

Short Notes

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Hydrostatic Pressure and Plastic Deformation of the Alkali Halides

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The effect of hydrostatic pressure on the plastic deformation of metal single crystals is not very important (1); a small rise in flow stress can be interpreted in terms of the work done against pressure to produce the volume increase associated with plastic deformation. This volume increase is due to anharmonic effects in the long range elastic field of dislocations, the core effects being negligible (2). On the other hand alkali halides show a marked dependence of flow stress on hydrostatic pressure (3, 4). The purpose of this note is to show that in ionic solids the presence of dislocations with dissociated cores on (110) planes (5) is compatible with the observed pressure effect.

In alkali halides the stacking fault energy $\gamma(x)$ for a $(x/\sqrt{2})$ [110] (110) fault is quite well approximated by (5)

$$\gamma(x) = \gamma_0 \sin^2(\pi x/b),$$

where b is the absolute value of the perfect Burgers vector of the structure and γ_0 the energy of a $b/2$ Burgers vector fault. Faulting introduces a strong dilatation ϵ between the two planes adjacent to the stacking fault. ϵ is a maximum for the $b/2$ fault being then equal to $\epsilon_0 (\epsilon = \delta d_{(110)}/d_{(110)}$ with $d_{(110)} = b/2$). Taking into account electronic polarization of the ions in the neighbourhood of the fault, computed values are $\gamma_0 = 330 \text{ erg cm}^{-2}$, $\epsilon_0 = 0.27$ for lithium fluoride, and $\gamma_0 = 195 \text{ erg cm}^{-2}$, $\epsilon_0 = 0.32$ for sodium chloride. $\gamma(x)$ has no minimum in the range $0 < x < b$. Thus the stacking fault cannot extend all through the crystal on a (110) plane since it is not even a metastable defect. It is possible, however, to speak of a dissociated core of a dislocation, the repulsion between partial dislocations stabilizing the stacking fault. Since there is no local minimum in $\gamma(x)$ one considers a continuous distribution of partial dislocations of a density $\rho(x)$. In a more

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quantitative approach we choose ρ to be constant in the range $-d \leq x \leq d$. Since for the total dislocation

$$\int_{-d}^{+d} b\rho(x) dx = b$$

$\rho(x) = 1/2d$ for $|x| < d$, and 0 otherwise, the centre of the dislocation being at $x = 0$. At x the absolute value of the Burgers vector defining the stacking fault is equal to

$$b(x) = \int_{-d}^{+d} b\rho(x) dx = b \frac{x+d}{2d}$$

for $|x| < d$ and 0 otherwise.

Thus between x and $(x + dx)$ we have a strip of stacking fault with the energy

$$\gamma [b(x)] dx = \gamma_0 \cos^2(\pi x/2d) dx$$

for $|x| < d$.

The width d of this function defining the dissociation is obtained by minimizing the total energy with respect to d . This total energy consists of five contributions.

1. The energy of the stacking fault strips

$$\int_{-d}^{+d} \gamma [b(x)] dx = \gamma_0 d$$

2. The interaction energy between partials which is about

$$- [\mu b^2 / 2\pi(1-\nu)] \int_{-d}^{+d} \int_{-d}^{+d} dx dx' \rho(x)\rho(x') \log(|x-x'|/b) \\ = - [\mu b^2 / 2\pi(1-\nu)] (\log(2d/b) - 3/2),$$

where μ is the shear modulus and ν the Poisson ratio.

3. The interaction energy between "Frank partials" due to the dilatation ϵ perpendicular to the fault. To get a rough estimate of this energy we assume that ϵ varies linearly from 0 for $x = -d$ to ϵ_0 for $x = 0$. The interaction energy between Frank partials of the continuous distribution so introduced is then equal to

$$- [\mu \epsilon_0^2 b^2 / 8\pi(1-\nu)] (\log(d/4\pi) - 3/2).$$

The self-energy of the partials is $\mu b^2 / 2 \int_{-d}^{+d} \rho(x) dx = \mu b^2 / 2$ for the first distribution and $\mu \epsilon_0^2 b^2 / 4$ for the Frank partial distribution.

