

Effect of Various Factors Upon the Curie Temperature SOV/48-22-12-17/33
of Piezoelectrics With the Structure of the Perovskite Type

type of the piezoactive cation , as proposed in references 8, 9, 13 promotes the solution of the problem discussed. Therefore, they have been investigated again in this paper. It was attempted to explain the differences of the Curie temperature in piezoelectrics with perovskite structure in the same way, by using only such characteristics as polarizability, charges and radii. The degree of covalence of the bindings in the respective compounds was neglected. The authors started from an approximate theoretical estimation. They used the results from references 15, 16, determined in the investigation of the effect of various parameters of cations upon the internal field of piezoelectrics with perovskite structure. The conclusions drawn on the basis of theoretical estimations agree with the few experimental results obtained by the authors of this article and Sawaguchi (Ref 7). As soon as new experimental data will be obtained it will be possible to check also the theoretical results still improved.

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Effect of Various Factors Upon the Curie Temperature SOV/48-22-12-17/33
of Piezoelectrics With the Structure of the Perovskite Type

There are 2 tables and 26 references, 12 of which are Soviet.

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova
(Physico-Chemical Institute imeni L. Ya. Karpov)

Card 3/3

AUTHORS: Venevtsev, Yu.N., Zhdanov, G.S., Solov'yev, S.P. and
Ivanova, V.V.

TITLE: On Internal Fields in Ferroelectric PbTiO_3 (O vnutrennikh
polyakh v segnetoelektrike PbTiO_3)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 255-257 (USSR)

ABSTRACT: Calculations of the internal fields in PbTiO_3 crystals
have been made by the Madelung-Hagedorn method
(R. Hagedorn - Ref 3) which is more accurate than
Kozlovskiy's method used before, according to the work
of Yu.N. Venevtsev et al (Ref 1). These fields E_i are
Pb 1.4, Ti 6.9, O_I 6.1 and O_{II} , O_{III} 1.8×10^8 V/cm .
The contributions of the separate ions to the spontaneous
polarisation of 81×10^{-6} coulomb/cm² are tabulated. The
internal fields for model crystals of the PbTiO_3 type
but with ions of different polarisability are similarly
calculated. For BaTiO_3 the calculations by both methods

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SOV/70-4-2-26/36

On Internal Fields in Ferroelectric $PbTiO_3$

are in good quantitative agreement. Graphical examination of the parameters affecting the internal fields show their relative importance. In order they are: 1) lattice period; 2) charge on the ferroelectric cation; 3) polarisability of the ions of the oxygen octahedra; 4) polarisability of the ferroelectric cation; 5) polarisability of the non-ferroelectric cation. There are 1 figure, 2 tables and 5 references, 4 of which are Soviet and 1 German.

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova
(Physical-Chemical Institute im. L. Ya. Karpov)

SUBMITTED: November 14, 1958

Card 2/2

AUTHORS: Venevtsev, Yu.N., Solov'yev, S.P. and Zhdanov, G.S. ^{SOV/70-4-4-17/34}

TITLE: On the Structural Coefficients of the Internal Field in Ferroelectrics of the Perovskite Type

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 4, pp 575-578 (USSR)

ABSTRACT: The notation is carried over from an article by the same authors (Ref 1). The values of the projection of the structural coefficients $S_i(x,y,z) \cong C_{ik}$ for different orientations (cube edges, face or body diagonals) of the dipoles in a cubic perovskite-type cell are tabulated in terms of P and Q . ($P = -15.04102$ and $Q = 4.33387$). The coefficients C_{ik} are dimensionless and numerically equal to the field strength, additional to the Lorentz field, due to the sub-lattice of unit dipoles of the k -th sort of ion and acting on the i -th sort of ion. The derivation of expressions such as :

$$S_2(0, 1/2, 1/2) = S_3(0, 1/2, 1/2) = Q/\sqrt{3}$$

Card 1/2 and

SOV/70-4-4-17/34
'On the Structural Coefficients of the Internal Field in Ferro-
electrics of the Perovskite Type

$$S_2(1/2, 0, 0) = S_3(1/2, 0, 0) = P/\sqrt{5}$$

is given but all the other values are tabulated.
There are 1 table and 1 Soviet reference.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
Physico-chemical Institute imeni L. Ya. Karpov)

SUBMITTED: June 23, 1958

Card 2/2

24.2800, 24.7700

77108
SOV/70-4-6-9/31

AUTHORS: Zhdanov, G. S., Solov'yev, S. P., Venevtsev, Yu. N.,
Ivanova, V. V.

TITLE: Internal Fields in the Orthorhombic Modification of
BaTiO₃

PERIODICAL: Kristallografiya, 1959, Vol 4, N 6, pp 855-861 (USSR)

ABSTRACT: Internal fields in orthorhombic (pseudomonoclinic) barium titanate are computed according to ionic-displacement data reported in Phys. Rev., 105, 3, 856, 1957. Computations are based on the assumption that point ionic charges are displaced parallel to the edges of monoclinic unit cells, twice as small as orthorhombic cells, and are superposed by the similarly displaced point dipole moments. The latter's magnitude is determined as the product of ionic polarization and the affecting internal field. The known equation:

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$$E_x = p_x \sum \frac{2x_i^2 - y_i^2 - z_i^2}{(x_i^2 + y_i^2 + z_i^2)^{3/2}} + p_y \sum \frac{3x_i y_i}{(x_i^2 + y_i^2 + z_i^2)^{3/2}} + p_z \sum \frac{3x_i z_i}{(x_i^2 + y_i^2 + z_i^2)^{3/2}}$$

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SOV/70-4-6-9/31

Internal Fields in the Orthorhombic
Modification of BaTiO₃

that defines the field along the X axis in terms of equal dipoles p and coordinates x₁, y₁, z₁ of l-th dipole, is reduced, substituting the three sums, for the sake of brevity, by h_{xx}, h_{xy}, h_{xz}. In cubic and tetragonal BaTiO₃, h_{xy}, h_{xz}, h_{yz} are equal to zero. Using various calculation methods the authors proved that h_{xy} in "monoclinic" BaTiO₃ is vanishingly small relative to h_{xx} and can be disregarded, while h_{xx} remains about the same as in cubic BaTiO₃. Thus dipole moments p_k for each projection upon l(x,z) axis become defined by:

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$$\sum_{k=1}^5 (\delta_{ik} - (f_1)_{ik}) \frac{p_k \cos \varphi_{kl}}{v} = \sum_{k=1}^5 \frac{e_k}{a^3} (f_1)_{ik}$$

where k = 1, 2, ..., 5 is number of unlike atoms in the unit cell; e_k is charge of a k-type ion; a and c are edgelengths of monoclinic cells; (f₁)_{ik} is structure factor whose magnitude equals the field intensity affecting l-th atom in the sublattice formed by k-type atoms; φ_{kl} is angle between l axis and k-type dipole;

Internal Fields in the Orthorhombic
Modification of BaTiO₃

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$$\delta_{ik} = \begin{cases} 0 & \text{for } k \neq i \\ \frac{1}{a_i} & \text{for } k = i; \end{cases}$$

Spontaneous polarization is computed according to:

$$P_{s1} = \sum_{k=1}^5 \frac{P_k \cos \varphi_{k1}}{v} + \sum_{k=1}^5 \frac{e_k \cdot s_{k1}}{v}$$

where s_{k1} denotes displacement of k-type atoms along 1 axis. The computed values (Table 2) are about the same as in tetragonal BaTiO₃. The computed spontaneous polarization proved to be equal to the experimental one. Ti atoms are subjected to the highest field intensity and Ba atoms to the lowest. The fields affecting both atoms and oxygen O_{II} are parallel to the polar axis and to the displacements of the respective atoms, while the fields affecting O_I and O_{III} are symmetrically inclined to the polar axis; they are under 29° to the displacement directions, and 90°30' to X and Z axes.

