NASA TECHNICAL TRANSLATION NASA TT F-14,932

TEMPERATURE DEPENDENCE OF ELASTIC CONSTANTS AND THE DEBYE TEMPERATURE OF NaCl AND KCl SINGLE CRYSTALS

A. V. Sharko, A. A. Botaki

Translation of: "Temperaturnaya Zavisimost' Uprugikh Postoyannykh i Temperatura Debaya Monokristallov NaCl i KCl," Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika; vol. 13, no. 6, 1970, pp 22-28.

NASA-TT-F-14932) TEMPERATURE DEPENDENCE OF ELASTIC CONSTANTS AND THE DEBYE TEMPERATURE OF NaCl AND KCl SINGLE (Linguistic Systems, Inc., Cambridge, Mass.) 13 p HC $3.00 CSCL 20L

N73-25801

Unclas
G3/26 06259

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
WASHINGTON, D.C. 20546 JUNE 1973

NASA TT F-14,932

TEMPERATURE DEPENDENCE OF ELASTIC CONSTANTS AND THE DEBYE TEMPERATURE OF NaCl AND KCl SINGLE CRYSTALS /22*

A. V. Sharko, A. A. Botaki

Measurement of the temperature changes of elasticity constants are promising in the regard that they provide the possibility of determining many hard to measure physical characteristics of solids. Thus, for example, the Debye temperature and energy of a crystal lattice may be found according to the temperature changes of the elasticity constant of single crystals of the halides of alkali metals.

The temperature changes of the elastic properties of single crystals of NaCl and KCl are determined in the present study and the Debye temperature of these compounds is found. The measurements were made by the ultrasonic pulse method with the use of the DUK-6V flaw detecter. Using the method of relative measurement, we determined $C_{l\infty}$ —the longitudinal wave propagation velocity in an infinite medium, C_l —the longitudinal wave propagation velocity in a thin rod, the cross section of which is much less than the length of elastic waves in the sample and $C_\perp$ is the transverse wave propagation velocity. The essence of the method of relative measurements is the following: the apparent length l' of the test specimen was determined according to the scale of the depth gage of a DUK-6V ultrasonic pulse flaw detecter, adjusted according to a standard sample with a known ultrasonic propagation velocity C_0; its true length l_0 was measured with the use of a micrometer. Having designated the elastic wave propagation velocities, respectively C and C_0 in the investigated and standard samples and

* Numbers in righthand margin indicate pagination of foreign text.

n—the number of the multiple echo pulse reflection, a desired value of a velocity C may be determined from the relationship

$$l' = n\frac{C_0}{C} l_0. \tag{1}$$

The samples for the measurements have the form of rectangular bars with faces coinciding with the cleavage planes of the single crystal. In order to remove internal stresses and the consequences of mechanical treatment, the samples were subjected to a kneeling at a temperature of 600°C with subsequent slow cooling. Particular attention was given to the surface quality of the working faces of the samples and the orientation relative to the planes {100}. In /23 recording the temperature dependences of the propagation velocities of the ultrasonic oscillations the specimen was glued to the flaw detecter sensor with a mixture consisting of 88% epoxy resin and 12% polyethylene polyamine, and placed in a cryostat. The values of the elastic constant C_{11} and Young's modulus E_{100} were determined from the well-known formulas

$$C_{l00} = \sqrt{\frac{C_{11}}{\rho}}; \quad C_l = \sqrt{\frac{E_{100}}{\rho}}, \tag{2}$$

where ρ is the density of the substance, determined for different temperatures according to the formulas from [1]:

$$\rho(t) = 2{,}1680(1 - 1{,}12\cdot 10^{-4} t - 5\cdot 10^{-8} t^2] \quad \text{for NaCl,} \tag{3}$$

$$\rho(t) = 1{,}9920\,[1 - 10{,}5\cdot 10^{-5} t - 0{,}4\cdot 10^{-7} t^2] \quad \text{for KCl,} \tag{4}$$

here t is the temperature in °C. Variations in the length of the specimen l(t) in relation to temperature was calculated according

to the formula

$$l(t) = l_0 \left[1 + \int_t^{t_0} \alpha(t)\, dt \right] \tag{5}$$

where $\alpha(t)$ is the coefficient of linear expansion, which, according to Henglein [2] may be determined according to the formula

