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DISLOCATIONS AND SLIP IN THE NaCl-STRUCTURE

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Résumé. — Les contraintes de cisaillement critique de NaCl ont été mesurées dans les plans $\{110\}$ et $\{001\}$. Leur rapport, l'anisotropie plastique, est expliqué en termes d'interaction des impuretés bivalentes avec les dislocations-cœur qui dépendent de la structure du cœur des dislocations.

Abstract. — The critical shear stresses of NaCl were measured on $\{110\}$ and $\{001\}$ planes. Their ratio, the plastic anisotropy, is explained in terms of the interaction of divalent impurities with edge dislocations which depends on the core structure of the dislocations.

1. Crystals of NaCl-structure normally slip on $\{110\}$ planes in $\langle 1\bar{1}0 \rangle$ directions—unless their ions are highly polarisable like in PbS, PbTe where $\{001\}$ slip planes are found dominating [1]. A typical experiment [2] is a constant strain rate compression test of a specimen whose long axis is parallel to $\langle 100 \rangle$. The active slip planes are identified by electron microscopy of surface replicas sputtered onto the crystals right after deformation in vacuum so that the slip steps are preserved before water vapour can wash them out [3]. Although a $\langle 100 \rangle$ crystal has 4 equivalent $\{110\}$ $\langle 1\bar{1}0 \rangle$ slip systems it is found that above the CRSS NaCl essentially deforms by single slip on one of these systems [4], figure 1. The work hardening rate is small (stage I in Fig. 2). At larger strains work hardening increases (stage II), especially for compression axes other than $\langle 100 \rangle$. Slip steps on oblique $\{110\}$ and on $\{001\}$ planes become visible then, accounting for about 10 or 1 % respectively of the total slip at the end of the stage II [3]. H. Strunk [Stuttgart, unpublished] has succeeded in doing electron transmission microscopy on $\langle 100 \rangle$ oriented NaCl compressed at room temperature. In stage II he finds dislocations of two $\{110\}$ $\langle 1\bar{1}0 \rangle$ slip systems, figures 3 and 4, which are in oblique orientation to each other, see figure 1. While the primary (edge) dislocations are relatively straight, the secondary dislocations (in contrast in Fig. 4) are rather joggy indicating that they have cross-slipped. That part of them which is parallel to the primary edges must have cross-slipped via $\{001\}$ planes in agreement with the replica results. In stage III, cross slip (of screw dislocations) becomes frequent. Matucha observes $\{001\}$ and $\{111\}$ cross slip traces on replicas, figure 5 (Franzbecker [6] also saw $\{112\}$ cross slip traces). This is confirmed by Strunk's transmission electron microscopy, which reveals also higher indices cross slip planes, figure 6. It is evident therefore that screw

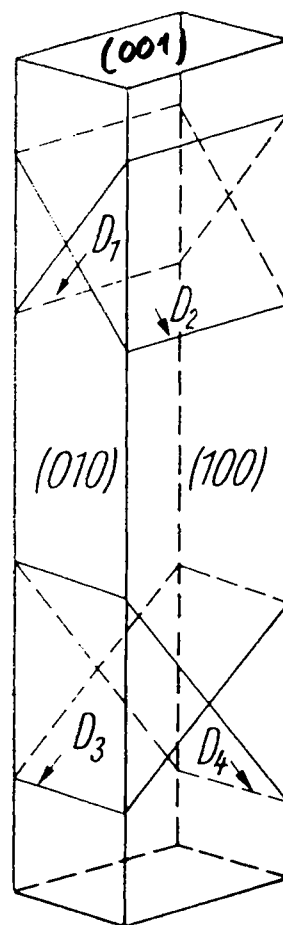


FIG. 1. — The four equally stressed $\{110\}$ $\langle 1\bar{1}0 \rangle$ slip systems of a $\langle 100 \rangle$ compression specimen, D_1 is orthogonal to D_2 , oblique to D_3 etc.

dislocations can move on planes $\{hkl\}$ other than $\{110\}$ at stresses not much higher than the CRSS $\tau_0 \{110\}$. If those $\{hkl\}$ planes are not observed as common slip planes it must be due to the difficulties edges encounter moving on these planes.