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Internal Fields in the Orthorhombic
Modification of BaTiO₃

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TABLE

| ION | $E_i \cdot 10^{-6}$, v/cm | | | $P_i = 3.1 \cdot 10^{-10}$ k/cm ² $P_{ix} = -2.2 \cdot 10^{-10}$ k/cm ² $P_{iz} = 2.2 \cdot 10^{-10}$ k/cm ² | | | | | |
|------------------|----------------------------|-------|------|---|------|----------------------------|------|----------------------------|-----|
| | E_x | E_z | E | $(P_{ix} + P_{iz}) \cdot 100\%$ | | $P_{ix} / P_i \cdot 100\%$ | | $P_{iz} / P_i \cdot 100\%$ | |
| | | | | x | z | x | z | x | z |
| | Ba | -0,08 | 0,08 | 0,12 | -1,3 | 1,3 | -1,3 | 1,3 | 0 |
| Ti | -3,60 | 3,60 | 5,09 | -15,0 | 15,7 | -5,3 | 5,3 | -9,7 | 9,7 |
| O _I | -0,44 | 2,62 | 2,66 | -12,3 | 57,1 | -8,3 | 49,9 | -4,1 | 7,2 |
| O _{II} | -0,47 | 0,47 | 0,67 | -13,8 | 13,8 | -9,0 | 9,0 | -4,8 | 4,8 |
| O _{III} | -2,62 | 0,44 | 2,60 | -57,1 | 12,3 | -49,9 | 8,3 | -7,2 | 4,0 |

Assistance of the late G. I. Skanavi is acknowledged.
There are 3 figures; 3 tables; and 11 references,
4 U.S., 3 Soviet, 2 German, 2 Danish. The U.S.
references are: G. Shirane, H. Danner, R. Pepinsky,
Phys. Ref., 105, 3, 856, 1957; J. C. Slater, Phys.
Rev., 78, 748, 1950; S. Triebwasser, J. Phys. Chem.
Solids, 3, 1/2, 53, 1957; H. H. Wieder, Phys. Rev.,
99, 1161, 1955.

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Internal Fields in the Orthorhombic
Modification of BaTiO_3

77108
SOV/70-4-6-9/31

ASSOCIATION: Physicochemical Institute imeni L. Ya. Karpov
(Fiziko-khimicheskiy institut imeni L. Ya. Karpova)

SUBMITTED: September 16, 1959

Card 5/5

82509

54600(A)
247800

S/070/60/005/004/009/012

AUTHORS:

Venevtsev, Yu.N., Zhdanov, G.S., Solov'yev, S.P.,
Bezus, Ye.V., Ivanova, V.V., Fedulov, S.A. and
Kapyshev, A.G.

TITLE:

Crystal Chemical Investigations of Substances with
the Perovskite Type of Structure Which Has Special
Dielectric Properties

PERIODICAL: Kristallografiya, 1960, Vol. 5, No. 4.
pp 620 .. 626

TEXT: In $BaTiO_3$ the dielectrically-active ion is the Ti but
in $PbTiO_3$ it is the Pb ion. The $(Pb.Ba)TiO_3$ system may, there-
fore, be expected to show peculiarities where these two effects
interact. The variation in structure, dielectric and piezo-
electric properties is not continuous from one end-member to
the other. Experimentally, solid solutions with 7, 9, 11, 14
and 24 wt. % $PbTiO_3$ showed anomalies not explicable as due to
loss of PbO. $NaNbO_3$ undergoes several phase transitions in a
short temperature interval. Dielectric and optical observations
give transitions at 360, 470, 520 and 640 °C. X-ray data contra-
dict all but the first of these. Polycrystalline material was
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S/070/60/005/004/009/012
E132/E360

Crystal Chemical Investigations of Substances with the Perovskite Type of Structure Which Has Special Dielectric Properties

studied by X-ray methods up to 700 °C and transitions at 360, 430, 470, 520 and 640 °C were found. Below 360 °C NaNbNO_3 is

monoclinic with $a \neq c \neq b$ and $\beta > 90^\circ\text{C}$. Above 360 °C it is monoclinic with $a \neq c \neq b$ and $\beta > 90^\circ\text{C}$ (true symmetry orthorhombic). The transition from orthorhombic to tetragonal is not at 360 but at 430 °C. The X-ray method is no less sensitive than the optical and dielectric methods. From an examination of solid solutions $\text{BaTiO}_3 \cdot (\text{Ca}, \text{Sr})(\text{Zr}, \text{Sn})\text{O}_3$,

it is concluded that, other things being equal, the Curie temperature of perovskite type ferroelectrics is higher, the smaller is the period of the lattice and the higher is the polarisability of the active cation.

BiTiO_3 with added $\text{Bi}_2\text{O}_3 \cdot \text{Cr}_2\text{O}_3$ and $\text{Bi}_2\text{O}_3 \cdot \text{Al}_2\text{O}_3$ has been synthesised and specimens showed properties like those found in BaTiO_3 containing $\text{Bi}_4\text{Ti}_3\text{O}_{12}$.

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Crystal Chemical Investigations of Substances with the Perovskite Type of Structure Which Has Special Dielectric Properties

BiFeO_3 and specimens in the system PbTiO_3 - BiFeO_3 have been synthesised. The former has a rhombohedral distortion

($a = 3.963 \text{ \AA}$, $\alpha = 89^\circ 24'$) and a susceptibility about 80. At 200 °C the susceptibility has a maximum of about 1200. In the solid solution up to 70% by wt. of BiFeO_3 there is also

a tetragonal modification. The Curie point of BiFeO_3 appears to be higher than that of PbTiO_3 .

General methods for calculating the internal field have been developed for structures of any dipole configurations. These have been applied to the orthorhombic structure of CaTiO_3 .

Here, the internal electric field is zero at the Ti sites.

There are 29 references: 2 Japanese (in English), 8 English, 2 international, 1 Swiss, 1 German and 15 Soviet.

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S/070/60/005/004/009/012

E132/E360

Crystal Chemical Investigations of Substances with the Perovskite Type of Structure Which Has Special Dielectric Properties

ASSOCIATION: Fiziko-khimicheskiy institut
im. L. Ya. Karpova
(Physico-Chemical Institute imeni
L.Ya. Karpov)

SUBMITTED: February 23, 1960

Card 4/4

S/070/60/005/005/006/017
E132/E360

AUTHORS: Solov'yev, S.P., Venevtsev, Yu.N. and
Zhdanov, G.S.

TITLE: On a Method of Calculating the Internal Fields in
Complex Dipole Structures

PERIODICAL: Kristallografiya, 1960, Vol. 5, No. 5,
pp. 718 - 725

TEXT: A method is proposed for calculating the internal field in complex dipole structure. In general, the problem comes down to the solution of a system of linear equations with $3m$ unknowns, where m is the number of atoms in the elementary cell. If the symmetry of the structure is taken into account the number can be decreased to $3n$ where n is the number of complexes and where n is less than m . Ewald's method can be successfully applied to calculating all the structure sums necessary for estimating the fields. The method is generally applicable in all cases where the structure has been determined. The calculation of the structure sums enables the idealisation of the structure to be avoided as these sums can be calculated in any case. Sometimes, however, in spite of the methods

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S/070/60/005/005/006/017
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On a Method of Calculating the Internal Fields in Complex
Dipole Structures

available for reducing the tediousness of the calculation of the fields in real structures, the number of unknowns may be too big to enable the system of equations obtained to be solved by hand methods. This raises no difficulty as modern computing machines can deal with such systems of equations with extreme speed. In fact, the systematic calculation of the fields in real antiferroelectric crystals and in other structures is best done by a machine appropriately programmed. There are 1 figure and 14 references: 5 Soviet, 1 Swiss, 5 English and 3 German. ✓

ASSOCIATION: Fiziko-khimicheskiy institut imeni
L.Ya. Karpova (Physics-chemical Institute
imeni L. Ya. Karpov)

SUBMITTED: March 1, 1960

Card 2/2

24,7800 (1142, 1144, 1162)

84996

S/O48/60/024/010/005/033
B013/BC63

AUTHORS: Solov'yev, S. P., Venevtsev, Yu. N., Zhdanov, G. S., and Ivanova, V. V.

