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DISSOCIATION OF DISLOCATIONS AND PLASTICITY OF IONIC CRYSTALS

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Abstract. — The dissociation of dislocations in the NaCl structure is discussed in terms of Fontaine's model. There are no well-defined partials in the dissociation of the Burgers vector $a/2[110]$ on the $(110)$ slip plane. The stacking fault on this plane is connected with a dilatation normal to $(110)$. This leads to an unique effect of hydrostatic pressure on the frequency of cross slip. Cross slip in stage III occurs via the $(111)$ and $(001)$ planes. On the $(001)$ plane dislocations are not dissociated while dissociation on $(111)$ probably is intermediate. On $(001)$ and $(111)$ planes edge dislocations interact strongly with multivalent impurities while screw dislocations move relatively freely. This strong electrostatic interaction is thought to be responsible for the choice of slip plane and for the unusually strong latent hardening observed in the NaCl structure. The dissociation of dislocations on the other hand appears to influence dislocation climb and creep determined by climb.

1. The width of dissociation. — For a long time dislocations of Burgers vector $b = a/2[110]$ in the NaCl structure were thought not to be dissociated. Fontaine in his thesis [1] has, however, shown that the electrostatic interaction between the ions forming this structure in fact favors the formation of stacking faults: Figure 1 shows that by a partial shear of $a/4[110]$, ions of opposite sign approach each other across a $(110)$ slip plane. The stacking fault energy $\gamma_0$ associated with this shear would be negative if the exchange energy between the ions did not oppose their close approach. The latter interaction leads to a positive $\gamma_0$ and to a dilatation $\varepsilon_0 \approx 0.3$ of the lattice normal to the $(110)$ stacking fault in the alkali halides, described by the reaction

$$\frac{a}{2}[1,1,0] \rightarrow \frac{a}{4}[1-2\varepsilon_0,1+2\varepsilon_0,0] + \frac{a}{4}[1+2\varepsilon_0,1-2\varepsilon_0,0].$$

A closer look shows, however, that the $a/4[110]$ shear actually corresponds to metastable atom positions and that there is no energetically stable partial shear at all on the $(1\bar{1}0)$ plane. Instead Fontaine describes the stacking fault energy due to $a\frac{\chi}{\sqrt{2}}[110]$ shear by a

![Figure 1. Dissociated edge dislocation in the NaCl structure according to Fontaine.](http://dx.doi.org/10.1051/jphyscol:1974718)
Table I

<table>
<thead>
<tr>
<th>Substance</th>
<th>$\varepsilon_0$</th>
<th>$\gamma_0(110)$</th>
<th>$\gamma_0(1\overline{1}0)$</th>
<th>$d/b(1\overline{1}0)$</th>
<th>$\gamma_0(111)$</th>
<th>R (max)</th>
<th>Polarizability $(10^{-24} \text{ cm}^3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiF</td>
<td>0.287</td>
<td>359</td>
<td>330</td>
<td>8</td>
<td>595</td>
<td>3.85</td>
<td>1.0</td>
</tr>
<tr>
<td>NaCl</td>
<td>0.327</td>
<td>206</td>
<td>195</td>
<td>6</td>
<td>220</td>
<td>2.15</td>
<td>3.9</td>
</tr>
<tr>
<td>KCl</td>
<td>0.340</td>
<td>166</td>
<td>161</td>
<td>6</td>
<td>158</td>
<td>1.60</td>
<td>4.5</td>
</tr>
<tr>
<td>KJ</td>
<td>0.345</td>
<td>123</td>
<td>128</td>
<td>19</td>
<td>110</td>
<td>1.87</td>
<td>7.9</td>
</tr>
</tbody>
</table>

$\gamma_0' = \gamma_0 + \text{corrections for electronic and ionic polarisation.}$

d/b calculated with $\gamma_0'$ and $b'(x) = b/2 \ d$ for $|x| < d$, $b' = 0$ otherwise.

c) The interaction energy $E_c$ between the Frank components of the partials describing the dilatation $s$ perpendicular to the fault. Assuming

$$e(x) = \varepsilon_0(\ d - |x|)/d$$

we obtain

$$E_c = -\left[\mu\varepsilon_0^2 b^2/8\pi(1-v)\right] \ln(2 \ d/b) - 3/2).$$

(d) The self energy $E_d$ of the partials is

$$\mu b/2 \int_{-\infty}^{+\infty} b'(x) \ dx = \mu b^2/2$$

for the Shockley and $\mu b^2/2$ for the Frank components.

e) The work $E_a$ done against the hydrostatic pressure $p$ in producing the $\varepsilon(x)$ dilatation is

$$E_a = p \varepsilon_0 \ b d/2.$$
Comparing eq. (7) and (8) one recognizes with the help of table I that in general $d(110) \geq 1.5 d(111)$ implying that the dissociation on (111) planes is not negligibly small.