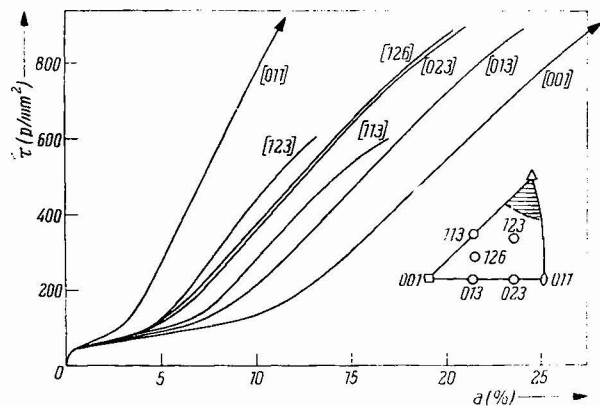


FIG. 2. — Shear stress, shear strain curves of NaCl compressed in various directions (given) at 294 K; strain rate $\dot{\epsilon} = 9.5 \times 10^{-3} \text{ s}^{-1}$ [2].

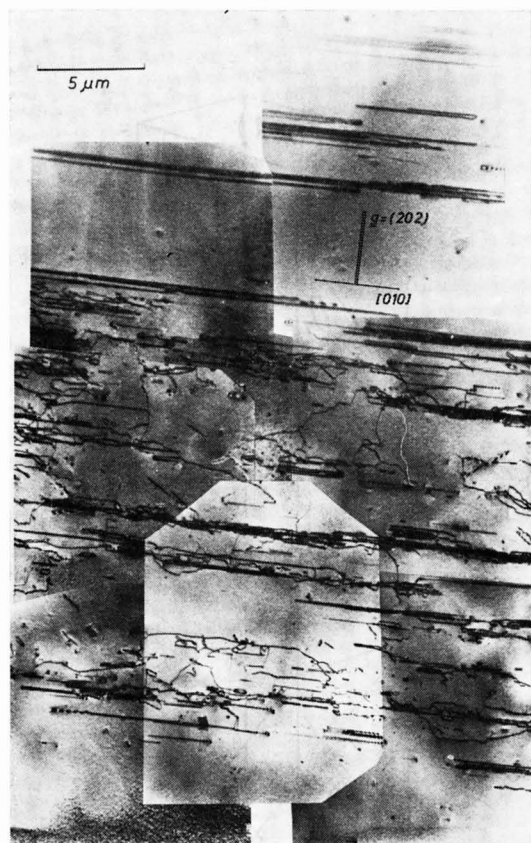


FIG. 3. — Electron transmission of NaCl, compressed parallel to $\langle 001 \rangle$, cut perpendicular to primary slip vector; traces of primary slip planes.

Crystals compressed along $\langle 111 \rangle$ do not get any outer shear stress on $\{110\}$ planes. They deform by a combination of $\{001\}$ and $\{111\}$ slip — at a very high work hardening rate [5].

In order to get a quantitative measure for the stress necessary to move (edge) dislocations on $\{001\}$ planes, shear tests have been performed [6]. A crystal layer thin compared to its width was sheared on a $\{001\}$ plane in $[110]$ direction. Only slip traces due to this slip system were visible on replicas taken

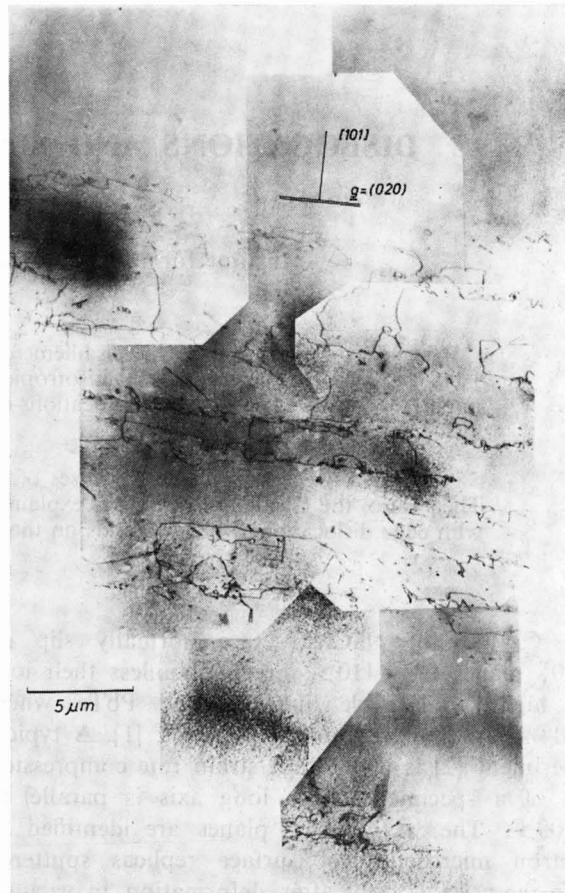


FIG. 4. — As figure 3, only secondary dislocations in contrast. Both pictures by H. Strunk (unpubl.).