TITLE: Method of Calculating Inner Electric Fields in Complicated Dipole Structures and Their Application to CaTiO₃ 1

PERIODICAL: Izvestiya Akademii nauk SSSR. Seriya fizicheskaya, 1960, Vol. 24, No. 10, pp. 1191 - 1194

TEXT: A general method is suggested for calculating the inner electric fields in complicated structures, in which there may take place both parallel and antiparallel ionic displacements in an arbitrary direction. This method, which was applied to the calculation of fields in CaTiO₃ ✓

type crystals, constitutes a generalization of the methods that are used for calculating the fields in piezoelectric substances of an ABO₃-type structure, and proceeds from the respective structure model of the compound concerned. A total of six different cases were examined. The calculation was made at the vychislitel'nyy tsentr MGU (Computer

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84996

Method of Calculating Inner Electric Fields in S/048/60/024/010/005/033
Complicated Dipole Structures and Their B013/B063
Application to CaTiO_3

Center of MGU) with the computer "СТРЕЛА" (Strela). The calculation of the fields in CaTiO_3 shows that the distribution of fields in this compound depends only little on the polarizability of Ca ions. It is all the more dependent, however, on the effective ion charge, up to the change of the signs of the fields acting upon the oxygen ions, although the qualitative picture remains unchanged. The fields acting upon Ca ions are only little varied in this connection. In all of the six cases examined the fields are considerably smaller than is the case with the piezoelectric ABO_3 compounds. In this case, as may be seen from the structure symmetry, the field acting upon the Ti ions is exactly vanishing. In BaTiO_3 and PbTiO_3 (Refs. 8 and 9), on the contrary, fields of maximum strength act upon the Ti ions. The basic difference between the fields in CaTiO_3 and in the piezoelectric ABO_3 compounds related to it, is connected with the fact that in the latter the octahedra are greatly deformed, while they are nearly ideal in CaTiO_3 . The relationship

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Method of Calculating Inner Electric Fields in Complicated Dipole Structures and Their Application to CaTiO_3 S/O48/60/024/010/005/033 B013/B063

between the anomaly of dielectric properties and the deformation of BO_6 octahedra can be also observed in the case of such ABO_3 compounds as are, e.g., PbZrO_3 , PbHfO_3 , NaNbO_3 . It can be stated that the presence of a deformation of B - O is an indispensable prerequisite for an antipiezoelectric phase transition. The authors thank N. P. Trifonov, collaborator of the computer center of MGU for his assistance in the computations. The present paper was read at the Third Conference on Piezoelectricity, which took place in Moscow from January 25 to 30, 1960. There are 1 figure and 12 references: 4 Soviet.

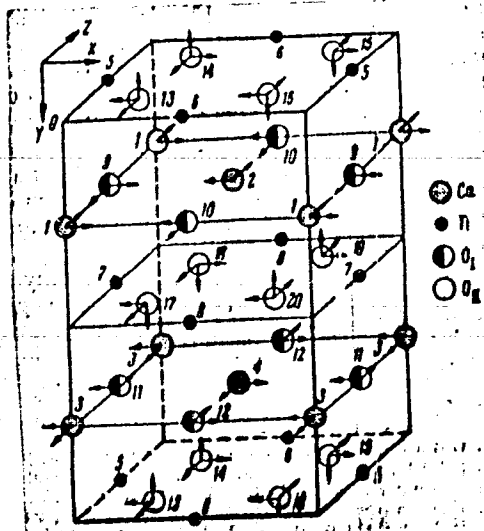
ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova (Physicochemical Institute imeni L. Ya. Karpov)

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S/048/60/024/010/005/033
B013/B063

Legend to Fig.:
The CaTiO_3 unit cell



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FEDULOV, S.A.; VENEVITSEV, Yu.N.; ZHDANOV, G.S.; SMAZHEVSKAYA, Ye.G.

X-ray and electric investigation of solid solutions in the system
 $PbTiO_3 - SrSnO_3$. Fiz. tver. tela 3 no. 3:959-963 Mr '61.
(MIRA 14:5)
(Lead titanate) (Strontium stannate) (Solutions, Solid)

30783

3/101/61003/011/020/056

5125/B104

15.2650

AUTHORS: Fedulov, S. A., and Venevtsev, I. N.

TITLE: Investigation of structure and dielectric properties of solid solutions $(\text{Pb,Sr})(\text{Ti,Zr})\text{O}_3$

PERIODICAL: Fizika tverdogo tela, v. 3, no. 11, 1961, 3371-3375

TEXT: The authors found a continuous series of solid solutions in the $\text{PbTiO}_3 - \text{SrZrO}_3$ system. The temperature dependences of the dielectric constant ϵ , the conductivity σ , and $\tan \delta$ were investigated by employing UM-3 (UM-3) and MOM-4 (MOM-4) type bridges and a KB-1 (KV-1) type Q-meter. ϵ and $\tan \delta$ were mainly determined for 1,000 cycles. Part of the samples with pseudomonoclinic distortion were investigated with Cr radiation in PKA-143 (RKD-143) type chambers (built by the Fiziko-khimicheskiy institut im. Karpova (Physicochemical Institute imeni Karpov)). At room temperature, these solid solutions of the $\text{PbTiO}_3 - \text{SrZrO}_3$ system are found in three modifications: tetragonal, cubic, and pseudomonoclinic (Fig. 1). Period

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B125/B104

Investigation of structure and dielectric ...

c becomes smaller in the tetragonal modification but period a increases. Fig. 2 shows the behavior of ratio c/a . Period a shows a steady increase in the cubic system. In the pseudomonoclinic range, monoclinic angle β and periods $a=c$ increase while the ratio b/a of the monoclinic axes decreases. Solid solutions $(Pb,Sr)(Ti,Zr)O_3$ with 32.5% by weight (40 mole%) of $SrZrO_3$ show a Curie temperature of more than $20^\circ C$. Fig. 3 shows the temperature dependence of ϵ for solid solutions of various types. The temperature dependence for a sample with 15% by weight of $SrZrO_3$ was established at 500 kilocycles, that for the other samples at 1 kilocycle. Conductivity of solid solutions and $\tan \delta$ will decrease with increasing concentration of $SrZrO_3$. From these data, it is possible to compile part of a phase diagram for solid solutions investigated (Fig. 6). When writing down the composition of ferroelectrics of perovskite-type structure in the general form ABO_3 , solid solutions are formed through simultaneous substitution of ions A and B in the systems $PbTiO_3 - SrZrO_3$, $PbTiO_3 - SrSnO_3$, and $PbTiO_3 - SrTiO_3$. The Curie temperature shows its

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Investigation of structure and dielectric ...

strongest decrease in samples investigated if SrSnO_3 is introduced, and it is less affected by SrZrO_3 and SrTiO_3 . A similar behavior was observed in analogous series of solid solutions where A-type ions are either Pb^{2+} or Ba^{2+} ions. The monoclinic structure may be caused for the cubic cell in the series SrTiO_3 , SrSnO_3 , and SrZrO_3 by a decrease of the geometrical factor t from 0.96 to 0.88. G. S. Zhdanov is thanked for a discussion of results and interest in the paper. There are 6 figures and 16 references: 10 Soviet and 6 non-Soviet. The three most recent references to English-language publications read as follows: J. Phys. Soc. Japan, 14, 10, 1286, 1959.; F. J. Kulscar. J. Am. Cer. Soc., 42, 1, 49, 1959.; J. Smith, A. J. E. Welch. Acta Cryst., 13, 8, 653, 1960.