$$\alpha(t) = \frac{\rho(t) - \rho_0}{\rho(t)\, t}, \tag{6}$$

where $\rho(t)$ and ρ_0 are the densities respectively at t and 0°C. In order to find the shear modulus, pulses of transverse waves at a frequency of 2.5 mHz were sent into the specimen, using prismatic search heads with an angle of inlet of the ultrasonic oscillations of 50°, which made it possible to transform longitudinal waves into shear waves. In the general case, with the incidence of an ultrasonic wave onto a plane parallel plate at a certain angle to the normal, both longitudinal and transverse waves arise in the latter. At the chosen angle of incidence of the ultrasonic wave, complete internal reflection of longitudinal wave takes place, and only the transverse wave, oriented at a certain angle to the crystallographic axes, is propagated in the specimen. Taking account of this angle made it possible to determine the orientation factor $F(\gamma)$ [3]

$$F(\gamma) = \gamma_1^2\gamma_2^2 + \gamma_2^2\gamma_3^2 + \gamma_1^2\gamma_3^2, \tag{7}$$

where γ are the direction cosines of the angles, formed by the transverse wave propagation direction with the crystallographic axes.

According to the measured values of $C_\perp$ we find the values of the shear modulus G_α in the direction of propagation of the shear

waves according to the formula

$$C_{\perp} = \sqrt{\frac{G_a}{\rho}}, \tag{8}$$

Calculation of the remaining elasticity constants was performed with the use of the following equations:

$$S_{11} = \frac{1}{E_{100}}; \quad C_{11} = \frac{S_{11} + S_{12}}{(S_{11} - S_{12})(S_{11} + 2S_{12})};$$
$$\frac{1}{G_a} = S_{44} + 4\left[(S_{11} - S_{12}) - \frac{1}{2} S_{44}\right] \cdot F(\gamma); \quad C_{44} = \frac{1}{S_{44}}; \tag{9}$$

/24

$$C_{12} = \frac{-S_{12}}{(S_{11} - S_{12})(S_{11} + 2S_{12})}; \quad \sigma = \frac{1 - 2\left(\frac{C_{\perp}}{C_{l\infty}}\right)^2}{2 - 2\left(\frac{C_{\perp}}{C_{l\infty}}\right)^2};$$
$$\varkappa = 3(S_{11} + 2S_{12}).$$

Here σ is Poisson's ratio and κ is the uniform compression coefficient.

Extrapolation of the experimental values of the low temperature dependences of the elastic constants to 0°K gives the following values:

For NaCl $C_{11} = 5.625 \cdot 10^{11}$ dyne/cm^2; $C_{12} = 0.973 \cdot 10^{11}$ dyne/cm^2;
$C_{44} = 1.310 \cdot 10^{11}$ dyne/cm ; $S_{11} = 0.1784 \cdot 10^{-11}$ cm^2/dyne;
$S_{12} = -0.0290 \cdot 10^{-11}$ cm^2/dyne; $S_{41} = 0.7368 \cdot 10^{-11}$ cm^2/dyne;

For KCl $C_{11} = 4.950 \cdot 10^{11}$ dyne/cm^2; $C_{12} = 0.610 \cdot 10^{11}$ dyne/cm^2; /25
$C_{44} = 0.658 \cdot 10^{11}$ dyne/cm^2; $S_{11} = 0.2073 \cdot 10^{-11}$ cm^2/dyne;
$S_{12} = -0.020 \cdot 10^{-11}$ cm^2/dyne; $S_{44} = 1.527 \cdot 10^{-11}$ cm^2/dyne.