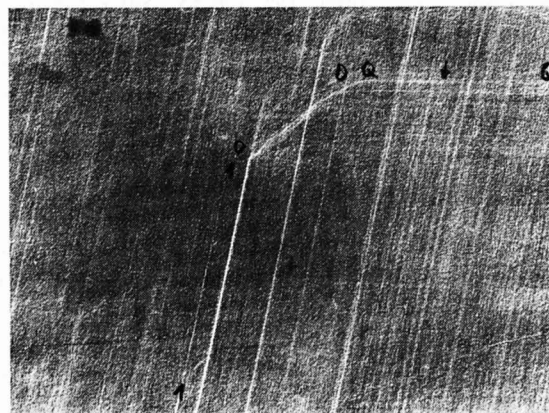


FIG. 5. — Slip steps on $\{100\}$ surface of crystal deformed from 9 to 11 % shear strain under $\tau \{110\} = 0.6 \text{ kg/mm}^2$. 1 — 1 = $\{110\}$; 0 — 0 = $\{111\}$; Q — Q = $\{100\}$ [3].

after deformation. For comparison, shear tests on the $\{110\} \langle 110 \rangle$ system gave the same CRSS $\tau_0 \{110\}$ as did compression tests. The work hardening curve in shear showed no stage II, however, but continued with a slope similar to that in stage I. The results of these tests, $\tau_0 \{110\}$ and $\tau_0 \{001\}$ for crystals of different Ca^{++} contents, deformed at various temperatures, are shown in figure 7. τ_0

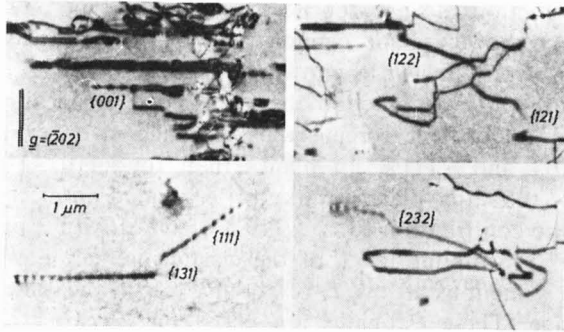


FIG. 6. — Jogs of primary dislocations in compressed NaCl after cross slip. Electron transmission (400 kV, 10^{-3} A/cm², 15 K) by H. Strunk (unpubl.).

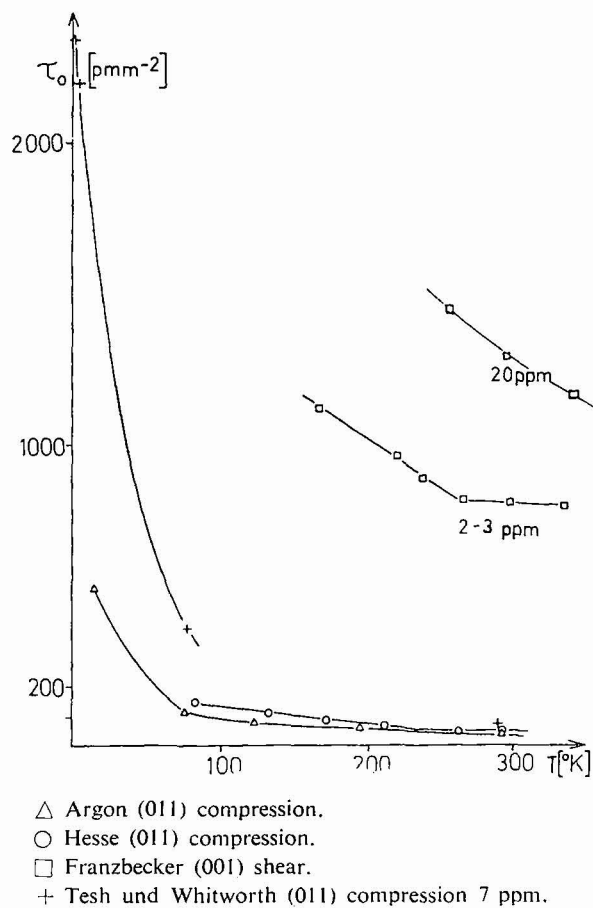


FIG. 7. — Critical shear stresses of NaCl plus various ppm Ca⁺⁺ vs. temperature for {110} and {001} slip, [6], [11], [2], [18].

increases at low temperatures and becomes temperature independent at higher temperatures: Here $\tau_0 \{001\} \approx 20 \times \tau_0 \{110\}$. Furthermore $\tau_0 \{001\} \approx 1200$ g/mm² with 20 ppm Ca⁺⁺ while $\tau_0 \{110\}$ is still below 80 g/mm² for the same doping (at 300 K).