ASSOCIATION: Nauchno-issledovatel'skiy fiziko-khimicheskiy institut im. L. Ya. Karpova Moskva (Scientific Physicochemical Research Institute imeni L. Ya. Karpov)

SUBMITTED: June 7, 1961

Card 3/8 J

2002

S/O70/61/006/001/002/011
E032/E314

7.2181 (2303, 1144)
24.7800 (1142, 1385, 1136)

AUTHORS: Solov'yev, S.P., Venevtsev, Yu.N., Zhdanov, G.S.
and Ivanova, V.V.

TITLE: Calculation of Internal Electric Fields in
Perovskite Crystals (CaTiO_3)

PERIODICAL: Kristallografiya, 1961, Vol. 6, No. 1,
pp. 78 - 85

TEXT: In a previous paper (Ref. 13) the present authors gave an account of a general method for the calculation of internal fields in structures having an arbitrary disposition of dipoles. The aim of the present paper is to apply this method to the calculation of fields in the antiferro-electric dipole structure of CaTiO_3 , using a model based on the real structure reported by Kay and Baily in Ref. 14. In the method described by the present authors in Ref. 13, it is assumed that the polarisabilities and effective ion charges are known. The polarisabilities of Ca and O ions were taken from the book by Kittel' (Ref. 15) ($\alpha_{\text{Ca}} = 1.1 \cdot 10^{-24} \text{ cm}^3$),

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S/070/61/006/001/002/011
E032/E314

Calculation of Internal Electric Fields

$\alpha_0 = 2.4 \times 10^{-24} \text{ cm}^3$). It is further assumed that the effective charges of the ions in BaTiO_3 are approximately equal to one-half of the total ion charges. In order to estimate the effect of the assumed magnitude of the charges and polarisabilities on the field distribution six different variants of the calculation were carried out, in which the charges and polarisabilities were varied within reasonable limits. The results obtained are summarised in Table 3, which gives the internal fields in CaTiO_3 . The first five variants are based on the real structure of CaTiO_3 , shown in Fig. 2. For comparison, variant 6 is based on values of the f and h sums calculated for undispersed positions of the ions. All the calculations were carried out on the electronic computer "Strela" at the Computation Centre of MGU.

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S/070/61/006/001/002/C11
E032/E314

Calculation of Internal Electric Fields

Acknowledgments are expressed to N.P. Trifonov and
A. Tel'nova of the Computation Centre of MGU, who carried
out the numerical calculation on the "Strela" computer.
There are 2 figures, 3 tables and 17 references: 7 Soviet
and 10 non-Soviet.

ASSOCIATION: Fizikokhimicheskiy institut im. L.Ya.Karpova
(Physicochemical Institute im. L.Ya. Karpov)

SUBMITTED: March 1, 1960

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S/G70/61/006/001/002/011
E032/E314

Calculation of Internal Electric

Table 3: 1 - Variants; 2 - $E \cdot 10^{-8}$, V/cm; 3 - Projection Axis;
CGSE = esu

| E·10 ⁻⁸ в/см | Ось проекции 3 | Варианты | | | | | |
|----------------------------|----------------------|--|---|--|-----------------------------------|---|----------|
| | | 1 | 2 | 3 | 4 | 5 | 6 |
| 2 | 3 | 1/2 αCa: α, εCa = 1.0 εTl = 2.0 εO = -1.0 | 2αCa: αO εCa = 1.0 εTl = 2.0 εO = -1.0 | αCa: αO εCa = 0.5 εTl = 2.5 εO = -1.0 | αCa: αO εTl = 1.5 εO = -1.0 | αCa = 1.1·10 ⁻¹⁰ см ² ; αO = 2.1·10 ⁻¹⁰ см ² ; εCa = 1.0 CGSE; εTl = -2.0 CGSE; εO = -1.0 CGSE | |
| E _{Ca} | X | -0,0708 | -0,136 | -0,0972 | -0,0720 | -0,0846 | -0,0072 |
| | Y | 0 | 0 | 0 | 0 | 0 | 0 |
| | Z | 0,494 | 0,751 | 0,517 | 0,601 | 0,557 | 0,422 |
| E _{Tl} | X | 0 | 0 | 0 | 0 | 0 | 0 |
| | Y | 0 | 0 | 0 | 0 | 0 | 0 |
| | Z | 0 | 0 | 0 | 0 | 0 | 0 |
| E _{O1} | X | 0,767° | 0,876° | 2,053° | -0,477 | 0,792° | 0,856° |
| | Y | 0 | 0 | 0 | 0 | 0 | 0 |
| | Z | 0,0215 | 0,302 | -0,499° | 0,080 | 0,0906 | -0,0714° |
| E _{O11} | X | 0,470° | 0,545° | 0,928° | 0,0578° | 0,489° | 0,544° |
| | Y | -0,875 | -0,892 | -1,887 | 0,134° | -0,880 | -0,942 |
| | Z | -0,0068 | -0,085 | -0,570 | 0,519 | -0,0258 | -0,520 |

esu

Card 4/5

20024

8/070/61/006/001/002/011
E032/E314

Calculation of Internal Electric Fields

Fig. 2:

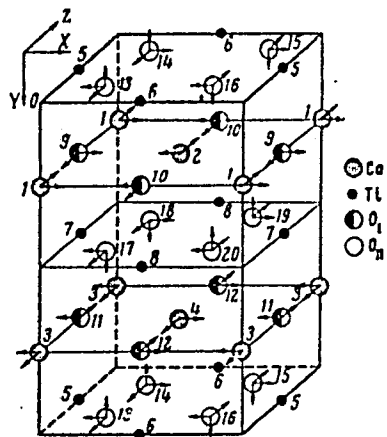


Рис. 2. Элементарная ячейка CaTiO₃.

Card 5/5

SOLOV'YEV, S.P.; ~~VEKSTEV, D.S.~~; ZHDANOV, G.S.

X-ray diffraction study of phase transitions in NaNbO_3 . Kris-
tallografiia 6 no.2:218-224 Mr-Ap '61. (MIRA 14:9)

1. Fiziko-khimicheskiy institut im. L.Ya.Karpova.
(Sodium niobate) (X rays--Diffraction)

22791

S/070/61/006/003/002/009
E021/E435

24,7100 (1160, 1136, 1142)

AUTHORS: Venkovtsev, Yu.N., Bondarenko, V.S., Zhdanov, G.S.,
Chkalova, V.V. and Stember, N.G.

TITLE: Anomalous changes in the lattice parameters, the dielectric and piezoelectric properties of (Ba, Pb)TiO₃ solid solutions

PERIODICAL: Kristallografiya, 1961, Vol.6, No.3, pp.375-380

TEXT: Samples were prepared from chemically pure titanium dioxide and barium and lead carbonates. X-ray investigations showed that solid solutions of (Ba, Pb)TiO₃ had a tetragonal-distorted cell of the perovskite type. Results of precision measurements on the parameter of the cell are given in Fig.1, where changes in lattice parameters and volume are plotted against weight % PbTiO₃. The curves are not continuous and there are sharp changes at 5.5, 9.2, 11.2 and 13.5% PbTiO₃. Fig.1a shows the periods of the crystal lattice c and a; Fig.1b shows c/a; Fig.1b shows the volume v of the elementary cell against weight % PbTiO₃. The results of measurements of the dielectric constant ε against temperature (°C) are shown in Fig.2 (the numbers on the curves correspond to the % PbTiO₃). The values of Card 1/7

X

22791

Anomalous changes ...

S/070/61/006/003/002/009
E021/E435

the dielectric constant at the Curie point ϵ_{\max} are plotted against concentration (wt.%) PbTiO_3 in Fig.3. There are sharp maxima at 5.5, 9.2, 11 and 13.7% PbTiO_3 . The curves in Fig.2 enable the Curie point and the positions of the second and third phase transformations to be found. On the basis of these measurements, the phase diagram at the BaTiO_3 rich end can be drawn (Fig.4). The change in the piezo-modulus d_{33} with composition is shown in Fig.5. There are maxima at 5.5, 11.2 and 13.5 wt.% PbTiO_3 . The obtained data agree in many respects with those of previous work when commercially pure materials were used. The results, as well as published data, lead to the conclusion that the observed anomalies are characteristic of the solid solutions of $(\text{Ba}, \text{Pb})\text{TiO}_3$ and they may be due to the differences in the properties of the barium and lead titanates. A change in the type of ferroelectrically active cations probably takes place in the concentration range of 11.2 to 13.5 wt.% PbTiO_3 when the second and the third phase transitions, which are characteristic for barium titanate, ceased to exist. Other observed anomalies are also attributed to the differences in the properties of the titanates of barium and lead. Acknowledgments are expressed to Senior
Card 2/7

22791

Anomalous changes ...