2. The choice of slip planes. — Most workers in the field of deformation of the NaCl structure, all the way back to M. J. Buerger [3] and more recently following J. Gilman [4], try to explain the choice of the slip planes in these crystals by the core structures of the dislocations on these planes, see Granzer [23]. Fontaine’s calculation seems to support such an argument since the widest dissociation favors indeed the observed {110} slip plane. Dislocations on {001} from this point of view have the highest core energy and no dissociation while on {111} the dissociation is intermediate. Connected with a narrow dislocation core is a large Peierls-Nabarro force which could determine the critical resolved shear stress (CRSS) at low temperatures.

The present author Haasen [5] has opposed the view that the width of dislocation or the Peierls-Nabarro force is responsible for the choice of slip planes and the CRSS above about 100 K in NaCl for the following reasons: First, slip steps on {001}, {111} and {112} planes are in fact observed during stage II and III deformation of NaCl crystals compressed along other than $<100>$ directions (Matucha [6], Franzbecker [7]). Second, the CRSS for slip on (001) measured in shear tests shows a typical impurity plateau, i.e. becomes independent of temperature, for $T \gtrsim 300\, \text{K}$ and $[\text{Ca}^{++}] \approx 2-3$ ppm (Franzbecker [7]). Third, Strunk [8] has shown by transmission electron microscopy of NaCl that screw dislocations appear to have freely cross-slipped on {001}, {111}, {121} and other planes leaving edge dislocation jogs which on the other hand seem to be rather immobile on these planes. This is exactly what is expected from a calculation by Haasen [5] of the electrostatic interaction of straight edge dislocations on various $\{hkl\}$ planes with divalent impurities: The extra half plane of a dislocation on {111} or {001} ends with rows of ions of the same sign of charge and therefore interacts more strongly with a multicharged ion than on {110} where the last ion rows in the core alternate in the sign of the charge. For screw dislocations on the other hand such a charged core does not exist on any plane. The calculation gives the right magnitude for the plateau stress in {001} shear of NaCl doped with (2-3) ppm Ca$^{++}$ relative to that for (110) shear. On the other hand the dislocation facing an impurity ion on its slip plane may not remain in straight edge orientation, but rather bend around into screw orientation as far as possible where it has less electrostatic interaction. Strunk and Frydman [9] are trying to explain the flow stress of NaCl by the drag of impurity anchored edge jogs. As the ions forming crystals with NaCl structure become more polarisable, non-{110} slip should become easier also for edge dislocations-all the way to AgCl which shows pencil slip on numerous planes containing the {110} Burgers vector. A shear investigation of {001} slip of a series of compounds with NaCl structure is under way in Göttingen.

3. Cross slip in NaCl. — The stress-strain curve of NaCl shows the three-stage behaviour typical for fcc metals. Figure 2 indicates that the stress $\tau_{111}$ at the end of the linear stage II of strong work hardening decreases with increasing temperature (Hesse [10]). The same is observed for a decreasing strain rate $\dot{\varepsilon}$ such that the experimental results in the range $266\, \text{K} \leq T \leq 368\, \text{K}$, $9.5 \times 10^{-5}\, \text{s}^{-1} \leq \dot{\varepsilon} \leq 1.9 \times 10^{-3}\, \text{s}^{-1}$ are well represented by the equation following from Seeger et al.’s [11] cross slip model

$$\ln (\tau_{111}/\mu) = \ln (\tau_{111}/\mu)_{T=0} - \frac{kT}{u} \ln \left( \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right).$$

The activation energy $u$ is related to $\gamma_0$ approximately as $u \approx \mu^2 b^4/\gamma_0$, see Haasen [24]; from Hesse’s experiments $u = 0.13\, \text{eV}$ (while in $\dot{\varepsilon}_0/\dot{\varepsilon} = 13$, $\dot{\varepsilon}_0 = 44\, \text{s}^{-1}$ for $\dot{\varepsilon} = 10^{-4}\, \text{s}^{-1}$). The stacking fault energy calculated from $u$ is about $\gamma_0^{\text{sf}} \approx 110\, \text{erg/cm}^2$ for NaCl, compared to 195 erg/cm$^2$ according to table I.