2. What is the reason for the high and impurity-sensitive CRSS for edges on {001} planes of NaCl? The classical explanation, going back to M. J. Buer-

ger [7], is based on the core structure of dislocations in NaCl: One notes that after half a glide step $b/2$ on a {001} plane in the $\langle 110 \rangle$ direction, any ion directly above the slip plane is at equal distance from the same number of positive and negative ions directly below the slip plane, so that electrostatic binding forces cancel while the repulsive forces between their cores are at a maximum. The corresponding expansion of the lattice corresponds to a high energy state which the dislocation producing slip avoids except under a high (Peierls) stress. On {110} on the other hand the half glide position is a low energy state which made Fontaine [8] propose that it is always connected with dislocations, i. e. that $\langle 110 \rangle$ dislocations dissociate into partial dislocations. The width of dissociation on {110} planes is about $6b$ for NaCl [9]; there is also a lattice expansion across the stacking fault which makes plastic deformation of NaCl sensitive to hydrostatic pressure. On {001} planes dislocations are less widely dissociated; on {111} probably more so. This is due to the homogeneous charge on either side of the slip plane: positive ions above, negative below or vice versa. If a slip step on such a plane is formed at the surface, charge of one sign is exposed creating a strong electric field. It is indeed surprising that {111} slip steps are observed at all. None of the above arguments for or against non — {110} slip differentiates between edge and screw dislocations — contrary to the experimental observations described under 1.

The most detailed calculation of the structure and energies of the core of an edge dislocation on {110} and {001} has been performed by F. Granzer [10] using a variational method. The following contributions to the interaction potential between atom rows parallel to the dislocation line are considered: a) The electrostatic interaction; b) Two forms of a repulsion potential according to Born-Pauling or Born-Mayer-Huggins; c) A van der Waals-interaction; d) A polarisation potential. At the boundary of the core the displacements are fitted to those of the isotropic or anisotropic elastic theories. Figures 8 and 9 show the atomic positions in the cores of edge dislocations on {110} and {001} planes, the latter for two symmetry positions. The assumed symmetries did not allow for a dissociation into partials, though. The maximum slope of the potential energy of the dislocation between these two symmetry positions is the Peierls force. It gives the stress τ_{po} necessary to move the (edge) dislocation at $T = 0$. At finite temperatures kink formation becomes possible and the dislocation moves already under a smaller stress: In fact this stress should fall continuously with increasing temperature and should not show a high temperature « plateau ». Granzer calculates $\tau_{po} \{110\} = (1.4 \dots 2.1)$ kg/mm² which is of the same magnitude as the CRSS $\tau_0 \{110\}$ of NaCl measured at 4 K [11]. According to these measurements $\tau_0 \{110\}$

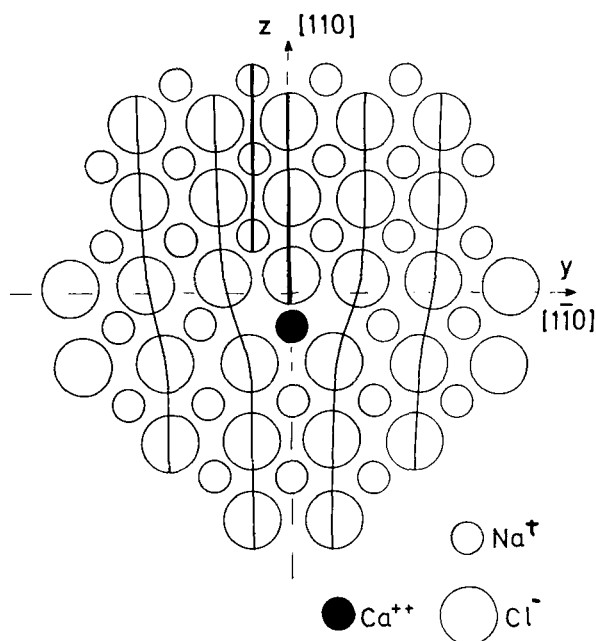


FIG. 8. — Core structure of edge dislocation on $\{110\}$ calculated by Granzer [10].

