# short note

reprinted from

# physica
# status
# solidi

Materials Research Center, Allied Chemical Corporation, Morristown, New Jersey (a),

and Department of Geology and Geophysics, Yale University, New Haven, Connecticut (b)

On the Deformation of Alkali Halide Single Crystals at High Pressure[1]

By

L. A. DAVIS (a) and R. B. GORDON (b)

In a recent note in this journal (hereafter referred to as I) Fontaine and Haasen (1) consider the influence of pressure, P, on the dissociation width, d, of $a/2\langle 110 \rangle$ dislocations on $\{110\}$ planes in alkali halide single crystals. Fontaine (2) has calculated the stacking fault energy for $(1\bar{1}0)$ faults which are formed by the dissociation

$$\frac{a}{2}[110] \rightarrow \frac{a}{4}[110] + \frac{a}{4}[110] + \varepsilon_o \frac{a}{4}[1\bar{1}0] + \varepsilon_o \frac{a}{4}[1\bar{1}0].$$

Separation of the Shockley partials to a distance of the order of that in pure metals ($\approx 5b$) is expected. The latter two "Frank partials", where $\varepsilon_o \approx \delta d_{110}/d_{110} \approx 0.3$, represent a strong local dilatation of the lattice; this relaxes the exchange energy contribution resulting from the closed shell repulsion of unlike ions which come into juxtaposition when the Shockley partials are formed. For the above dissociation the change in d/b with pressure is given in I as

$$\frac{d}{b} = \frac{\mu b \left( 1 + \frac{\varepsilon_o^2}{4} \right)}{2\pi(1-\nu)\left( \gamma_o + \frac{\varepsilon_o b \Delta P}{2} \right)} \tag{1}$$

Because $\varepsilon_o$ is large, equation (1) predicts a significant reduction in d/b with increasing $\Delta P$. This should lead to reduced flow stress, $\sigma$, when deformation is controlled by the recombination and cross slip of partial dislocations. Such considerations are not pertinent to an explanation of data for the change of $\sigma$ with pressure in stages I and II deformation of the alkali halides (3), because in each case the observed $d\sigma/dP$ is positive, i.e., it is of opposite sign to the effect predicted

due to reduced dissociation of the slip dislocations. An increase in $\sigma$ with pressure is consistent with control of the flow stress by elastic interaction processes or by processes involving point defect generation and/or diffusion.

It is pertinent to consider the importance of stacking faults in stage III deformation of the alkali halides; according to Seeger et al. (4) stage III deformation in f.c.c. metal single crystals is controlled by the thermally activated cross slip of screw dislocations. Hesse (5) has shown that $\sigma_{III}$, the stress for initiation of stage III, is a logarithmic function of T in single crystal NaCl, a relationship predicted by the cross slip theory of Seeger et al. Matucha and Haasen (6) have observed profuse cross slip traces on entering stage III in NaCl. Hence, we may suppose that dynamic recovery in the alkali halides is governed by cross slip and if so, a pressure-induced decrease in d/b should cause a decrease in $\sigma_{III}$. Indeed, a pronounced reduction in $\sigma_{III}$ has been recently observed (7) in NaCl and KCl at 4.3 kbar. The results for $\Delta\sigma_{III}/\sigma_{III}$ are summarized in Table 1. (These results in fact appear to represent strong, although indirect, evidence for the presence of stacking faults in the alkali halides.) Thus the prediction in I that pressure should effect d appears valid.

To a first approximation, in equation (1) $\mu$ and $\gamma_{110}$ (= $\gamma_o + \epsilon_o b \Delta P/2$) are the important functions of pressure so one may write for the fractional change of d/b with pressure

$$\frac{\Delta(d/b)}{(d/b)} \approx \frac{\Delta\mu}{\mu} - \frac{\Delta\gamma}{\gamma} \approx \frac{\Delta K}{K} - \frac{\Delta\gamma}{\gamma} , \qquad (2)$$

where we have replaced $\gamma_{110}$ by $\gamma$ and $\mu$ by K, the edge ($K_e$) or screw ($K_s$) dislocation stress field elastic constant in the NaCl structure, or some average of the two. For $\Delta K/K$ we use an average of $\Delta K_s/K_s$ and $\Delta K_e/K_e$, which may be computed from data in the literature, (see (3)) and $\Delta\gamma/\gamma$ follows easily from the linear approximation.

Table 1 lists the various parameters for $\Delta P = 4.3$ kbar and it is evident that for $\epsilon_o \approx 0.3$ the change in $\gamma$ outweighs the increase in elastic constants with a resulting decrease in d/b. It is expected that the larger the decrease in d/b, the larger will be the decrease in $\sigma_{III}$: the experimental results are just the reverse

Table 1

Change of selected parameters with pressure (4.3 kbar)

|       | $(\Delta\sigma_{III}/\sigma_{III})$ | $\varepsilon_0$ | $\Delta K/K$ | $\Delta\gamma/\gamma$ | $\Delta(d/b)/(d/b)$ |
|-------|-------------------------------------|-----------------|--------------|-----------------------|---------------------|
| NaCl  | $-0.50 \pm 0.10$                    | 0.33            | 0.070        | 0.146                 | $\approx -0.076$    |
| KCl   | $-0.11 \pm 0.05$                    | 0.34            | 0.067        | 0.205                 | $\approx -0.14$     |
| KI    | $0 \quad \pm 0.05$                  | 0.35            | 0.124        | 0.295                 | $\approx -0.17$     |

of this expectation (see Table 1). To improve the correlation of the observations with the simple model of I, therefore we would have to require, for example, that $\varepsilon_0$ be substantially less (by $\approx 1/2$ in KI) in the materials of greater ionic polarizability; while this does not appear in Fontaine's stacking fault theory (2), it does not seem unreasonable.

### References

(1) G. FONTAINE and P. HAASEN, phys. stat. sol. <u>31</u>, K67 (1969).

(2) G. FONTAINE, J. Phys. Chem. Solids <u>29</u>, 209 (1968).

(3) L. A. DAVIS and R. B. GORDON, J. appl. Phys. <u>39</u>, 3885 (1968).

(4) A. SEEGER, R. BERNER, and H. WOLF, Z. Phys. <u>155</u>, 247 (1955).

(6) J. HESSE, phys. stat. sol. <u>9</u>, 209 (1965).

(6) K. H. MATUCHA and P. HAASEN, Nachr. Akad. Wiss. Göttingen <u>17</u>, 219 (1967).

(7) L. A. DAVIS and R. B. GORDON, to be published in J. appl. Phys.