S/070/61/006/003/002/009
E021/E435

laboratory assistant B.G.Nikolov, Technician I.I.Moreva,
Engineer V.A.Ulitin and Laboratory assistant G.V.Bazhanova for
their assistance. There are 5 figures and 9 references:
4 Soviet-bloc and 5 non-Soviet-bloc. The three references to
English language publications read as follows: H.D.Megaw, Proc.
Phys.Soc., 58, 133, 1946; G.Shirane, F.Jona, R.Pepinsky, Proc.IRE,
43, 12, 1738, 1955; B.Joffe, R.S.Roth, S.Marzullo, J.Res.Nat.Bur.
Standards, 55, 5, 239-254, 1955.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya.Karpova
(Institute of Physics and Chemistry imeni
L.Ya.Karpov)

SUBMITTED: August 24, 1960

Card 3/7

2016
S/070/61/006/005/004/011
E132/E560

15 2640
x4,7200 (1144,1160)

AUTHORS: Fedulov, S.A., Venevtsev, Yu.N., Zhdanov, G.S. and Rez, I.S.

TITLE: X-ray crystallographic and electrical studies of specimens of the system $PbTiO_3 \cdot BaZrO_3$

PERIODICAL: Kristallografiya 1961, Vol. 6, No. 5, pp. 681-685

TEXT: Hitherto the system $PbTiO_3 - BaZrO_3$ has hardly been studied. The $PbTiO_3$ synthesized had a tetragonally-distorted perovskite structure with $a = 3.899$ and $c = 4.155 \text{ \AA}$ giving $c/a = 1.065$. The $BaZrO_3$ was cubic with $a = 4.190 \text{ \AA}$. These agree with previously published data (Ref. 6, H. Megaw, Proc. Phys. Soc., 58, 133, 1946). Fig. 1 shows the variation of cell dimensions with composition for intermediate compositions in the continuous series of solid solutions obtained. The volume changes without discontinuity. The two phases appeared to co-exist over the composition range 37.5 to 40% (by weight). At the high $PbTiO_3$ end of the composition range, measurements of the dielectric constant were hindered by the high conductivity. The log of the conductivity was a linear function of $1/T$ (the absolute temperature). The

Card 1/4

X-ray crystallographic and

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E152/E560

dielectric constant was measured at 530 kc for the compositions 20-25% BaZrO₃ and at 1 kc otherwise. Graph shows the variation of d.c. with temperature for various compositions of material. The existence of a two-phase region between the ferroelectric (tetragonal) and the paraelectric (cubic) modifications is not new but has been found also in PbTiO₃-BaTiO₃. This is expressed in the spreading of the maxima in the curves of d.c. against T and corresponds to the statistical distribution of the cations in the two phases. This statistical distribution gives rise to strains in the crystal lattices and as a result the ferroelectric-paraelectric transformation takes place over a finite temperature interval. The rhombohedral phase found by T. Ikeda (Ref. 1, J. Phys. Soc. Japan, 14, 2, 168, 1959) was not encountered. The absence of a piezoelectric effect in the range from 40-42.4% also confirms that there was no rhombohedral phase in this case. Work reported by others on the system PbZrO₃-BaTiO₃ is contradictory.

Acknowledgments are expressed to Ye. G. Snazhevskaya and N. A. Kabalkina for their assistance. There are 6 figures and 11 references, 6 Soviet and 5 non-Soviet. The English-language

Card 2/4

X-ray crystallographic and ...

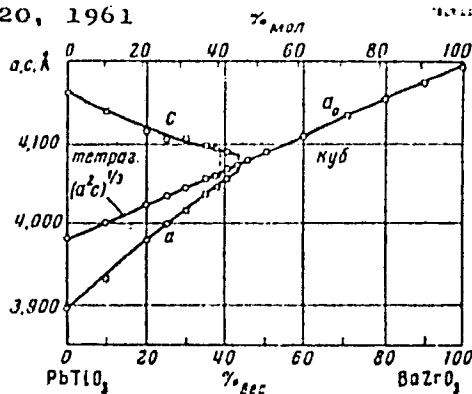
S/070/61/006/005/004/011
E132/E560

referencea road as follows: Ref.1 (quoted in text); Ref.7:K.Suzuki, J. Phys. Soc. Japan, 6,5,340, 1951; Ref.8: B. Jaffe, R.S.Roth, S. Marzullo, J.Res.Nat.Bur. Standards, 55, 239, 1955; Ref.9: S. Nomura, S. Sawada, J.Phys.Soc. Japan. 10, 2, 1955.

ASSOCIATION: Fiziko-khimicheskiy institut imeni L. Ya. Karpova
(Physico-Chemical Institute imeni L. Ya. Karpov)

SUBMITTED: January 20, 1961

Fig.1.



Card 3/4

15 2450

24,7200(1144,1160)

26651

S/070/61/006/005/009/011

E032/E114

AUTHORS: Fedulov, S.A., Venevtsev, Yu.N., Zhdanov, G.S., and Smazhevskaya, Ye.G.

TITLE: High-temperature X-ray and thermographic studies of bismuth ferrite

PERIODICAL: Kristallografiya, 1961, Vol.6, No.5, pp. 795-796

TEXT: In previous papers, Ref.1 (I.S. Rez. Tezisy dokl. Tret'yego soveshchaniya po segnetoelektricheskoy "Abstracts of the Third Conference on Ferroelectrics", Izd-vo AN SSSR, p.51, 1960) and Ref.2 (Yu.N. Venevtsev, G.S. Zhdanov, S.P. Solov'yev, Ye.V. Bezus, V.V. Ivanova, S.A. Fedulov, A.G. Kapyshev, Kristallografiya, Vol.5, 4, 620, 1960) the present authors et al. reported the existence of the compound BiFeO_3 with perovskite type structure, and suggested that this compound is a ferroelectric having a higher Curie temperature than lead titanate. The Curie temperature of BiFeO_3 and also of the solid solutions belonging to the system $\text{PbTiO}_3\text{-BiFeO}_3$ cannot be determined from dielectric measurements owing to the high conductivity of the specimens. The present authors have therefore carried out high

Card 1/4

High-temperature X-ray and

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E032/E114

Y

temperature X-ray and thermographic studies of BiFeO_3 . Specimens were prepared from a mixture of Bi_2O_3 and Fe_2O_3 by heating them to 800°C for one hour and subsequently repeating this process. The X-ray photographs were obtained with copper radiation and the ЭРКА-114 (VRKD-114) camera (designed at the Physicochemical Institute imeni L.Ya. Karpov). The synthesized specimens consisted of a single phase and had a rhombohedral distorted cell of the perovskite type with $a = 3.963 \text{ \AA}$ and $\alpha = 89^\circ 24'$. The latter is in agreement with the results reported in Ref. 2 (room temperature). Fig. 1 shows the variation of a and α with temperature. Analysis of the X-ray photographs obtained led to the conclusion that at 700°C the BiFeO_3 began to decompose and weak lines belonging to a second phase appeared. The decomposition is an irreversible process. The thermographic study was carried out with the aid of the UKTA-58 (UKTA-58) apparatus. Fig. 2 shows the thermogram obtained for BiFeO_3 . It follows from the form of the differential curve (D), the contraction curve (Y) and the weight-loss curve (B) that up to about 850°C no phase transformations occur in the specimen. In the temperature ranges

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High-temperature X-ray and

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S/070/61/006/005/009/011
E032/E114

875-930 °C, 970-1030 °C and 1030-1090 °C endothermic effects were observed and there was an appreciable contraction of the specimen which became noticeable immediately after the endothermic effect near 875-930 °C. It is concluded that the Curie temperature of BiFeO₃ should be greater than or equal to 850 °C. BiFeO₃ can therefore be used as a basis for ferroelectric solid solutions with high Curie temperatures. In addition, this substance will be useful in the development of materials which have both magnetic and ferroelectric properties. Acknowledgments are expressed to V.I. Rivkin and Yu.M. Toropov for assistance in the thermographic studies.