TABLE 1

Ultrasonic Propagation Velocity in a NaCl Single Crystal

$T°$ K	ρ g/cm3	Propagation velocity of ultrasonic vibrations, m/sec		
		$C_{l\infty}$	C_l	$C_\perp$
300	2,1613	4697	4410	2426
290	2,1639	4710	4427	2426
280	2,1663	4724	4447	2427
270	2,1687	4737	4471	2427
260	2,1711	4759	4492	2427
250	2,1732	4771	4512	2427
240	2,1759	4790	4551	2427
230	2,1782	4803	4556	2427
220	2,1806	4813	4574	2427
210	2,1829	4829	4594	2427
200	2,1851	4848	4615	2427
190	2,1874	4866	4635	2428
180	2,1896	4873	4662	2428
170	2,1919	4882	4673	2428
160	2,1943	4895	4693	2428
150	2,1962	4909	4714	2428
140	2,1984	4921	4731	2429
130	2,2005	4935	4751	2429
120	2,2025	4951	4772	2429

TABLE 2

Ultrasonic Propagation Velocity in a KCl Single Crystal

$T°$ K	ρ g/cm3	Propagation velocity of ultrasonic vibrations, m/sec		
		$C_{l\infty}$	C_l	$C_\perp$
300	1,9864	4481	4402	1774
290	1,9884	4501	4412	1776
280	1,9906	4515	4424	1777
270	1,9926	4527	4452	1778
260	1,9948	4550	4463	1780
250	1,9968	4562	4475	1781
240	1,9988	4581	4483	1780
230	2,0008	4598	4500	1781
220	2,0030	4616	4519	1780
210	2,0049	4631	4539	1781
200	2,0069	4646	4553	1781
190	2,0087	4660	4569	1782
180	2,0107	4672	4581	1784
170	2,0127	4683	4594	1785
160	2,0147	4698	4612	1785
150	2,0165	4719	4629	1786
140	2,0185	4733	4643	1787
130	2,0203	4741	4658	1787
120	2,0221	4756	4663	1789
110	2,0241	4766	4683	1789
100	2,0259	4785	4696	1788
90	2,0277	4799	4710	1789
80	2,0297	4811	4734	1790

Measurement of the elasticity constants are given in Tables 1, 2, 4 and 5.

TABLE 4

Elasticity Constants and Elasticity Coefficients of NaCl

T°K	Elasticity constants $\times 10^{-11}$ dyne/cm^2			Elasticity Coefficients $\times 10^{11}$ cm^2/dyne		
	C_{11}	C_{12}	C_{44}	S_{11}	$-S_{12}$	S_{44}
300	4.769	1.314	1.273	0.2380	0.0514	0.7855
290	4.801	1.306	1.274	0.2357	0.0504	0.7849
280	4.831	1.298	1.276	0.2334	0.0491	0.7837
270	4.863	1.291	1.277	0.2306	0.0484	0.7831
260	4.908	1.282	1.279	0.2284	0.0473	0.7819
250	4.948	1.271	1.280	0.2263	0.0464	0.7812
240	4.994	1.260	1.282	0.2238	0.0452	0.7800
230	5.025	1.252	1.283	0.2212	0.0443	0.7794
220	5.052	1.244	1.285	0.2192	0.0433	0.7782
210	5.091	1.233	1.286	0.2169	0.0423	0.7776
200	5.134	1.218	1.287	0.2148	0.0414	0.7770
190	5.178	1.202	1.289	0.2127	0.0402	0.7756
180	5.200	1.194	1.290	0.2105	0.0393	0.7752
170	5.224	1.185	1.292	0.2088	0.0386	0.7740
160	5.258	1.169	1.294	0.2068	0.0376	0.7726
150	5.294	1.155	1.295	0.2049	0.0367	0.7722
140	5.323	1.145	1.297	0.2032	0.0360	0.7710
130	5.359	1.128	1.298	0.2012	0.0350	0.7702
120	5.399	1.111	1.299	0.1992	0.0340	0.7698

Tables 3 and 6 contain values as a function of time of the anisotrophy factor $a = (S_{11} - S_{12}) - \frac{1}{2} S_{44}$ and $A = C_{44} : \frac{C_{11} - C_{12}}{2}$, the uniform compression coefficients κ, Poisson's ratio σ and cubic elasticity $k = \frac{C_{11} + 2C_{12}}{3}$, the measure of the resistance to deformation, expressed by the shear stress, applied in the plane {110} in the direction ⟨100⟩ $C' = \frac{C_{11} - C_{12}}{2}$ and the ratio C_{44}/C_{12}, characterizing the deviation from the Cauchy relation $C_{12} = C_{44}$. From Tables 3

and 6 it is obvious that the elastic anisotropy factor $\left(C_{44}: \frac{C_{11}-C_{12}}{2}\right)$ of KCl and NaCl monocrystals increases with an increase in temperature. Extrapolation of the experimental data to the fusing temperature shows that the elastic anisotropy factor up to the fusing temperature remains less than unity, that is, there is no point of elastic anisotropy in a potassium chloride single crystal, which agrees with the data of references [4, 5].

