A SINGLE SLIP LINE IN KCl:Pb

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Sometimes single slip lines are observed in KCl:Pb upon compression of samples in the <100> direction. These lines should be macrodislocations with Burgers vector along <110>, built up at the intersection of a subboundary and a <110> slip plane.

In the course of a study on the optical [1] and the piezospectroscopic [2] properties of KCl:Pb we noticed some singular phenomena. Upon compression of KCl:Pb samples single slip lines appeared in addition to the usual slip systems, when the samples were observed through a polarizing microscope. In fig. 1 we present a photograph of such a single slip line against the background of the usual $\{1\bar{1}0\}<110>$ systems. In other crystal directions similar lines can be observed. In fig. 2 such lines are shown seen end-on. What can they be ?

The first question to be solved is whether dislocations are involved. This must be the case because before stressing and after annealing of the samples the line was not observed.

The second question is what the photographs present. Fig. 1 was taken with the polarizer and analyzer of the polarizing microscope along

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<110> directions, fig. 2 with the polarizer and analyzer along <100>. In these positions the greatest contrast is obtained. As the main stresses around the dislocations are directed parallel and perpendicular to the Burgers vector, the Burgers vector must be directed along <110> in fig. 2. The projection in the plane of fig. 1 is then parallel to <100>. Comparison with the literature shows that these phenomena have not yet been reported in KCl, but that there is a striking similarity with pictures of single dislocations in Ge and Si, see fig. 60, 65 and 121 in Amelinckx's review [3]. Of course, it is not likely that one dislocation can be observed with the magnification used, but a macrodislocation is quite possible. It consists of a great number of parallel dislocations with the same Burgers vector along <110>, i.e. normal dislocations as produced by the stress.

The last question is how the macrodislocation is formed. It is probable that the constituent dislocations are pinned at a specific subboundary, the
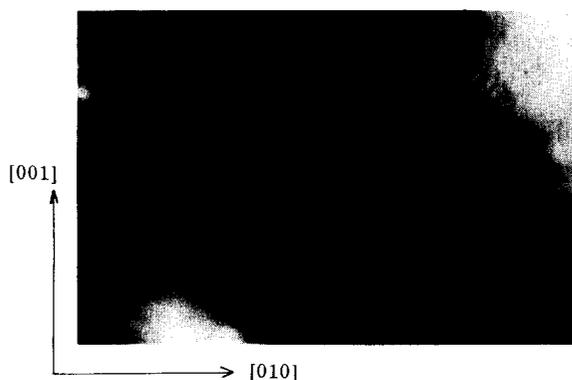

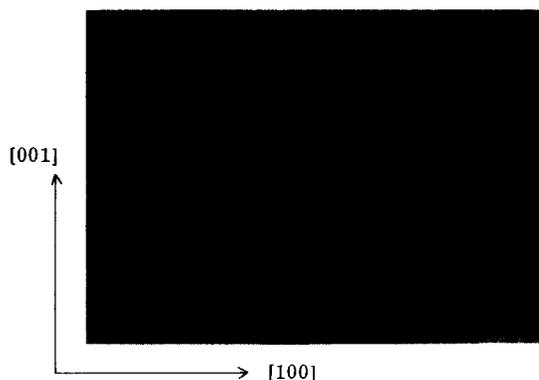Fig. 1. Single slip line in KCl:Pb seen along a ⟨110⟩ direction (×40).

Fig. 2. Similar lines as in fig. 1 seen end-on along a ⟨100⟩ direction (×100).

very same line often reappearing at the same place upon annealing and reloading of the samples. Where do the dislocations come from ? One might think of two alternative solutions: the source is situated far from the subboundary somewhere in the crystal, or the subboundary itself acts as a source. In the first case the pinned dislocations have predominantly edge character, and in the second case screw character. Arguments can be found for and against both possibilities. Fig. 2 supports the idea of edge dislocations [3], but it is not clear why dislocations from the one source are pinned, while dislocations from another source are passed. This difficulty is not present if the subboundary itself is a source, for it is very well conceivable that only special parts of it generate dislocations. Some authors, however, state that screw dislocations do not give rise to birefringence [4].

References
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THE INFLUENCE OF THE POTENTIAL ON ELECTRON ENERGY BANDS IN ALKALI HALIDE CRYSTALS

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The electronic band structure of NaCl is investigated using six different types of potentials in order to explain the difference in the results obtained for NaCl by Kunz from that obtained by Clark and Kliewer. It is found that the "muffin-tin" treatment of the potential produces significant changes in the conduction band structure.

In recent months several calculations on the electronic band structure of NaCl have become available [1-3]. The methods of calculation used differ significantly, as do certain of the results. The calculation of Kunz features the orthoganalized plane wave method and a potential which is a superposition of free ion potentials for the Na^+ and Cl^- ions [1]. The calculation of Clark and Kliewer involves the augmented plane wave method and a "muffin tin" potential [2]. The third calculation given by Fong and Cohen involves an empirical pseudopotential [3].

While results of Kunz and Cohen are quite similar in many qualitative features, the bands computed by Clark and Kliewer differ greatly from those of Kunz in many ways. In particular Clark and Kliewer find that the d-like conduction bands lie much higher above the s like conduction bands than do these of Kunz or of Fong and Cohen. Clark and Kliewer find that at the point X in the first Brillouin zone, X_1, which is s-like, lies lower than X_3, which is d-like, whereas both Kunz and Fong and Cohen find the reverse to be true. In this paper we examine the band structure of NaCl for six choices of crystal potential in order to understand the differences between the calculations.

Firstly results are obtained using the Hartree-Fock-Slater potential with the Latter tail [4]. This potential is also reused in the "muffin tin" approximation using the prescription of Clark and Kliewer [2]. Thirdly the many body exchange potential of Robinson et al is used [5]. The fourth and fifth potentials are two Lindgren exchange potentials [6] which have the form

$$rV_{ex}(r) = c[81/4\pi^2)]^{\frac{1}{3}} r^{\frac{1}{3}n} \rho(r)^{\frac{1}{3}m} \qquad (1)$$