There are 2 figures and 4 Soviet references.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
(Physicochemical Institute imeni L.Ya. Karpov)

SUBMITTED: January 20, 1961

Card 3/4

VENEVTSSEV, Yu.N.; SOLOV'YEV, S.P.; ZHDANOV, G.S.

Methods for the X-ray diffraction study of small deformations
of cubic primary cells. Zav.lab. 27 no.9:1112-1115 '61.

(MIRA 14:9)

1. Nauchno-issledovatel'skiy fiziko-khimicheskiy institut
imeni L.M. Karpova.

(Electric batteries)

(X-ray--Diffraction)

VENEVTSSEV, Yu. N.

"Investigation of some solid solutions based on the ferroelectric-antiferromagnetic BiFeO_3 ."

report presented at the Symposium on Phase Transitions in Solids, 6th General Assembly, Intl. Union of Crystallography, Rome, Italy, 16-18 Sep 1963.

(Karpov Institute of Physical Chemistry, Moscow, USSR)

VENEVITSEV, Yu. N.

"The Calculations of the internal electric fields and electric-field gradients in the perovskite-type compounds with special dielectric properties."

report presented at the Symposium on Phase Transitions in Solids, 6th General Assembly, Intl. Union of Crystallography, Rome, Italy, 16-18 Sep 1963.

(Karpov Institute of Physical Chemistry, Moscow, USSR)

VENEVTSSEV, Yu. N., LYUBIMOV, V. N. , SOLOV'YEV, S. P., Viskov, A. S. and ZHDANOV, G. S.

"Calculation of Internal Electric Fields and Field Gradients in Perovskite Type Compounds with Special Dielectric Properties."

report presented at the Symposium on Ferroelectricity and Ferromagnetism, Leningrad, 30 May - 5 June 1963.

217300

S/181/62/004/005/041/055
B102/B104

AUTHORS: Lyubimov, V. N., and Venevtsev, Yu. N.
TITLE: Calculation of potentials in hyperstructures
PERIODICAL: Fizika tverdogo tela, v. 4, no. 5, 1962, 1352 - 1357

TEXT: The potentials of hyperstructures of crystals of the type ABO_3 with 5 atoms per unit cell are investigated theoretically. The hyperstructures are complexes of unit cells with, for example 20 atoms ($CaTiO_3$, $CdTiO_3$) or 40 atoms (e.g. $PbZrO_3$). In the formation of hyperstructures not only the lattice constants become larger but also the crystallographic axes change their directions in space. Some fundamental considerations are made for the very complicated problem of potential calculation and some general relations written down. A formula is obtained for the relationship between the potentials of the structure field of a unit cell and the potentials of the structure field of a hypercell (which consists of an integral number of unit cells, such as 4 or 8). Formulas giving the relations between the structure coefficients of the
Card 1/2

√B

Calculation of potentials . . .

S/181/62/004/005/041/055
B102/B104

internal field of the unit cell and hyperstructure are derived for some concrete cases. Not only the nature of electrical properties but also that of other properties of hyperstructures which depend on the potential distribution may be derived from potential calculations. The results obtained make it possible to study the differences in the behavior of the various modifications. There are 2 figures.

JB

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova Moskva
(Physicochemical Institute imeni L. Ya. Karpov, Moscow)

SUBMITTED: January 25, 1962

Card 2,2

LYUBIMOV, V.N.; VENEVTSEV, Yu.N.; ZHDANOV, G.S.

Ferroelectricity and antiferroelectricity in polar crystals.
Fiz. tver. tela 4 no.8:2123-2127 Ag '62. (MIRA 15:11)

1. Fiziko-khimicheskiy institut imeni L.Ya. Karpova, Moskva.
(Crystals--Electric properties)

S/181/62/004/012/027/052
B125/B102

AUTHORS: Lyubimov, V. N., Venevtsev, Yu. N., Solov'yev, S. P.,
Zhdanov, G. S., and Bakushinskiy, A. B.

TITLE: The dipole structure and the internal electric fields in
 PbZrO_3

PERIODICAL: Fizika tverdogo tela, v. 4, no. 12, 1962, 3543-3550

TEXT: The most probable values of the internal electric fields and field-induced electron dipoles are calculated for a PbZrO_3 crystal on the basis of the model of point dipole structure. Using the method developed by S. P. Solov'yev, Yu. N. Venevtsev, G. S. Zhdanov (Kristallografiya 3, 473, 1958), the determination of the 28 different projections of the electron dipole moments was reduced to the solution of a system of 28 linear algebraic equations for 28 unknowns. The structural sums which are necessary for the set-up of these equations describe the fields of the infinite sublattices of the unit charges and unit dipoles, the number of which exceeds by far 1000. Both the structural sums and the system of
Card 1/3

The dipole structure and the ...

S/181/62/004/012/027/052
B125/B102

equations itself were calculated in various modifications using the electronic computer "Strela". The effect of all structure sublattices on each of the 40 atoms incorporated in the elementary cell was taken into account. The variant P_S was determined by extrapolation for the parameters $e_{Pb} = 1.27$, $e_{Zr} = 1.73$, $e_O = -1$, $\alpha_{Pb} = 4.32 \cdot 10^{-24} \text{ cm}^3$, $\alpha_{Zr} = 0.80 \cdot 10^{-24} \text{ cm}^3$, $\alpha_O = 2.26 \cdot 10^{-24} \text{ cm}^3$. e_i denotes the effective charges and α_i denotes the electron polarizabilities of the ions. The small value of P_S within a certain temperature interval makes it possible to establish a correlation between the data obtained from structure and those from dielectric studies. At room temperature, the ion polarization for the above-mentioned values of the parameters is compensated by electron polarization. Hence, the $PbZrO_3$ crystal is antipolarized and very similar to an anti-electret. Results, similar in principle, are obtained for any of the ten crystallographic polar classes of pyroelectrics (electrets). It is assumed that at least the direction of most of the projections of the electron dipole moments and of the internal fields corresponds to the

Card 2/3

The dipole structure and the ...

S/181/62/004/012/027/052
B125/B102

real structures of PbZrO_3 at room temperature. The displacement of the atoms may be attributed to nonelectrostatic forces. The highest field strength acts on the Zr ion. In general the internal field strength increases with decreasing ion polarizability. The rules found for PbZrO_3 resemble those governing the ferroelectric crystals BaTiO_3 and PbTiO_3 . It would be useful to investigate PbZrO_3 under pressure. There are 7 tables. ✓

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova, Moskva
(Physicochemical Institute imeni L. Ya. Karpov, Moscow)

SUBMITTED: July 9, 1962

Card 3/3

34729
S/070/62/007/001/002/022
E032/E314

24,700 (1153, 1454)

AUTHORS: Lyubimov, V.N., Venevtsev, Yu.N. and Zhdanov, G.S.