TABLE 3 /26

Elastic Properties, the ratio C_{44}/C_{12} and Anisotropy of NaCl

T°K	$G' \times 10^{-11} \frac{dyne}{cm^2}$	$\frac{C_{44}}{C_{12}}$	$K \times 10^{-11} \frac{dyne}{cm^2}$	A	$-a \times 10^{11} \frac{cm^2}{dyne}$	$E_{100} \times 10^{-11} \frac{dyne}{cm^2}$	$\varkappa \times 10^{11} \frac{cm^2}{dyne}$	σ
300	1,728	0,969	2,466	0,737	0,1033	4,201	0,4056	0,3181
290	1,747	0,976	2,471	0,729	0,1063	4,242	0,4047	0,3194
280	1,768	0,983	2,476	0,722	0,1090	4,285	0,4038	0,3207
270	1,788	0,989	2,484	0,714	0,1126	4,335	0,4026	0,3221
260	1,813	0,997	2,491	0,706	0,1152	4,380	0,4014	0,3242
250	1,838	1,007	2,497	0,696	0,1179	4,422	0,4005	0,3254
240	1,867	1,018	2,501	0,687	0,1210	4,467	0,3993	0,3273
230	1,886	1,024	2,510	0,680	0,1242	4,520	0,3984	0,3286
220	1,904	1,033	2,513	0,675	0,1266	4,561	0,3975	0,3295
210	1,929	1,043	2,519	0,667	0,1296	4,609	0,3969	0,3311
200	1,958	1,057	2,523	0,657	0,1323	4,655	0,3963	0,3327
190	1,988	1,073	2,527	0,648	0,1350	4,700	0,3957	0,3336
180	2,003	1,081	2,529	0,644	0,1378	4,750	0,3954	0,3348
170	2,020	1,091	2,531	0,640	0,1396	4,788	0,3951	0,3357
160	2,044	1,107	2,533	0,633	0,1420	4,835	0,3948	0,3369
150	2,069	1,121	2,535	0,626	0,1445	4,880	0,3945	0,3381
140	2,088	1,132	2,539	0,621	0,1463	4,922	0,3939	0,3389
130	2,115	1,150	2,539	0,614	0,1499	4,970	0,3939	0,3401
120	2,144	1,169	2,541	0,606	0,1517	5,020	0,3936	0,3409

TABLE 5

Elasticity Constants and
Elasticity Coefficients of KCl

T°K	Elasticity Constants X 10^{-11}, dyne/cm^2			Elasticity Coefficients X 10^{11}, cm^2/dyne		
	C_{11}	C_{12}	C_{44}	S_{11}	$-S_{12}$	S_{44}
300	3.989	0.725	0.625	0.2597	0.0452	1.600
290	4.028	0.724	0.627	0.2581	0.0443	1.595
280	4.060	0.724	0.629	0.2564	0.0433	1.590
270	4.095	0.723	0.630	0.2532	0.0426	1.587
260	4.130	0.723	0.632	0.2516	0.0418	1.582
250	4.155	0.722	0.633	0.2500	0.0412	1.580
240	4.195	0.722	0.633	0.2488	0.0404	1.580
230	4.230	0.721	0.635	0.2469	0.0395	1.575
220	4.268	0.720	0.635	0.2445	0.0390	1.575
210	4.300	0.719	0.636	0.2421	0.0380	1.572
200	4.330	0.717	0.637	0.2404	0.0373	1.570
190	4.360	0.715	0.638	0.2387	0.0365	1.567
180	4.390	0.712	0.640	0.2367	0.0355	1.562
170	4.415	0.710	0.641	0.2353	0.0350	1.560
160	4.450	0.705	0.642	0.2333	0.0340	1.558
150	4.490	0.704	0.643	0.2315	0.0335	1.555
140	4.520	0.700	0.644	0.2299	0.0330	1.553
130	4.542	0.692	0.645	0.2282	0.0320	1.550
120	4.575	0.690	0.647	0.2273	0.0310	1.546
110	4.600	0.685	0.648	0.2252	0.0305	1.543
100	4.640	0.680	0.648	0.2237	0.0295	1.543
90	4.670	0.675	0.649	0.2222	0.0290	1.541
80	4.700	0.670	0.650	0.2196	0.0280	1.538

The point of elastic anisotropy of NaCl single crystals is found /27
near the temperature 680°K, which also agrees with the analogous temperature measurements of [6, 7].