The microscopic process of cross slip in NaCl probably does not fit Seeger’s model developed for fcc crystals. Replica electron microscopy (Matucha and Haasen [12]) shows that stage III deformation is related to the appearance of cross slip steps leading from a {110} first to a {111} slip plane and then to a {001} plane. In fcc metals on the other hand, main and cross slip planes all are of the {111} type. It is tempting to relate the complicated cross slip series observed in NaCl to the order of increasing stacking fault energies $\gamma_0(110) < \gamma_0(111) < \gamma_0(001)$. Accord-
ingly, \(\{111\}\) appears as a first cross slip plane because it offers a limited dissociation although continued slip on \(\{111\}\) leads to the appearance of free charge at the crystal surface; this could force cross slip finally onto the non-dissociative \(\{001\}\) plane. The continuously dissociated-dislocation-model introduced above for the \((110)\) slip plane allows part of the Burgers vector of a screw to change into the \((111)\) plane and to dissociate there while the other part is still dissociated on \((110)\) thus making a full constriction unnecessary and cross slip easier.

A cross slip model for fcc crystals which allows for redissociation on the cross slip plane during the thermally activated transition has been worked out by Escaig [13] following Friedel. Assuming \(\langle \tau_{\text{III}} b/\gamma_0 \rangle < 1\) the theory results in

\[
3 \cdot \frac{\tau_{\text{III}}}{\mu} \approx \frac{\gamma_0}{\mu b} - \frac{kT}{\mu b^3} \left( \frac{\gamma_0}{\mu b} \right)^2 \frac{1860}{\left( \ln \left( \mu b / 15 \gamma_0 \right) \right)^{1/2}} \ln \left( \frac{\alpha_0}{\alpha} \right)^3.
\]

Applying eq. (10) to the experimental data of Hesse (which actually fit eq. (9) better than eq. (10)) one obtains for the strain rate sensitivity \(\left( \frac{d\tau_{\text{III}}}{d \ln \alpha} \right)\), the measured quantity which is independent of the second unknown (besides \(\gamma_0\)), \(\dot{\alpha}_0\):

\[
\left( \frac{\mu b^3}{kT} \right) \frac{d\tau_{\text{III}}}{d \ln \alpha} \approx \frac{\mu}{\tau_{\text{III}}} \cdot 40
\]

from experiment, see eq. (9);

\[
\approx \left( \frac{\gamma_0}{\mu b} \right)^2 \frac{620}{\left( \ln \left( \mu b / 15 \gamma_0 \right) \right)^{1/2}}
\]

from theory, eq. (10).

The comparison yields \(\gamma_0 = 16 \text{ ergs/cm}^2\) for NaCl, a value at least a factor 12 smaller than the theoretical one, see table I. The cross slip theory as it stands does not fit the data on NaCl.

4. The effect of hydrostatic pressure. — Hydrostatic pressure has only a small effect on the plastic deformation of fcc metals (Haasen and Lawson [14]). It can be explained by changes of the elastic constants, lattice parameters, and probably of the rate of point defect production with pressure. The same is true for alkali halides during the work hardening stages I and II. There is, however, a strong and unique decrease of work hardening with increase of pressure in stage III of the deformation of NaCl, see figure 3 (Davis and Gordon [15], Aladag et al. [16], Davis [17]). An increase of pressure during stage III deformation leads to work softening just like an increase of temperature. It is tempting to interpret the change of the cross slip initiation stress \(\tau_{\text{III}}\) as an effect of hydrostatic pressure on the dilatation connected with a \((110)\) stacking fault, see eq. (6) (Fontaine and Haasen [2], Haasen et al. [18]). Figure 4 shows \(\tau_{\text{III}}(p)\) for NaCl deformed at two strain rates at 300 K according to Davis [17]. \(\tau_{\text{III}}\) decreases with increase of pressure up to \(p = 5 \text{ kbar} = 50 \text{ kg/mm}^2\) and then remains independent of \(p\) and \(\dot{\alpha}\) at a value of \(\tau_{\text{III}} \approx 30 \text{ bar} = 0.3 \text{ kg/mm}^2\). We want to compare now the experimental values of \(\tau_{\text{III}}(p, \dot{\alpha})\) with the theory for the width of the stacking fault, eq. (7), leading to \(\dot{\alpha} \gamma_{\text{eff}} = \gamma_0 + \dot{\alpha} b \phi / 2\), by means of eq. (9) and (10).

