium.

If xy is the slip plane, x is the direction of the Burgers' vector, and σ_{xz} is the resolved shear stress, then the total strain caused by the motion of all the dislocations in one slip system, i.e., ϵ_{xz}, is given by[1]

$$\epsilon_{xz}=S\sigma_{xz}. \tag{1}$$

Assuming that S is a constant and the same for all slip systems, the total contribution to the strain can be obtained. The procedure for obtaining the total dislocation contribution to the strain is as follows.

Using the cubic axes of the crystal for reference and assuming an arbitrary stress field σ_{ij}, the value of σ_{xz} for each system is found in terms of σ_{ij}. Using Eq. (1), the dislocation contribution to the strain ϵ_{xz} is obtained and its components with respect to the reference axes evaluated. Adding the contribution from all the slip systems, the total dislocation contribution to the strain $\delta\epsilon_{ij}$, referred to cubic axes and expressed in terms of the applied stress, is obtained.

The results of calculation for the bcc crystals are

$$\begin{aligned}
\delta\epsilon_{11}&=\tfrac{8}{3}S\sigma_{11}-\tfrac{4}{3}S\sigma_{22}-\tfrac{4}{3}S\sigma_{33},\\
\delta\epsilon_{22}&=-\tfrac{4}{3}S\sigma_{11}+\tfrac{8}{3}S\sigma_{22}-\tfrac{4}{3}S\sigma_{33},\\
\delta\epsilon_{33}&=-\tfrac{4}{3}S\sigma_{11}-\tfrac{4}{3}S\sigma_{22}+\tfrac{8}{3}S\sigma_{33},\\
\delta\epsilon_{23}&=\tfrac{4}{3}S\sigma_{23},\\
\delta\epsilon_{31}&=\tfrac{4}{3}S\sigma_{31},\\
\delta\epsilon_{12}&=\tfrac{4}{3}S\sigma_{12}.
\end{aligned}$$

The slip systems for bcc crystals are listed in Table I. For cubic crystals, the relation between stress and strain is

$$\begin{aligned}
\epsilon_{11}&=S_{11}\sigma_{11}+S_{12}\sigma_{22}+S_{12}\sigma_{33},\\
\epsilon_{22}&=S_{12}\sigma_{11}+S_{11}\sigma_{22}+S_{12}\sigma_{33},\\
\epsilon_{33}&=S_{12}\sigma_{11}+S_{12}\sigma_{22}+S_{11}\sigma_{33},\\
2\epsilon_{23}&=S_{44}\sigma_{23},\\
2\epsilon_{31}&=S_{44}\sigma_{31},\\
2\epsilon_{12}&=S_{44}\sigma_{12}.
\end{aligned}$$

Thus, it can be seen that the apparent change in S_{ij}, due to dislocations, is given by

$$\begin{aligned}
\delta S_{11}&=8/3S,\\
\delta S_{12}&=-4/3S,\\
\delta S_{44}&=8/3S.
\end{aligned}$$

The values of the factor S in the two specific cases,[1] $\theta=0$ (all screw) and $\theta=\pi/2$ (all edge), are

$$S_0=\frac{(\pi/6)N(\langle l\rangle_{\mathrm{av}},0)\langle l^2\rangle_{\mathrm{av}}}{[\ln(R/r_0)][K+(d^2K/d\theta^2)]_{\theta=0}},$$

$$S_{\pi/2}=\frac{(\pi/6)N(\langle l\rangle_{\mathrm{av}},\pi/2)\langle l^2\rangle_{\mathrm{av}}}{[\ln(R/r_0)][K+(d^2K/d\theta^2)]_{\theta=\pi/2}}.$$

The correct value of S is expected to lie between S_0 and $S_{\pi/2}$. Here, $N(\langle l\rangle_{\mathrm{av}},0)$ and $N(\langle l\rangle_{\mathrm{av}},\pi/2)$ represent the density of screw and of edge dislocations, respectively, which are associated with one slip system. The

TABLE I. Slip systems for the body-centered cubic crystals.