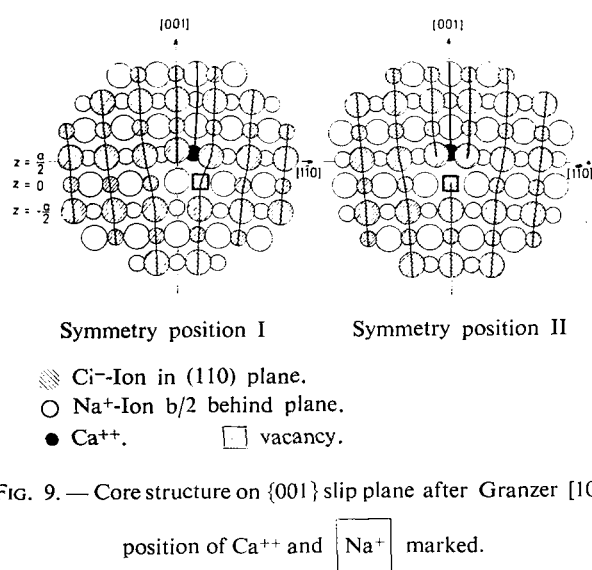


FIG. 9. — Core structure on $\{001\}$ slip plane after Granzer [10];

position of Ca^{++} and Na^+ marked.

drops rapidly to $1/10 \times \tau_{po} \{110\}$ already at 77 K. The Peierls stress $\tau_{po} \{001\}$ estimated by Huntington *et al.* [12] is ten times larger than $\tau_{po} \{110\}$. Granzer [10] estimates a core energy ratio for dislocations on $\{001\}$ and $\{110\}$ planes of 1.6 for NaCl and of 1.1 for AgCl and takes this as crude measure of the «plastic anisotropy» of these ionic crystals. All of these arguments fail, however, in explaining the large, rather temperature-insensitive but impurity sensitive CRSS $\tau_0 \{001\}$ of NaCl between 250 and 350 K, see figure 7.

3. It is tempting to ascribe $\tau_0 \{001\}$ in this temperature range to the interaction between dislocations and (divalent) impurities. It is well known that such an interaction affects edges more than screws. *Elastic*

interactions do not depend much on the type of slip plane, however, and cannot easily explain the plastic anisotropy. It will be shown in the following that the *electrostatic* interaction between edge dislocations and multivalent foreign ions is much stronger for $\{001\}$ and $\{111\}$ slip planes than for $\{110\}$ [13]. For the latter plane Frank [14] estimated an electrostatic contribution to $\tau_0 \{110\}$ of NaCl with 2 ppm Ca^{++} of about 15 % of the elastic interaction with the same ions at low T , of about 25 % in the plateau range. These estimates are based on Fleischer and Schöck-Seeger types of solution hardening theories and give $\tau_0 \sim \sqrt{c_{\text{Ca}^{++}}}$ or $\tau_0 \sim c_{\text{Ca}^{++}}$, respectively, for the dependence on calcium ion concentration $c_{\text{Ca}^{++}}$. Frank assumed furthermore a charge density on the dislocation of one e per (12-20) atomic sites as is suggested by experiments [15].

The different strengths of the electrostatic interaction with a foreign ion close to the slip plane results from the different ionic arrangements along the extra half plane of an edge dislocation on various slip planes, figures 10 and 11: On $\{110\}$ positive and negative ions alternate in each row along the dislocation while on $\{001\}$ each row consists of ions

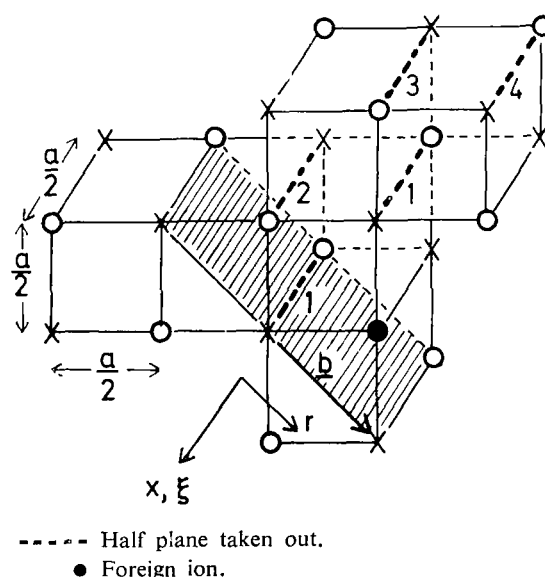


FIG. 10. — Geometry of half planes to be neutralized for dislocation on $\{110\}$; $\bullet = \text{Ca}^{++}$.