Eq. (9) from the theory of Seeger et al. yields approximately

\[
\frac{d \ln \tau_{\text{III}}}{d p} \mid_{\text{atm}} = -820 \frac{kT \gamma_0}{\mu^2 b^4} \ln \left( \frac{\alpha_0}{\alpha} \right) \left\{ \frac{d \ln \gamma_{\text{eff}}}{d p} - 2 \frac{d \ln \mu}{d p} - 4 \frac{d \ln b}{d p} \right\}.
\]
The first, second and third terms in the brackets are (in units of \(10^{-12}\) cm\(^2\) dyn) + 30.8, -29.4 and + 5.7, respectively. The total effect calculated
\[
\frac{d \ln \tau_{\text{HI}}}{dp} \text{calc} \approx -0.015/\text{kbar}
\]
therefore depends on a delicate balance between about equal, but opposing factors and is only in rough agreement with the measured effect, see figure 4,
\[
\frac{d \ln \tau_{\text{HI}}}{dp} \text{exp} \approx -0.25/\text{kbar}.
\]
The pressure dependence of the strain rate sensitivity has the advantage of being independent of \(a_0\). It follows from (11)
\[
S = \frac{d}{dp} \left( \frac{d \ln \dot{\alpha}}{d \ln a_0} \right) \approx \frac{1}{\ln \dot{\alpha}/a_0} \frac{d \ln \tau_{\text{HI}}}{dp} \approx +10^{-2}/\text{kbar}
\]
while experimentally \(S \approx -3 \times 10^{-2}/\text{kbar}\), see figure 4. Here we even obtain the wrong sign for the effect due to the balance effect mentioned above. For any thermally activated process with a stress as well as pressure dependent activation energy \(U(\tau, p)\) one obtains
\[
kT \frac{\partial}{\partial p} \left( \frac{\partial \ln \dot{\alpha}}{\partial \tau} \right) = -\frac{\partial^2 U}{\partial p \partial \tau}.
\]
Defining an activation area \(A\) by
\[
-\frac{\partial U}{\partial \tau} = Ab = 1bd,
\]
one expects for thermally activated cross slip \(d\) to be proportional to the width of dissociation. This width should decrease with increasing pressure, therefore, \(\partial^2 U / \partial p \partial \tau > 0\) so the experimentally found sign of
\[
\frac{\partial}{\partial p} \left( \frac{\partial \tau_{\text{HI}}}{\partial \ln a_0} \right) < 0
\]
appears to be correct. If \(\sigma_0\) were about 20\% smaller (or \(\gamma_0\) larger) than predicted from theory, the pressure dependence calculated for the strain rate sensitivity would change sign according to eq. (10). The same sign difficulty arises with Escaig’s theory, eq. (10); the numerical discrepancies are even worse. It appears, however, that the idea of cross slip determining state III of NaCl via a pressure dependent stacking fault energy is basically correct. According to Davis and Gordon (unpublished) pressure has no effect on work hardening of crystals compressed along \(< 111>\) which indeed slip on \{111\} and \{001\} planes (Franzbecker [7]).

5. Creep by dislocation climb. — Climb should be reduced by a dissociation of the dislocations. At high temperatures creep of single crystals is usually considered to be controlled by dislocation climb. The stationary creep rate follows a relation
\[
\dot{\alpha}_s = bNL \left( \frac{V_j}{h} \right) c_j b
\]
where:
- \(N\) is the mobile dislocation density,
- \(L\) their mean free path of glide,
- \(V_j = \frac{D}{kT} n b^2 \tau\) the drift velocity of a jog under a stress \((\tau r)\) for a diffusion constant \(D\),
- \(c_j\) the number of jogs per unit length of dislocation,
- \(h\) the height of the obstacle the dislocation has to climb over.

