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THE STRENGTH OF SINGLE CRYSTALS OF INORGANIC SALTS UNDER HIGH PRESSURE, III

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Based on the results of the plastic deformation of five alkali halide single crystals shown in Part II of this series the values of the distance L over which a dislocation can be propagated in the crystal given in Taylor's equation were calculated. The obtained values of L are about 2×10^{-4} cm for lithium fluoride and sodium chloride, 5×10^{-4} cm for potassium chloride and potassium bromide, and 16×10^{-4} cm for potassium iodide. Also, the pressure effects on the various factors in Taylor's equation were investigated, and the values of L under high pressure were calculated. 1.4×10^{-4} cm for lithium fluoride and sodium chloride, and 2.8×10^{-4} cm for potassium chloride were obtained under hydrostatic pressures up to 1000 kg/cm^2.

In Part II of this series[1], the plastic deformation by compressive stress on five alkali halide single crystals: lithium fluoride, sodium chloride, potassium chloride, potassium bromide and potassium iodide, were measured under the atmospheric and some hydrostatic pressures up to 1000 kg/cm^2. The results obtained were shown in five diagrams of the compressive strain as a function of the time at each constant compressive stress. Also, the stress-strain curves after one hour loading were shown in another diagram.

In the present paper, based on the above results, some considerations will be described on the relations between the magnitude of the strain for the same constant stress and their physical constants. And then, applying Taylor's theory, the values of L, the distance over which a dislocation can be propagated in the crystal, were calculated. Moreover, for the purpose of applying this theory to the conditions under hydrostatic pressure, the effects of pressure on the various factors in Taylor's equation were investigated, and the values of L on lithium fluoride, sodium chloride and potassium chloride under high pressure were calculated.

Arrangements of the Results

The experimental results shown in Fig. 2 of Part II give the variation of strain with time under constant stress. Therefore, the slope of the tangential line of each curve shows the rate of deformation, *i.e.* the creep rate. The true strain or the basic strain except the effect of creep is given as the value extraporated to the zero time at each curve, supposing that there holds a linear relation between the strain and time after a certain loading time. Table 1 shows the relation between compressive stress σ and extraporated compressive strain $(h_0-h)/h_0$, where h_0

1) K. Inoue, *This Journal*, 27, 54 (1957)

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Table I Experimental results

Hydrostatic pressure, P kg/cm²	Atmospheric pressure		200		1000	
Crystal	Compressive stress σ & strain $(h_0-h)/h_0$					
	σ, kg/cm²	h_0-h/h_0, %	σ, kg/cm²	h_0-h/h_0, %	σ, kg/cm²	h_0-h/h_0, %
LiF	220	6.2	220	5.7	220	5.2
	480	12.6	500	10.6	530	10.4
	520	—	670	16.0	740	25.0
NaCl	100	2.6	190	4.9	190	4.5
	340	14.9	350	11.4	350	10.8
	460	21.4	470	19.8	480	18.0
KCl	100	6.9	100	5.6	100	3.6
	180	11.7	180	11.4	260	9.4
	350	27.2	420	28.0	430	26.8
KBr	90	7.6	90	6.7	90	6.0
	170	13.2	170	11.3	180	9.7
	300	23.9	330	28.0	420	29.4
KI	50	4.4	90	9.4	90	6.2
	90	11.2	160	18.1	170	13.0
	140	27.6	200	—	200	26.8

and h are the initial height and that corresponding to the stress σ respectively.

In Table I, the magnitude of compressive strain, corresponding to the same compressive stress, has larger value in the following order: lithium fluoride<sodium chloride<potassium chloride< potassium bromide<potassium iodide. Also, according to the same crystal, it is shown that the higher the hydrostatic pressure, the lesser is the strain at constant compressive stress.

Generally, the plastic deformation of a single crystal under the process of tension or compression is represented with the shear strain which occurs in the direction parallel to the glide plane, and in the present case, all kinds of the crystals have the same structure, the simple cubic lattice; hence the glide occurs to the $[1\bar{1}0]$ direction in the (110) plane. Then the above-mentioned order of the magnitude of the strain by a constant stress on alkali halide single crystals is considered to be caused more effectively by the difference of the physical constants of the crystals than by that of the condition of the defects in the crystals used in this experiment.

