but measurements of any changes in atomic positions are obviously of prime importance to the formulation of a more complete theory of ferroelectricity in the KH<sub>2</sub>PO<sub>4</sub> class of ferroelectrics. Such changes have been found in our study, and these are presented briefly in this letter. Only minor refinements of secondary importance to the physical picture of the transition remain to be considered. Publication of a complete paper is being deferred until these have been checked.

The procedure followed was that of solving the tetragonal structure just above the Curie temperature, and then using these results to proceed to the more difficult structure just below. The observation temperatures were 126°K and 116°K. Intensities from a small single crystal were recorded photographically, and for any one oscillation range the observations at the two temperatures were recorded side-by-side by use of a movable camera in conjunction with a multi-layerline shield. The problem of spot splitting and superposition of nonequivalent reflections caused by domain structure was eliminated by choosing the base diagonal of the "F" cell as rotation axis. This will be discussed in more detail in the full publication. The tetragonal structure was redetermined at 126°K (instead of working from West's structure) for several reasons: (1) to study temperature corrections for the intensities, (2) to discover any changes relative to the room temperature structure that might be important to the transition, (3) to provide a closer comparison to the 116°K structure. One of the significant results was that of finding that a rather strong anisotropy in thermal vibrations had developed along the c-axis, in which direction the crystal spontaneously polarizes at the transition temperature. This was corrected for in the calculated structure factors rather than the observed.

The results of the two structure analyses and West's room temperature structure are compared in Table I. The interatomic distances are based on the tabulated cell dimensions. Those for the room temperature structure are not the ones presented in West's paper, but are obtained from the more accurate values found by Ubbelohde and Woodward by transforming from the "I" to the "F" cell. A combination of the thermal contraction data of these authors with that of de Quervain was found to check very well for the low temperature values.

The O, O distance refers to oxygens of the same elevation in the c-direction for a given PO4 group. O, O' refers to oxygens of opposite elevation. K, O refers to distances between a potassium and closest oxygens belonging to P's having the same (x, y)coordinates as the K, while K, O' refers to closest oxygens belonging to P's displaced by  $(\pm \frac{1}{4}, \pm \frac{1}{4}, \pm \frac{1}{2})$  from the K.

On cooling to 126°K it is noted that the slightly elongated O<sub>4</sub> tetrahedra at room temperature have become perfectly regular. A marked contraction in the hydrogen bond has occurred. It is noticeable also that while each K was surrounded by two equidistant sets of oxygens at room temperature, the K, O distances are distinctly larger than the K, O'. These elongated distances have their principal component along the c axis, which is just the direction along which the preferential thermal vibration has developed and is the direction of polarization after the transition.

TABLE I. Interatomic distances and lattice dimensions in KH<sub>2</sub>PO<sub>4</sub> above and below the Curie point.

	Room temp.	126°K	116°K
Sp. Gp.	$F\overline{4}d2$	$F\overline{4}d2$	Fdd
P, O	1.56A	1.57A	{1.59A 1.54
0,0	2.46	2.57	2.55
0,0'	2.60	2.57	2.55
0 – H · · · 0	2.53	2.45	2.49
К, О	2.79	2.85	
К, О′	2.82	2.78	2.77 2.78
a	10.516	10.48	10.53
b	10.516	10.48	10.44
c	6.945	6.90	6.90

After the transition, it is seen that the O<sub>4</sub> tetrahedron has remained regular, but that the P's have "sagged" from their central positions. This displacement, which is parallel to the c axis, is calculated to be 0.03A. The hydrogen bond has expanded, which suggests an increased order in agreement with the Slater theory. The c-axial component of the K displacement is calculated to be 0.08A relative to the P's and 0.05A relative to the O<sub>4</sub> tetrahedra. This is particularly interesting not only because of the heretofore unsuspected role of the K's in contributing to the polarization, but also because their behavior suggests that they may even trigger the transition. This could be of importance in explaining the pecularities of the  $\rm NH_4H_2PO_4$  transition.  $^5$  These matters will receive more attention in the complete report.