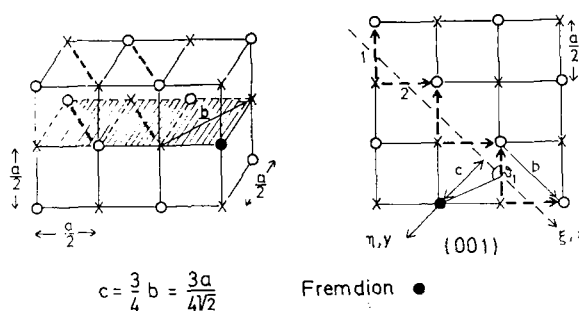


FIG. 11. — Geometry of half planes to be neutralized for dislocation on $\{001\}$; $\bullet = \text{Ca}^{++}$.

of the same sign. The maximum interaction energy U_{\max} of the dislocation with a divalent impurity has been estimated in two approximations:

a) A $\{1\bar{1}0\}$ half plane is electrically neutralized by superposing ions of opposite charge. The interaction of these ions with the Ca^{++} ion close-by is calculated according to Madelung [16].

b) Changes in this interaction are estimated when the $\{1\bar{1}0\}$ half plane is actually removed and the surrounding lattice allowed to relax.

CASE a), SLIP PLANE $\{110\}$. — The potential at the position (x, y) of each neutralising row, figure 10, is:

$$\varphi(x, y) = \frac{1}{\varepsilon} \int \frac{\rho(\xi) d\xi}{\sqrt{(x - \xi)^2 + r^2}};$$

$$\rho(\xi) = \sum_n \rho_n \exp\left(\frac{2\pi i n \xi}{a}\right) = e \delta(\xi) - e \delta\left(\xi - \frac{a}{2}\right) \quad (1)$$

ε is the static dielectric constant.

The integral leads to the function $K_0(2\pi n r/a)$ which is rapidly converging, so that only $n = 1$ needs to be considered asymptotically

$$\varphi(x, y) = \frac{2e}{\varepsilon a} \cos \frac{2\pi x}{a} \sqrt{\frac{a}{r}} \exp\left(-\frac{2\pi r}{a}\right). \quad (2)$$

The potential is a maximum for a Ca^{++} position one half period above the slip plane, figure 10, at which (to within 10 %) only the two rows No. 1 contribute

$$\left. \begin{aligned} \Phi &\approx 2 \varphi\left(0, \frac{a}{2}\right) \approx \frac{e}{\varepsilon a} \cdot 0.21 \\ U_{\max}^{\text{Ca}^{++}\{110\}} &= 2 e \varphi \approx 0.2 \text{ eV} \end{aligned} \right\} \quad (3)$$

Frank [14] estimates the maximum *elastic* interaction energy to 0.7 eV for this case.

CASE b), $\{110\}$. — Allowing the ion rows near the eliminated ones now the relax to their equilibrium positions in a dislocation, figure 8, there will be a strong interaction only with Ca^{++} sites in the core which have a strongly distorted neighborhood. Due to the extremely short range of the potential (2), we expect only the position in figure 8 to be of importance. The interaction energy will then be of the magnitude given by eq. (3). Interesting enough there is no 2nd position of similar interaction strength but opposite sign for the Na^+ -vacancy which is associated with a Ca^{++} at this position at not too high temperatures.

CASE a), $\{001\}$ is more difficult to treat because the ions in a row have the same sign, see figure 11. We combine pairs of rows into dipoles 1 and 2 of strength $p = e/2 \cdot a/2$ each, but of orthogonal orientations. The potential at the position $(0, c, z)$, see

figure 11, which each neutralizing double row produces, is then

$$\varphi(0, c, z) = -\frac{p}{\varepsilon} \int \frac{\rho_1 \cos \theta_1 + \rho_2 \cos \theta_2}{\xi^2 + c^2 + z^2} d\xi \quad (4)$$

with

$$\rho_1(\xi) = \delta\left(\xi - \frac{b}{4}\right); \quad \rho_2 = \delta\left(\xi - \frac{3}{4}b\right); \quad r^2 = c^2 + z^2;$$

$$\sqrt{2} \cos \theta_{1,2} = \frac{\pm \xi - r}{\sqrt{\xi^2 + r^2}};$$

$$\rho_j = \sum_n \rho_n^{(j)} \exp\left(\frac{2\pi i n \xi}{b}\right).$$

Using for $n \neq 0$ again the K_0 representation asymptotically, only the $n = 1$ term is important and only for $z = 0$

$$\varphi_{10}(0, c, 0) \approx \frac{-e}{a\varepsilon} 0.51 \gg \varphi_{11}\left(0, c, \frac{a}{2}\right). \quad (5)$$

Furthermore for the Fourier term $n = 0$ eq. (4) becomes

$$\begin{aligned} \varphi_{0m}(0, c, z_m) &= (-1)^m \frac{2pr}{\varepsilon \sqrt{2} b} \int \frac{d\xi}{(\xi^2 + r_m^2)^{3/2}} \\ &= (-1)^m \frac{2\sqrt{2}p}{\varepsilon b r_m}. \end{aligned} \quad (6)$$

The $n = 0$ term, summed over all $z_m = ma/2$ ($m=0, 1, \dots$) converges so slowly that it is imperative to take into account the distorted lattice quantitatively.