Unit vector normal to slip plane	Unit vector in direction of **b**
$2^{-\frac{1}{2}}\langle 110\rangle$	$3^{-\frac{1}{2}}\langle 1\bar{1}1\rangle$
	$3^{-\frac{1}{2}}\langle \bar{1}11\rangle$
$2^{-\frac{1}{2}}\langle 011\rangle$	$3^{-\frac{1}{2}}\langle 11\bar{1}\rangle$
	$3^{-\frac{1}{2}}\langle 1\bar{1}1\rangle$
$2^{-\frac{1}{2}}\langle 101\rangle$	$3^{-\frac{1}{2}}\langle 11\bar{1}\rangle$
	$3^{-\frac{1}{2}}\langle \bar{1}11\rangle$
$2^{-\frac{1}{2}}\langle 1\bar{1}0\rangle$	$3^{-\frac{1}{2}}\langle 111\rangle$
	$3^{-\frac{1}{2}}\langle 11\bar{1}\rangle$
$2^{-\frac{1}{2}}\langle 01\bar{1}\rangle$	$3^{-\frac{1}{2}}\langle 111\rangle$
	$3^{-\frac{1}{2}}\langle \bar{1}11\rangle$
$2^{-\frac{1}{2}}\langle 10\bar{1}\rangle$	$3^{-\frac{1}{2}}\langle 111\rangle$
	$3^{-\frac{1}{2}}\langle 1\bar{1}1\rangle$

[1] J. S. Koehler and G. deWit, Phys. Rev. **116**, 1121 (1959).

TABLE II. Values of $[K+(d^2K/d\theta^2)]$ and S for edge and screw dislocations in lithium, with $r_0=3\times10^{-8}$ cm, $R=5\times10^{-4}$ cm, $N=4\times10^6$ cm^{-2}, and $l=3\times10^{-4}$ cm.

$[K+(d^2K/d\theta^2)]_{\theta=0}$ (dyn/cm^2)	$[K+(d^2K/d\theta^2)]_{\theta=\pi/2}$ (dyn/cm^2)	S_0 (cm^2/dyn)	$S_{\pi/2}$ (cm^2/dyn)
2.417×10^{11}	0.361×10^{11}	0.067×10^{-13}	0.45×10^{-13}

dislocation segments are supposed to have the same length $\langle l\rangle_{\mathrm{av}}$. R is the average dislocation separation and r_0 is the core radius of a dislocation. K is a function of the elastic constants of the crystal and the orientation with respect to crystal axes of both the Burgers' vector and the dislocation, and is related to the elastic energy per unit length of a long straight dislocation by $E=(b^2/4\pi)[\ln(R/r_0)](K)$, where b is the magnitude of the Burgers' vector. For an arbitrary orientation θ of the dislocation in an anisotropic crystal, where θ is the angle between the Burgers' vector and the dislocation, K is determined numerically.

We have estimated the dislocation contribution to the elastic constants for Li; the latter have been determined by Nash and Smith[2] to be $S_{11}=2.948$, $S_{12}=-1.348$, $S_{44}=0.929$ (all in units of 10^{-11} cm^2/dyn). Values of $[K+(d^2K/d\theta^2)]$ at $\theta=0$ and $\theta=\pi/2$ are obtained from the numerical computations of deWit and Koehler[3] and are given in Table II together with the values of S_0 and $S_{\pi/2}$. Table III gives the dislocation contribution to the different elastic moduli.

TABLE III. Percent dislocation contribution to elastic moduli.

	S_{11}	S_{12}	S_{44}
Screw	0.06	0.06	0.19
Edge	0.4	0.43	1.3

The present calculation indicates that the dislocation contribution to the elastic moduli is about a few percent. Edge dislocations contribute about seven times more than does a similar density of screw dislocations.

[2] H. C. Nash and C. S. Smith, J. Phys. Chem. Solids **9**, 113 (1959).

[3] G. deWit and J. S. Koehler, Phys. Rev. **116**, 1113 (1959).