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## The Production of Large Tensile Stresses by Dislocations\*

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ONSIDER n similar straight parallel dislocations moving on  $\checkmark$  the same glide plane; suppose that these dislocations are pushed up against an obstacle by a uniform external shearing stress t. Then Cottrell<sup>1</sup> and later Eshelby, Frank, and Nabarro<sup>2</sup> have shown that the force exerted towards the obstacle on the dislocation nearest the obstacle is tnb, where b is the magnitude of the Burger's vector of the dislocation. In this equilibrium situation the forward force is balanced by the force exerted by the obstacle. It is assumed in these calculations that the obstacle interacts only with the nearest dislocation. Since the forward force on a single dislocation is only tb, it is clear that such dislocation arrays are effective means for the concentration of shearing stresses. In fact, in reference 2 it is shown that the shearing stress on the glide plane ahead of the n jammed dislocations under stress t is approximately the same as that ahead of a twodimensional crack of width 4L under stress t. L is the distance along the glide plane occupied by the *n* dislocations; *L* is, of course, measured along a direction perpendicular to the axes of the dislocations.

It is the aim of this letter to show that an edge type dislocation array of the type described above has large tensile stresses associated with it. It will be shown that the maximum tensile stress is of the order of nt.

Let the dislocations be numbered 0, 1,  $2 \cdots j \cdots (n-1)$ , where the zeroth dislocation is the one nearest the obstacle. Suppose that the zeroth dislocation is at the origin of coordinates and the others are located along the plus x axis, the shearing stress t is such that it drives the dislocations towards negative x coordinates. The position of the jth dislocation is<sup>2</sup> approximately given by  $x_i = (\pi j)^2 A/8nt$ , where  $A = Gb/2\pi(1-\nu)$ . G is the modulus of rigidity and  $\nu$  is Poisson's ratio. The stresses near a single positive edge type dislocation are,<sup>3</sup>

$$\sigma_x = -A y (3x^2 + y^2)/r^4,$$
  

$$\sigma_y = +A y (x^2 - y^2)/r^4,$$
  

$$t_{xy} = +A x (x^2 - y^2)/r^4,$$
  
(1)

where x measures the distance of the field point from the dislocation along the glide plane, y measures the distance to the dislocation normal to the glide plane, and  $r^2 = x^2 + y^2$ . Consider first the tensile stress  $\sigma_x$  in the x direction. It is clear upon examination that the largest tensile stress will be found along the negative y axis (using the coordinates described for the array).

Since the equations of elasticity are linear, we have,

$$\sigma_x = -Ay \sum_{j=0}^{n-1} \frac{3\{(j\pi)^2 A/(8nt)\}^2 + y^2}{\{(j\pi)^2 A/(8nt)\}^2 + y^2\}^2}.$$

Upon introducing a dimensionless variable z such that

$$x = -\frac{8nt}{\pi^2} z \sum_{j=0}^{n-1} \frac{3j^4 + z^2}{(j^4 + z^2)^2}.$$

This series gives  $\sigma_x = \infty$  at z = 0. This singularity appears because the stresses near a single dislocation go as 1/r. Since we wish to investigate magnification of stresses by an array rather than the stress field of a single dislocation, we omit the term in the series having j=0; i.e., we calculate the tensile stress on the y axis produced by the (n-1) dislocations which are located along the plus x axis. The maximum tensile stress for this case is located at z = -0.766 and  $\sigma_x = 1.271(8nt)/\pi^2 \cong nt$ .

 $y=z(\pi^2A/8nt),$ 

If we consider the tensile stress along a line parallel to the yaxis which passes midway between the zeroth and the first dislocation, then Eq. (3) can be used except that we must replace i in it by  $(j-\frac{1}{2})$ . In this case no singularity is encountered on keeping *n* terms and we find that the coordinate and value of the maximum tensile stress are z = -0.171 and  $\sigma_x = 8.932(8nt)/\pi^2 \simeq 7nt$ . The series (3) converges very rapidly so that only the first 5 terms are needed to secure 1 percent accuracy in the sum. Actually the errors arising from the use of an approximate expression for the positions of the dislocations are of the order of 50 percent (i.e., the magnitudes of the maximum stresses given above are about 50 percent too large).

There are several points which should be made. First, the other stresses are also large. Consider the dilatation  $\Delta = (1+\nu)(\sigma_x + \sigma_y)$ . The maximum dilatation on the line midway between the first two dislocations is located at z = -0.25; the value of the dilatation there is  $4.11(8nt)\{(1+\nu)/\pi^2\}\cong 3.3(1+\nu)nt$  where we have again overestimated by about 50 percent. Second, these large stresses exist over regions which are in many cases several hundred angstroms in size. The unit of distance used here is  $\pi^2 A/8nt$ . If we consider copper and take n = 10 and  $t = 10^8$  dyne/cm<sup>2</sup>, then the unit of distance is 343A.