According to the relation between the physical constants and the magnitude of the strain, in due considerations of the existence of dislocation and its motion in the glide plane of the crystal, and also with the aid of the mathematical theory of elasticity, Taylor[2] gave the following theory. The author applied this theory to the results, and calculated the mean free path, L, of the dislocation in the crystals.

Taylor's Theory and its Application to the Results

In crystals, the plastic deformation occurs when the shear stress along the glide plane attains

2) G. I. Taylor, *Proc. Roy. Soc.* (*London*), **A145**, 362, 388, 405 (1934)

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over a certain value, the opposite centers of dislocation will escape from each other and migrate freely through the crystal. But their moving distance is subject to restriction with faults or flaws in the crystal. Assuming that L is the mean free path of the dislocation in the crystal, shear strain γ is given as the following equation,

$$\gamma=\frac{L}{C^2G^2\lambda}f^2, \tag{1}$$

where f is the shear stress, G the modulus of shear, λ the interval of the atoms in the direction of gliding, and C a constant depending on the particular arrangement of the centers of the dislocation. For the cubic lattice, $\lambda=\sqrt{2}/2\times$(side of unit cube). And C is equal to $1/\pi$ if the shear stress due to the nearest negative dislocation alone is considered, and practically, 0.17 was given by Taylor for square lattice of dislocations.

On the other hand, the relationship between the contraction of the specimen and the magnitude of the shear strain for cubic lattice is shown in the following equation,

$$\frac{\sigma}{\sqrt{\log(h_0/h)}}=2\sqrt{2}\frac{f}{\sqrt{\gamma}}, \tag{2}$$

and combinig Eq. (1) with Eq. (2),

$$\frac{\sigma}{\sqrt{\log(h_0/h)}}=2\sqrt{2}\,CG\sqrt{\frac{\lambda}{L}}$$

or

$$L=8C^2G^2\lambda[\sigma/\sqrt{\log(h_0/h)}]^{-2}. \tag{3}$$

The order of magnitude of L is 10^{-4}cm for rock salt as described by Taylor, which is the same order as the mean distance of the element of mosaic pattern obtained from the data of X-ray analysis by Bragg, Darwin and James[3], and also as the average distance apart of loose planes in structure from the work of Siedentopf[4] on the diffusion of the vapor of alkali metals into rock salt. There are many disputes with regard to the mosaic lattice pattern structure or the second lattice[5].

Using the experimental results under atmospheric pressure, the values of L calculated from Eq. (3) are shown in Table 2. The values of the modulus of shear G shown in the fifth column of Table 2 were calculated from the elastic constants C_{11} and C_{12} shown in the second and third columns[6]. It will be seen from Table 2 that the values of L of all alkali halide crystals in this study agreed with the above order of magnitude by Taylor for rock salt, and besides the order of magnitude of values corresponds substantially to the order of the lattice constant.

In the discussion on the values of L, Burgers[5] pointed out the indefiniteness of the values of C, when the values of L are compared with each other among the crystals having the

3) W. L. Bragg, C. G. Darwin and R. W. James, *Phil. Mag.*, **1**, 897 (1926)
4) H. Siedentopf, *Phys. Z.*, **6**, 855 (1905)
5) R. Houwink, *Elasticity, Plasticity and Structure of Matter*, **2nd** Ed., Dover Pub., Inc., New York (1952)
6) L. S. Combes, S. S. Ballard and K. A. McCarthy, *J. Opt. Soc. Am.*, **41**, 215 (1951)

Table 2 Physical constants and calculated L under atmospheric pressure

Crystal	C_{11}* 10^5 bar	C_{12}* 10^5 bar	λ** 10^{-8} cm	G*** 10^5 kg/cm²	σ kg/cm²	h_0/h	$\sigma/\sqrt{\log(h_0/h)}$ 10^3 kg/cm²	mean	L (C=0.17) 10^{-4} cm
LiF	9.74	4.04	2.84	2.908	220	1.066	1.32	1.65	2.0
					480	1.144	1.98		
NaCl	4.85	1.23	3.98	1.847	100	1.027	0.93	1.21	2.1
					340	1.175	1.28		
					460	1.272	1.42		
KCl	3.98	0.620	4.44	1.714	100	1.074	0.57	0.76	5.2
					180	1.132	0.78		
					350	1.374	0.94		
KBr	3.45	0.540	4.66	1.485	90	1.082	0.49	0.68	5.1
					170	1.152	0.69		
					300	1.314	0.87		
KI	3.32	0.578	4.98	1.399	50	1.046	0.36	0.38	16
					90	1.126	0.40		
					140	1.381	0.37		