Normally one assumes \(N \sim \tau^2, h \sim \tau^{-1}\) (for dislocation-dislocation interaction) and some stress dependence of the other parameters of the dislocation arrangement, so that eq. (12) becomes (with \(n = 4, ..., 5\) and a dimensionless constant \(C\))
\[
\dot{\alpha}_s = C \frac{D}{kT} n b (\frac{\tau}{\mu b})^x f(\frac{\gamma_0}{\mu b}).
\]
Empirically Mohamed and Langdon [19] find for eight fcc metals \(f(\gamma_0/\mu b) = (\gamma_0/\mu b)^3\). Such a decrease of \(\dot{\alpha}\) with stacking fault energy is not unreasonable, see eq. (12), as \(L\) decreases with \(\gamma_0\) because stronger obstacles (dissociated LC-dislocations) are formed, and \(c_j\) decreases as intersections of dissociated dislocations become more difficult. Using this function \(f\) and the constant \(C\) obtained from fcc metals as well as \(D\) for the anion, Mohamed and Langdon calculate from creep data the stacking fault energies of LiF, NaCl, KCl to 390, 235, 135 ergs/cm\(^2\), respectively: These figures compare well with those of Fontaine, see table I.

6. Latent hardening in the NaCl structure. — Latent hardening is defined as the increase in flow stress of potential, but macroscopically inactive glide systems by slip on the primary system. The phenomenon is described as the Latent Hardening Ratio \(R = (\tau_2/\tau_1)_{\text{ex}}\), where \(\tau_2\) and \(\tau_1\) are the shear stresses in the second and first slip systems, respectively, after a prestrain \(a_0\) in system 1. Latent hardening is particularly interesting in the NaCl structure where \(R \gg 1\) is found contrary to the results on metals (Alden [20], Sankaran and Li [21], Nakada and Keh [22]). Figure 5 shows a typical specimen with the slip systems (011) [011] and (011) [110] operating when it is compressed in direction 1. During the second compression in direction 2 the previously latent and not stressed systems (110) [110] and (110) [100] or (011) [011] and (011) [011] will operate. Each pair of slip systems has mutually orthogonal Burgers vectors the dislocations
of which therefore do no interact much. A system active during $a_1$ on the other hand interacts strongly with any oblique slip system operating during compression 2 and this leads to the large $\Delta \tau = A - C$ shown in figure 5. As a function of prestrain the ratio $R$ is a maximum for $a_1 \approx 1\%$ and decreases for larger prestrains, probably because $a_1$ then is no longer produced by primary slip alone. Latent hardening persists even at high temperatures where the primary flow stress becomes temperature independent (Nakada and Keh [22]). The (maximum) $R$ values obtained for various NaCl type crystals are given in table I.

The strong temperature-independent interaction between oblique systems leading to high $R$ values seems to be consequence of the dislocation reaction

$$\frac{a}{2} [011] + \frac{a}{2} [1\overline{1}0] \rightarrow \frac{a}{2} [101] \text{ along } [\overline{1}11]$$

in (0$\overline{1}$1) | in (110) | in (12$\overline{1}$)

This reaction leads to a 50 % decrease in dislocation energy and to a sessile edge dislocation since (1$\overline{2}$1) is an only rarely observed slip plane. The reason for this may be a high Peierls force. It is also possible that the electrostatic interaction with divalent impurities immobilizes edge dislocations on {112} planes as calculated by Haasen [5] for {111} planes. (The extra half plane of an edge on {112} ends in an staggered array of equally charged ion pairs.) This interaction decreases as ions become more polarizable — so does the ratio $R$ according to Alden and Nakada et al., see table I. The stacking fault width on the other hand increases with increasing polarizability. This makes somewhat stronger because extended sessile dislocations and should increase $R$, contrary to observation. Also the difference in magnitude of $R$ between fcc metals and ionic crystals cannot be explained by the strength of the sessile obstacle but only by its mobility. In this interpretation we differ from Fontaine [1]. A dislocation intersection and jog dragging model for the latent hardening in the NaCl structure is excluded by Nakada and Keh because of the relative temperature independence of $R$. Dr. J. Hesse kindly commented on this MS.

**References**