The fact that large tensile stresses do arise in a stressed material containing locked dislocations can be of importance for ductile fracture and for fatigue. In addition, the fact that large dilatation may exist over an appreciable volume may be of importance for precipitation.

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## The Abundance of CO in the Sun and in the Earth's Atmosphere\*

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THE recent observation<sup>1</sup> of CO in the sun has been confirmed further by the identification of about one hundred lines in the spectrum of the solar limb, in the region between  $\lambda 23,000$  and  $\lambda 24,000$ , on new tracings made with the Snow telescope and infrared spectrometer at the Mount Wilson Observatory. The lines originate from the 0-2, 1-3, 2-4, and 3-5 vibrational transitions in the ground electronic state. At the center of the disk the intensities of the strongest lines average about 0.030A in equivalent width. Sufficient data are available for preliminary estimates of the abundance of CO in the sun and of the vibrational temperature. Penner and Weber<sup>2</sup> have made precise measurements of

TABLE I.

Molecule	$\log N$
 СО	19.1
ĊŇ	16.3
CH	17.3
NH NH	13.0
<b>OH</b>	17.5

the integrated absorption coefficients for the 0-1 and 0-2transitions, obtaining  $2.88 \times 10^{-7}$  and  $1.99 \times 10^{-9}$  cm<sup>2</sup> sec<sup>-1</sup> per molecule, respectively. Generalized expressions for the theoretical intensities of vibrational transitions have also been derived by Scholz.<sup>3</sup> The intensity ratio between the fundamental and first overtone obtained by Scholz is in good agreement with the results of Penner and Weber. The relative values of the absorption coefficient computed by Scholz for the 0-2, 1-3, 2-4, and 3-5 bands were therefore adopted, together with the absolute value for the 0-2 transition measured by Penner and Weber. The resulting values of the temperature and abundance are  $T=4300^{\circ}$ K and  $N=1.1\times10^{19}$  molecules/cm<sup>2</sup> above the solar surface defined by the continuous absorption coefficient at  $\lambda 23,500$ . The temperature is in good agreement with other determinations<sup>4</sup> from molecular bands in the photographic region of the solar spectrum, and since its value is approximately the boundary temperature of the sun, it provides additional evidence apart from the strengthening of the lines toward the limb that CO is concentrated at relatively very small optical depths in the solar atmosphere. The abundance of CO is very high compared with those of other solar molecules for which abundance determinations<sup>4</sup> have been made, as is shown by Table I:

The high abundance of CO is not unexpected, however, in view of its relatively high dissociation potential of 9.6 ev.

The identification of CO in the sun makes possible certain conclusions concerning the abundance of this gas in the air above Mount Wilson, California, and Lake Angelus, Michigan. Migeotte<sup>5</sup> has identified a series of strong lines centered at  $4.67\mu$  in the solar spectrum as the result of the 0-1 band of CO in the earth's atmosphere. Migeotte and Neven<sup>6</sup> have also observed the same band from the Jungfraujoch, Switzerland. According to Migeotte, the intensity of the band was variable by a factor of two or three when observed at Columbus, Ohio, but no large intensity variations have been reported by Shaw, Chapman, Howard, and Oxholm,7 also working at Columbus, Ohio. The published tracings and measured wave numbers of both Migeotte and Neven and Shaw, et al., leave no doubt as to the correctness of the identification, inasmuch as the measured wave numbers agree with the laboratory values to within a few hundredths of a wave number. and the band shows a well-defined zero gap. Adel,<sup>8</sup> however, states that he finds no evidence for the existence of the fundamental band of CO on tracings made in 1941 at Flagstaff, Arizona, and concludes that CO occurs only in local concentrations, presumably over industrial centers.

The published tracings<sup>6,7</sup> of the 0-1 CO band suggest an atmospheric abundance of about 0.5 atmos-cm. It can easily be demonstrated, with the aid of the absorption coefficients measured by Penner and Weber,<sup>2</sup> that this amount of CO in the earth's atmosphere would produce strong lines of the 0-2 overtone band at  $2.35\mu$ , with equivalent widths of about 0.17A. Lines with onetenth this intensity can be detected with ease on tracings of the  $2\mu$  region made both at Mount Wilson and at Lake Angelus, but the tracings show no sign of the telluric 0-2 band. In fact, from tracings made on several days with the sun close to the horizon, it can be stated that no telluric lines of this band were present with intensities as great as 0.02A when the path length exceeded 10 air masses. In terms of abundances, this result implies that the total quantity of atmospheric CO in the zenith above Lake Angelus and Mount Wilson was no greater than 0.006 atmos-cm