* Reference 6)

** $\lambda=\sqrt{2}/2\times$(side length of unit cube)

*** $G=(C_{11}-C_{12})/2$

different structure. In the present case, since the crystals have the same lattice structure, there is no need of considering the absolute value of C, when L is compared with one another. Hence, it is induced that the relative differences of the values of L are not caused by the indefiniteness of C, but due to the property of the crystal.

Application of Taylor's Equation under High Pressure

In order to apply Taylor's equation against the stress-strain relations under high pressure, the effects of pressure on the factors in the equation, C, G and λ were considered.

The numerical factor C depends on the particular arrangement of centers of dislocation as above mentioned, so if it does not appear the structure change such as a phase transition, it may be held a constant value.

The pressure effect of the atomic distance along the slip plane λ, may be estimated from the compressibility of the crystals. The compressibility of lithium fluoride, sodium chloride, potassium chloride, potassium bromide and potassium iodide are 1.53, 4.18, 5.65, 6.68 and 8.56×10^{-6} respectively. The estimated values of $(\partial\ln\lambda/\partial p)_T$ are 5.1×10^{-7} for lithium fluoride, and 2.8×10^{-6} for pottassium iodide, and for others between these two values. Then the change of λ at 1000 kg/cm² hydrostatic pressure is of order of the magnitude $10^{-12}\sim10^{-11}$cm, and as compared with the fact that the order of λ is 10^{-8}cm, it seems negligible.

The modulus of shear G increases with increasing hydrostatic pressure, and the values of $(\partial\ln G/\partial p)_T$ are reported by Susse[7] and Lazarus[8] as 1.043×10^{-5} cm²kg^{-1}, 2.53 and 3.16×10^{-5} bar^{-1}

7) C. Susse, *Compt. rend.*, **250**, 1974 (1960)

8) D. Lazarus, *Phys. Rev.*, **76**, 545 (1949)

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for lithium fluoride, sodium chloride and potassium chloride respectively. Hence at the hydrostatic pressure of 1000 kg/cm², the value of G^2 of potassium chloride increases about 6 per cent.

From these considerations, using the G value corrected for pressure, the values of L under high pressure on three alkali halide single crystals above mentioned were calculated and shown in Table 3. The fourth column of the table shows the corrected values of G for the pressures shown in the third column.

Table 3 Physical constants and calculated L under hydrostatic pressures

Crystal	λ 10^{-5} cm	P kg/cm²	G 10^5 kg/cm²	σ kg/cm²	h_0/h	$\sigma/\sqrt{\log(h_0/h)}$ 10^3 kg/cm²	mean	L (C=0.17) 10^{-4} cm
LiF	2.84	200	2.914	220	1.060	1.38	2.03	1.4
				500	1.119	2.26		
				670	1.190	2.44		
		1000	2.939	220	1.055	1.44	2.00	1.4
				530	1.116	2.45		
				740	1.333	2.10		
NaCl	3.98	200	1.856	190	1.051	1.29	1.44	1.5
				350	1.129	1.52		
				470	1.247	1.52		
		1000	1.893	190	1.047	1.35	1.52	1.4
				350	1.121	1.57		
				480	1.219	1.64		
KCl	4.44	200	1.725	100	1.059	0.63	0.84	4.3
				180	1.129	0.78		
				420	1.389	1.11		
		1000	1.767	100	1.037	0.80	1.07	2.8
				260	1.104	1.25		
				430	1.366	1.17		

In Table 3, all the values of L for the crystals are smaller than those under atmospheric pressure. This may be understood from the fact that the mosaic lattice pattern or the second lattice above mentioned becomes smaller under high pressure than that at atmospheric pressure. Another characteristic in Table 3 is that the changing rate of the value of L with pressure is more effective in such a kind of crystal as has larger value of L under atmospheric pressure. It seems that this tendency has a direct connection with the essential difference of L between these crystals as above mentioned.

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