The Debye temperature of KCl and NaCl single crystals was determined according to values of C_{11}, C_{12}, and C_{44} extrapolated to 0°K. The calculation was performed according to the formula:

$$\Theta_D^3 = \left(\frac{9N}{4\pi V}\right)\left(\frac{h}{\kappa}\right)^3\left(\frac{C_{11}}{\rho}\right)^3 [9/(18+\sqrt{3})]\, f(S, t) \quad , \qquad (10)$$

where $S = \frac{C_{11} - C_{44}}{C_{12} + C_{44}}$, $t = \frac{C_{12} - C_{44}}{C_{44}}$; C_{ik}, V and ρ are respectively the elasticity constants, molar volume and crystal density determined for 0°K; N, h and k are the double Avogadro number (for the halogens of alkali metals) and the Planck's and Boltzmann's constants. The values of the function f(s, t) were determined /28 according to special tables [8, 9] with the use of Stirling's interpolation formula and were equal to 1.4068 for NaCl and 2.1129 for KCl. The density of the substance at 0°K was determined according to formulas (3) and (4) and the following results were obtained: $\rho_{NaCl} = 2.2260$ g/cm^3 and $\rho_{KCl} = 2.0432$ g/cm^3. After substitution of the values found in formula (10) $\Theta_D = 321.4$°K and $\Theta_D = 244.1$°K were found for NaCl and KCl single crystals respectively, which is in good agreement with data from heat measurement [10, 11].

TABLE 6 /27

Elastic Properties, Ratio C_{41}/C_{12} and Anisotropy of KCl

T °K	$C' \times 10^{-11} \frac{dyne}{cm^2}$	$\frac{C_{44}}{C_{12}}$	$K \times 10^{-11} \frac{dyne}{cm^2}$	A	$-a \times 10^{11} \frac{cm^2}{dyne}$	$E_{100} \times 10^{-11} \frac{dyne}{cm^2}$	$\varkappa \times 10^{11} \frac{cm^2}{dyne}$	Poisson's ratio σ
300	1,632	0,862	1,813	0,383	0,4949	3,850	0,5516	0,4070
290	1,652	0,866	1,825	0,379	0,4951	3,875	0,5480	0,4078
280	1,668	0,869	1,836	0,377	0,4953	3,900	0,5446	0,4082
270	1,686	0,871	1,847	0,374	0,4975	3,950	0,5415	0,4087
260	1,703	0,874	1,859	0,371	0,4977	3,975	0,5379	0,4096
250	1,716	0,877	1,866	0,369	0,4988	4,000	0,5358	0,4101
240	1,726	0,878	1,880	0,367	0,5008	4,020	0,5319	0,4111
230	1,755	0,881	1,890	0,362	0,5011	4,050	0,5291	0,4116
220	1,774	0,882	1,903	0,358	0,5040	4,090	0,5255	0,4126
210	1,791	0,885	1,913	0,355	0,5059	4,130	0,5228	0,4132
200	1,806	0,889	1,921	0,353	0,5073	4,160	0,5205	0,4147

TABLE 6 (continued)