TITLE: Internal electric fields in NaTaO_3 and CdTiO_3 crystals

PERIODICAL: Kristallografiya, v. 7, no. 1, 1962, 12 - 19

TEXT: The aim of the present calculations was to obtain some information on the electrical properties of the above crystals. It is stated that they have not been extensively investigated and that the published information is to some extent conflicting. Thus, G.A. Smolenskiy (Ref. 1 - Dokl. AN SSSR, 85, 985, 1952; Ref. 2 - Zh. tekhn. fiz., 20, 157, 1950 and Ref. 3 - Dokl. AN SSSR, 70, 405, 1950) reported that CdTiO_3 was a ferro-electric with a Curie point at 50 - 60 °K, while J.K. Hulm, B.T. Matthias and E.A. Long (Ref. 4 - Phys. Rev., 79, 885, 1950) did not find these properties. According to the experimental results of B.T. Matthias (Ref. 5 - Amer. Phys. Soc., 24, 28, 1949 and Ref. 6 - Phys. Rev., 75, 1771, 1949), NaTaO_3 should be regarded as a ferro-electric, while V.A. Isupov



Card 1/3

Internal electric fields

S/070/62/007/001/002/022
E052/E314

(Ref. 8 - Izv. AN SSSR, Ser. fiz., 22, 1504, 1958) describes it as "quasi-ferro-electric". In order to resolve these difficulties, the present authors calculate the internal electric fields of the above structures at room temperature. Use is made of a modified form of Eq. (10) in the paper by S.P. Solov'yev, Yu.V. Venetsev and G.S. Zhdanov (Ref. 10 - Kristallografiya, 5, 1960, 718) in order to abbreviate the calculations. The structural coefficients of $CdTiO_3$ were calculated by P.P. Ewald's method (Ref. 11 - Ann. Phys., 64, 253, 1921) using the Strela computer. Each structural coefficient was determined to four decimal places. The procedure used by the authors enabled them to reduce the number of points for which the coefficients had to be evaluated from 34 to 15. There are 9 structural coefficients for each of these 15 points. Of the resulting total number of 135, there are 74 which are equal to zero. The authors have used this theory to calculate the dipole moment of the superstructure cell and found its antiparallel components. The dipole moment and the contribution of ions to the spontaneous polarization

Card 2/5

Internal electric fields

S/070/62/007/001/002/022
E032/E314

are given (in units of 10^{-18} ESU) in Table 5. The internal fields (in units of 10^{-8} V/cm), the spontaneous polarization and the structural distortion of various crystals of type ABO_3 are given in Table 6. It is stated that further careful studies of the structural, dielectric and other characteristics of these substances are necessary. Acknowledgments are expressed to S.P. Solov'yev for advice and T.A. Osipova for evaluating the structural sums. There are 6 tables and 17 references: 10 Soviet-bloc and 7 non-Soviet-bloc. The four latest English-language references are: Ref. 4 (quoted in text); Ref. 7 - H.F. Kay, J.L. Miles - Acta crystallogr., 10, 213, 1957; Ref. 12 - H.F. Kay, P.C. Baily - Acta crystallogr., 10, 219, 1957 and Ref. 15 - J.R. Tessman, A.H. Kahn, W. Shockley - Phys. Rev., 92, 890, 1953.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
(Physicochemical Institute im. L.Ya. Karpov)

SUBMITTED: February 15, 1961

Card 3/5

S/070/62/007/001/007/022
E132/E460

AUTHORS: Fedulov, S.A., Venevtsev, Yu.N., Zhdanov, G.S.,
Smazhevskaya, Ye.G., Rez, I.S.

TITLE: X-ray and electrical studies of the system
PbTiO₃-BiFeO₃

PERIODICAL: Kristallografiya, v.7, no.1, 1962, 77-83

TEXT: X-ray powder photographs were taken at various temperatures up to about 800°C of specimens from the BiFeO₃-PbTiO₃ system and measurements were made of dielectric constant and electrical conductivity. Fig.1 shows the change in cell dimensions with composition, wt.%; Fig.7 shows the phase diagram. The rhombohedral phase near the composition BiFeO₃ has an exceptionally high Curie point, about 850°C, which is near its incongruent m.p. At lower concentrations of BiFeO₃ (65%) before the transition from tetragonal to rhombohedral, the tetragonal phase reaches a c/a ratio of 1.17, which is exceptionally high. As a base for ferroelectric structure, BiFeO₃ has wide possibilities and may lead to technical materials with both ferroelectric and ferromagnetic properties. There are 7 figures.

Card 1/2

Physics Center in Ya Karlov

3019

S/070/62/007/002/005/022
E132/E160

24,7100

AUTHORS: Lyubimov, V.N., Veneytsev, Yu.N., and Zhdanov, G.S.

TITLE: On a method of calculating the gradients of the internal electric fields in complex dipole structures

PERIODICAL: Kristallografiya, v.7, no.2, 1962, 229-233

TEXT: The problem of calculating the gradients q of the internal electric field in a crystal lattice of any symmetry made up of charges and dipoles is examined. As $q = \text{grad } \underline{E} = - \text{grad } V$ and $\partial E_x / \partial y = \partial E_y / \partial x$, q is a symmetrical tensor with 6 components. In the general case $6m$ quantities must be calculated to give the field if there are m atoms per unit cell. Inclusion of the symmetry of the unit cell may reduce this to $6n$ where n is the number of complexes, and simplify the formulae. The symmetry of the ions themselves introduces further simplifications.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
Card 1/1 (Physico-chemical Institute imeni L.Ya. Karpov)

SUBMITTED: April 26, 1961

FEDULOV, S. A.; VENEVTSEV, Yu. N.; DZHMUKHADZE, D. F.

X-ray diffraction and electric studies of the system
 $PbTiO_3$ - $LaAlO_3$. Kristallografiia 7 no.3:408-411 My-Je '62.
(MIRA 16:1)

1. Fiziko-khimicheskiy institut imeni Karpova.

(X-ray crystallography) (Dielectric constant)
(Systems (Chemistry))

S/070/62/007/005/011/014
E132/E460

AUTHORS: Lyubimov, V.N., Venevtsev, Yu.N.

TITLE: The formation of dipole configurations in certain structures with special dielectric properties

PERIODICAL: Kristallografiya, v.7, no.5, 1962, 793-794

TEXT: A. Jaskiewicz and H. Konwent (Bull. Acad. polon. Sci. Cl. III, v.9, 1961, 553) have examined the process of the formation of dipole structure in perovskites (ABO_3), although not entirely successfully. An attack on the structure of WO_3 (ReO_3 -type) proves simpler. Here, either the W or the O ions can be ferroelectrically active and the method of trial and error is practicable. For the case where the W ion is active and the dipolar structure is formed because, as a result of the thermal oscillations, the W ion in one cell possesses an initial dipole $(0,0,m_z)$, the field, acting on W ions in neighbouring cells, can be determined by the above method. This gives the case of tetragonal WO_3 consisting of chains of pseudocubic cells, where in each chain the polarization of the cells is directed in one way and in the neighbouring chain oppositely. This is the simplest
Card 1/2

The formation of dipole ...

S/O70/62/007/005/011/014
E132/E460

configuration known for WO_3 . The method cannot be pursued further to give other configurations but some results can be obtained for the NH_4Cl and NH_4Br structures (where the halide ions are active). These are found to be antiferroelectric. The method is only confirmatory and does not disclose new information. ✓

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya.Karpova
(Physico-chemical Institute imeni L.Ya.Karpov)

SUBMITTED: February 21, 1962

Card 2/2

24,5700

38380

S/070/62/007/003/009/026
E132/E460

AUTHORS: Fedulov, S.A., Venevtsev, Yu.N., Dzhmukhadze, D.F.