CASE b), $\{001\}$. — We obtain the distorted arrangement of ion rows from the undistorted one by adding rows of dipoles such that the undistorted ion positions are cancelled and the distorted ones established, see figure 12. We will calculate the potential φ_d

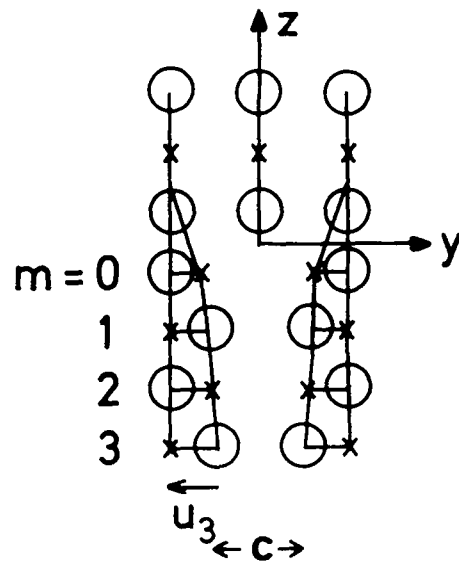


FIG. 12. — Displacement dipoles $e \cdot u_m(z)$ to produce dislocation on $\{001\}$; only half to the vertical ion rows shown.

of these dipole rows only at the Ca^{++} position of maximum distortion, which according to figure 9 has the coordinates $(0, c, z_1 = a/2)$. Interesting enough there is a second position of equal interaction of opposite sign below the $\{001\}$ slip plane which the Na^+ -vacancy will take if the $\text{Ca}^{++} - \boxed{\text{Na}^+}$ dipole is free to rotate (above 250 K).

The potential of the 2 dipole rows at z_m is according to eq. (6)

$$\varphi_{dm}\left(0, c, \frac{a}{2}\right) = \frac{4\sqrt{2}e}{\epsilon b} \frac{u_m(-1)^m}{\sqrt{\left(z_m - \frac{a}{4}\right)^2 + c^2}},$$

$$z_m = -\frac{2m+1}{4}a, \quad m = 0, 1, \dots \quad (7)$$

with

$$u_m = \frac{b}{2\pi} \left[\arctg \frac{z_m}{c} + \frac{z_m c}{2(1-\nu)(z_m^2 + c^2)} \right],$$

being the displacement field of an edge dislocation according to isotropic elasticity. The potentials of the planes $m = 0$ and 1, $\varphi_{d0} \approx -\varphi_{d1}$ just about cancel each other at the position $(0, c, a/2)$; the potentials of the more distant displacement dipoles ($m = 2, 3, \dots$) cancel those of the neutralisation dipoles according to eq. (6). The remaining interaction potential stems from the $n = 0$ terms of the first two rows of neutralizing dipoles, $m = 0$ and 1 of eq. (6), and is to be taken at the displaced position of the Ca^{++} in the plane

$$z = \frac{a}{2}, \quad y = \frac{5}{8}b.$$

The result is

$$\Phi = \frac{-e}{\epsilon a} \cdot 1.2 \quad \text{and} \quad U_{\max}^{++}\{001\} = -1.15 \text{ eV}.$$

The interaction is attractive as is the elastic one. A potential of similar strength but opposite sign is felt by a Na^+ -vacancy in the plane $z = -a/2$ as indicated in figure 9. If the Ca^{++} ion is associated with a Na^+ -vacancy and if this dipole is able to rotate freely as we expect it will in the temperature range of interest (see Fig. 7) then the interaction energy of the $\{001\}$ dislocation with the dipole is $2 U_{\max}^{++}\{001\} \approx 2.3 \text{ eV}$ which is 11 times the maximum interaction energy on $\{110\}$. This factor 11 enters linearly into the Schöck-Seeger flow stress of a solid solution of rotating solute dipoles (plateau stress) but to the 3/2 power ($= 36$) into the low temperature flow stress of a solid solution according to Fleischer [14]. Of course the elastic interactions must be superposed onto the electrostatic ones discussed above but it is clear that the latter can explain qualitatively the plastic anisotropy of NaCl as shown in figure 7.