The work done against the external hydrostatic pressure p to produce the dilatation ϵ . With the linear approximation for ϵ in 3., this term is simply equal to $\epsilon_0 b p d / 2$.

Minimizing the sum of the preceding five contributions with respect to d we obtain the dissociation width

$$d = \frac{\mu b^2 (1 + \epsilon_0^2 / 4)}{2\pi(1-\nu)(\gamma_0 + \epsilon_0 b p / 2)}$$

For typical values of d/b are 8 and 6 for LiF and NaCl, respectively. It is clear from the last equation that a hydrostatic pressure p must have some effect on $\epsilon_0 b p / 2$ becomes comparable to γ_0 . To obtain an order of magnitude we define a critical pressure p_c such that

$$\epsilon_0 b p_c / 2 = \gamma_0 / 10$$

For p_c are 6 kbar for LiF and 4 kbar for NaCl. Experimentally (3) no pressure effects are found for LiF at 4.3 kbar. At the same pressure effects are, however, detected for NaCl, and also for LiF tested at 13 kbar (3, 4) (observed is an increase in the flow stress and a decrease in dislocation mobility). Of course the agreement found here with our calculation must be considered to be only semi-quantitative because of the arbitrary definition of p_c . At least it explains the observed difference between LiF and NaCl. On the other hand, the action of p results in a narrower dissociated core, thus easier cross-slip which is difficult to associate with the observed increase in flow stress.

Finally such pressure effects can be expected in all cases where a dilatation occurs at stacking faults. For example in b.c.c. metals the $1/8 [110] (1\bar{1}0)$ fault produces a compression of the planes adjacent to the fault. These become closer $1/39$ as seen from hard sphere considerations (6). Thus hydrostatic pressure helps dissociation markedly for $p \geq p_c$. With $b p_c / 39 \approx \gamma_0 / 10$ and with $\gamma_0 = 0.135 \mu b$ for iron (6), $p_c \approx 42$ kbar. As far as we know, experiments on iron crystals under such high hydrostatic pressures have not yet been reported.

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Light-Induced Electron Paramagnetic Resonance of $^2S_{1/2}$ -State Impurity Centres in CdS and CdSe Single Crystals

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Recently $^2S_{1/2}$ -state impurities with $(ns)^1$ -configuration have become an interesting object of EPR investigations in II-VI compounds. Rüber and Schneider (1) observed spectra of Group-III elements, Sugibuchi and Mita (2, 3) the spectra of Group-IV elements in ZnS, and Suto and Aoki (4, 5) found spectra of Pb-associated centres in ZnTe. From the extremely large hyperfine splitting by the nuclear spins of some isotopes of the impurity centres, Rüber and Schneider, and also Sugibuchi and Mita concluded that the unpaired spin is strongly localized in the (ns) -orbital of the impurity ion. In contrast to the observations in ZnS, the investigations in Pb:Pb and ZnTe:Ge (6) show large g -shifts to values greater than the free-spin g and an additional superhyperfine structure, caused by the interaction with ^{67}Zn . Suto and Aoki (7), and Iida and Watanabe, who calculated the probability of finding the unpaired spin in the (ns) -orbital of only 0.23 for Ge and 0.19 for Pb (8), concluded that the paramagnetic centre is a hole, localized mainly on the four Te atoms around the Ge or Pb ion.

To get further information about the nature of these centres we extended the measurements to single crystals of CdS and CdSe with wurtzite structure. The EPR measurements were performed with an X-band rf-modulated JEOL spectrometer JES-3BQ. The samples were prepared by two methods. Either by growing single crystals of CdS and CdSe with the doping material or by growing the crystals from highly purified CdS and CdSe powder with an admixture of the doping material. In both cases strong EPR-spectra were observed at 77 °K after excitation with light in the visible range from an ordinary prism monochromator.