Elastic Properties, Ratio C_{41}/C_{12} and Anisotropy of KCl

T °K	$C' \times 10^{-11} \frac{dyne}{cm^2}$	$\frac{C_{44}}{C_{12}}$	$K \times 10^{-11} \frac{dyne}{cm^2}$	A	$-a \times 10^{11} \frac{cm^2}{dyne}$	$E_{100} \times 10^{-11} \frac{dyne}{cm^2}$	$\varkappa \times 10^{11} \frac{cm^2}{dyne}$	Poisson's ratio σ
190	1.822	0.892	1.930	0.351	0.5083	4.190	0.5181	0.4148
180	1.829	0.899	1.938	0.350	0.5088	4.225	0.5160	0.4148
170	1.852	0.902	1.945	0.346	0.5097	4.250	0.5142	0.4150
160	1.872	0.910	1.953	0.343	0.5117	4.285	0.5120	0.4157
150	1.893	0.913	1.966	0.340	0.5125	4.320	0.5086	0.4164
140	1.910	0.920	1.973	0.337	0.5136	4.350	0.5068	0.4169
130	1.925	0.930	1.975	0.334	0.5146	4.382	0.5063	0.4173
120	1.943	0.937	1.985	0.333	0.5148	4.400	0.5038	0.4176
110	1.957	0.946	1.990	0.331	5.5158	4.440	0.5025	0.4180
100	1.980	9.953	2.000	0.327	0.5183	4.470	0.5000	0.4188
90	1.997	0.961	2.007	0.325	0.5193	4.500	0.4983	0.4193
80	2.015	0.969	2.013	0.323	0.5212	4.550	0.4968	0.4197

REFERENCES

1. International Critical Tables (McGraw-Hill Company, N. Y.), v. 3, p. 43, 1928.

2. Henglein, Fr. A., Zeit. f. Physik Chemie, vol. 115, p. 91, 1925.

3. Byuren, V.: Defekty v Kristallakh [Defect in Crystals], Moscow, IL, vol. 27, 1962.

4. Niknarov, S. P. and Stepanov, A. V.: FTT, vol. 4, 9, p. 2576, 1962.

5. Norwood, M. N. and Briscoe, C. V.: Phys. Rev., vol. 112, p. 45, 1958.

6. Stepanov, A. V. and Eydus, I. M.: ZhETF, vol. 29, pp. 5, 669, 1955.

7. Overton, I. and Swim, R. T.: Phys. Rev., vol. 84, p. 758, 1951.

8. DeLaunay, J.: Chem. Phys., vol. 30, p. 91, 1959.

9. Botaki, A. A., Popova, Yu. Ya., Suslova, V. N. and Sharko, A. V.: Izv., TPI (in print).

10. Kittel, Ch.: Vvedeniye v fiziku tverdogo tela [Introduction to Solid State Physics], Izd. AN SSSR, Moscow, 1962.

11. Zeytts, F.: Sovremenaya teoriya tverdogo tela [Contemporary Solid State Theory], GITTL, Moscow, 1949.

STANDARD TITLE PAGE

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA TT F- 14, 932		

4. Title and Subtitle	5. Report Date
TEMPERATURE DEPENDENCE OF ELASTIC CONSTANTS AND THE DEBYE TEMPERATURE OF NaCl AND KCl SINGLE CRYSTALS	June 1973
	6. Performing Organization Code
7. Author(s)	8. Performing Organization Report No.
A. V. Sharko, A. A. Botaki	
	10. Work Unit No.
9. Performing Organization Name and Address	11. Contract or Grant No.
LINGUISTIC SYSTEMS, INC. 116 AUSTIN STREET CAMBRIDGE, MASSACHUSETTS 02139	NASW-2482
	13. Type of Report & Period Covered
	TRANSLATION
12. Sponsoring Agency Name and Address	
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION WASHINGTON, D C. 20546	14. Sponsoring Agency Code

15. Supplementary Notes

Translation of: "Temperaturnaya Zavisimost' Uprugikh Postoyannykh i Temperatura Debaya Monokristallov NaCl i KCl," Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika; vol. 13, no. 6, 1970, pp 22-28.

16. Abstract

The ultrasonic pulse method was used to measure the temperature changes, elasticity moduli, the constants C_{ik} and S_{ik}, the anisotropy factor, the uniform compression coefficient and Poisson's ratio in the temperature range 300 - 120°K for NaCl and 300 - 80°K for KCl. According to the values of the elastic constants, extrapolated to 0°K, the Debye temperature of the compounds is found.

17. Key Words (Selected by Author(s))	18. Distribution Statement
	UNCLASSIFIED - UNLIMITED

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price
UNCLASSIFIED	UNCLASSIFIED	11	

12