The electrostatic interaction will be still stronger for an edge dislocation on $\{111\}$ whose extra half planes end in rows of ions of the same sign. A rough estimate according to the arguments given above for the $\{001\}$ dislocation yields

$$U_{\max}^{++}\{111\} \approx 2.5 U_{\max}^{++}\{001\}$$

explaining observations that it is still more difficult to activate macroscopic $\{111\}$ slip (by compressing $\langle 111 \rangle$ oriented crystals) than it is to produce slip on $\{001\}$ [5]. Franzbecker [6] was unable to shear NaCl crystals on $\{111\}$; they always yielded on less favorably oriented $\{110\}$ planes [6]. It will be very interesting to measure the plastic anisotropy of other substances with NaCl structure which have more polarisable ions, see [17].

4. Conclusions. — The critical shear stresses of NaCl were measured on $\{110\}$ and $\{001\}$ planes. Their ratio, the plastic anisotropy, is explained in terms of the interaction of divalent impurities with edge dislocations which depends on the core structure of the dislocations.

References

- [1] GILMAN, J. J., *Acta Met.* **7** (1959) 608.
- [2] HESSE, J., *Phys. Stat. Sol.* **9** (1965) 209.
- [3] MATUCHA, K. H., *Phys. Stat. Sol.* **26** (1968) 291.
- [4] HESSE, J. and MATUCHA, K. H., *Scripta Met* **6** (1972) 865.
- [5] FRANZBECKER, W., Dipl. Thesis Göttingen (1969).
- [6] FRANZBECKER, W., ph. d. Thesis Göttingen (1972), *Phys. Stat. Sol.* **57** (1973) 545.
- [7] BUEGER, M. J., *Am. Mineral.* **15** (1930) 226; **16** (1931) 237.
- [8] FONTAINE, G., *J. Phys. Chem. Sol.* **29** (1968) 209.
- [9] FONTAINE, G. and HAASEN, P., *Phys. Stat. Sol.* **31** (1969) K 67.
- [10] GRANZER, F., Habil. Thesis Frankfurt (1970); GRANZER, F., WAGNER, G. and EISENBLÄTTER, J., *Phys. Stat. Sol.* **30** (1968) 587.
- [11] TESH, J. R. and WHITWORTH, R. W., *Phys. Stat. Sol.* **39** (1970) 627.
- [12] HUNTINGTON, H. B., DICKEY, J. E. and THOMSON, R., *Phys. Rev.* **100** (1955) 1117.
- [13] HAASEN, P. and FRANZBECKER, W., *Nachr. Göttg. Akad. Wiss.* (1973) in press.
- [14] FRANK, W., *Phys. Stat. Sol.* **29** (1968) 391 and private communication.
- [15] WHITWORTH, R. W., *Phil. Mag.* **15** (1967) 305.
- [16] MADELUNG, E., *Phys. Zeits.* **19** (1918) 524.
- [17] CHIN, G. Y., VON KITERT, L. G., GREEN, M. L. and ZYDZIK, G., *Scripta Met* **6** (1972) 475.
- [18] ARGON, A. S. and PADAWER, G. E., *Phil. Mag.* **25** (1972) 1073.

DISCUSSION

J. S. DRYDEN. — It is an experimental fact, that in alkali halides doped with divalent ions the shear stress is the same whether the divalent ion-vacancy pairs are present as individual pairs or in small clusters (possibly containing three divalent ion-vacancy pairs). Has this fact been considered by Dr. Haasen in his calculations ?

P. HAASEN. — I assume that the experimental observations cited by Dr. Dryden refer to [110] slip. I have shown that for this plane it is not possible to get both partners of a pair into positions of maximum attractive interaction with a dislocation. I assume therefore that associations of pairs does not change the strength of interactions. Of course the Snoek interaction (of rotating pairs) turns into the Fleischer interaction of static ones which is stronger. On the other hand the concentration of obstacles

decreases with the association of pairs. It appears possible to account for the observations by a combination of these effects.

H. L. FOTEDAR. — In your slide of yield stress dependence on temperature it is shown that the critical temperature at which yield stress becomes independent of temperature is very much impurity sensitive for [100] slip and not for [110] slip. Would you comment on what causes this impurity sensitivity of critical temperature for [100] and not for [110] slip in NaCl.

P. HAASEN. — For $\{001\}$ slip the critical temperature marks the transition between two processes, Fleischer and Snoek, by which impurities interact with a dislocation. The low temperature rise of the yield stress for $\{110\}$ slip on the other hand appears to be caused by the Peierls potential.