TITLE: X-ray diffraction and electrical studies of the
system $\text{PbTiO}_3 - \text{LaAlO}_3$

PERIODICAL: Kristallografiya, v.7, no.6, 1962, 408-411

TEXT: PbTiO_3 being ferroelectric and LaAlO_3 paraelectric, the pseudo-binary system is of interest. Pure PbCO_3 , Al_2O_3 , TiO_2 and La_2O_3 were used to make the materials, sintering being carried out at 800 to 1200°C and again at 1100 to 1400°C in each case for 1 hour. High precision X-ray powder photographs were taken of the products. The dielectric constant ϵ and the loss $\tan \delta$ were measured at 1 Kc/s on a bridge. The phase diagram is as shown in Fig.1. The cubic region widens with increasing temperature until at 500°C there is only a cubic phase at all compositions. The temperature dependence of ϵ was measured with increasing content of LaAlO_3 . A significant drop in the peak height takes place and the position of the maximum passes below 0°C for contents greater than 20%. A significant piezoelectric effect was found for specimens containing 5 and 7.5% LaAlO_3 . The Card 1/2

S/070/62/007/003/009/026
E132/E460

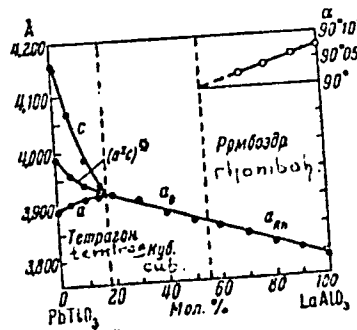
X-ray diffraction and ...

combination of high piezoelectricity and high Curie temperature (above 300°C) may be technically useful. Professor G.S.Zhdanov is thanked for his advice. There are 5 figures.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya.Karpova (Physicochemical Institute imeni L.Ya.Karpov)

SUBMITTED: July 10, 1961

Fig.1.



Card 2/2

43506

S/070/62/007/006/018/020
E132/E435

AUTHORS: Lyubimov, V.N., Venevtsev, Yu.N., Koyranskaya, Ye.Yu.

TITLE: Calculation of the gradients of the electric field in ionic crystals

PERIODICAL: Kristallografiya, v.7, no.6, 1962, 949-952

TEXT: It has been shown (E. Brun et al. Helv. phys. acta, v.34, 1961, 391) that the contribution of δE_d of the multipolarity of the ions to the field gradient may greatly exceed that, δE_p , of the point charges. This effect would be expected to be particularly great for ferroelectrics with dipole structures. The authors' formula (Kristallogr. v.7, no.2, 1962, 229-233) for calculating δE in a dipole structure is now applied to the tetragonal $BaTiO_3$ (or the general perovskite ABO_3). The structure sums were calculated on the "Minsk" computer. The dipolar contribution to δE of any atom does not exceed 0.7×10^{14} cgsu and is normally between 0.1 and 0.5×10^{14} . The true effective charges may, however, differ from those assumed by 20 to 30%. (Assumed $e_A = +1$; $e_B = +2$; $e_{O_I} = e_{O_{II}} = -1$)

Card 1/2

Calculation of the gradients ...

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E132/E435

If so, then the contributions of the A and B atoms to δE will not be zero and there will be a dipole contribution of the order of $\delta E_d = \text{approx } 0.5 \times 10^{14}$ cgsu. For the oxygen ions the charge contribution exceeds the dipolar contribution. Inasmuch as the electronic dipoles have the functions of effective charges and their values are only approximately known, their contribution to the dipole structure cannot be calculated accurately. The dynamic corrections to the effective charges can be calculated. For the oxygen this is $\alpha \cdot \delta E = \text{approx } 4 \times 10^{-10}$ cgsu. For the Ti the correction is significantly less and is about $0.1 e$ and the force acting on the charge greatly exceeds that acting on the dipole. This gives grounds for treating the movement of the ferroelectric ion as that of a point charge and not of a dipole. For the other ions the forces are of the same order. For calculating the fields at the nuclei (or nuclear quadrupole resonance, Moessbauer effect etc) quantum mechanical methods are necessary to calculate the Sternheimer constant γ_{∞} which must be included. There is 1 table.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya.Karpova (Physico-
SUBMITTED: March 27, 1962 chemical Institute im. L.Ya.Karpov)
Card 2/2

35597
S/O48/62/026/003/006/015
B107/B102

24.7100 (1153,1160)

AUTHORS: Ivanova, V. V., Kapyshev, A. G., Venevtsev, Yu. N., and Zhdanov, G. S.

TITLE: X-ray determination of symmetry of the elementary cells of the ferroelectrics $(K_{0.5}Bi_{0.5})TiO_3$ and $(Na_{0.5}Bi_{0.5})TiO_3$ and of the high-temperature phase transitions in $(K_{0.5}Bi_{0.5})TiO_3$

PERIODICAL: Akademiya nauk SSSR. Izvestiya. Seriya fizicheskaya, v. 26, no. 3, 1962, 354-356

TEXT: The ferroelectrics with perovskite structure, $(K_{0.5}Bi_{0.5})TiO_3$ and $(Na_{0.5}Bi_{0.5})TiO_3$ with the Curie point at 380 and 320°C, respectively, had been described in earlier papers (Ref. 1: G. A. Smolenskiy, A. I. Agranovskaya, Fiz. tverdogo tela, 1, no. 10, 1562 (1959); Ref. 2: G. A. Smolenskiy, V. A. Isupov, A. I. Agranovskaya, N. N. Kraynik, Fiz. tverdogo tela, 2, no. 11, 2982 (1960)). The radiographic examination with an PKY-114 (RKU-114) camera shows that the samples are single-phased at room
Card 1/3

X

S/048/62/026/003/006/015
B107/B102

X-ray determination of symmetry ...

temperature, and that K and Bi, and/or Na and Bi are statistically distributed in the sites of the elementary cell with the coordination number 12. Splitting of some lines was observed, but could not be measured accurately. CrK radiation and an PKA-143 (RKD-143) camera (produced at the FKhI imeni L. Ya. Karpov) were therefore used. The following lattice constants were determined from the splitting of the line with

$\sum h_i^2 = 8$: $(K_{0.5}Bi_{0.5})TiO_3$ is tetragonal with $a = 3.913 \pm 0.003 \text{ \AA}$,
 $c = 3.993 \pm 0.003 \text{ \AA}$, $V = 61.1 \pm 0.15 \text{ \AA}^3$; $(Na_{0.5}Bi_{0.5})TiO_3$ is rhombohedral

with $a = 3.891 \pm 0.002 \text{ \AA}$, $\alpha = 89^\circ 36' \pm 3'$, $V = 58.7 \pm 0.1 \text{ \AA}^3$. Furthermore, the change in the lattice constants with temperature up to 500°C was determined for $(K_{0.5}Bi_{0.5})TiO_3$. At 270°C the tetragonal passes over into a

pseudocubic phase. The slightly diffuse lines make more accurate determination impossible. On the basis of previous conclusions (Ref. 4: Yu. N. Venetsev, G. S. Zhdanov, Izv. AN SSSR. Ser. fiz., 21, 2275 (1957)) the distortion can be assumed to be tetragonal. The cubic phase occurring from 410°C onward makes the radiographs clearer. The authors thank V. A. Isupov who supplied the samples. There is 1 figure.

Card 2/3

X-ray determination of symmetry ...

S/048/62/026/003/006/015
B107/B102

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova
(Physicochemical Institute imeni L. Ya. Karpov)

X

Card 3/3

24.7800(1035, 1043, 1153)

35573
S/048/62/026/003/007/015
B117/B102

AUTHORS: Fedulov, S. A., Veneytsev, Yu. N., Zhdanov, G. S., and
Dzhmukhadze, D. F.

TITLE: X-ray and electrical analysis of the system $PbTiO_3-LaFeO_3$

PERIODICAL: Akademiya nauk SSSR. Izvestiya. Seriya fizicheskaya, v. 26,
no. 3, 1962, 357 - 361

TEXT: This paper was presented at the VII Nauchno-tekhnicheskoye
soveshchaniye po primeneniyu rentgenovykh luchey k issledovaniyu materialov
(7th Scientific-technical Conference on the Use of X-rays for the
Examination of Materials) held in Leningrad from June 22 to 29, 1961. The
system $PbTiO_3 - LaFeO_3$ was studied by means of X-ray and electrical
analysis. The specimens were prepared by double annealing (preliminary
annealing at 800 - 1100°C, final annealing at 1100 - 1400°C, for one hour
each) in lead oxide vapor. X-ray analysis was made with CuK_{α} and FeK_{α}
radiation in $PbY-114$ (RKU-114) and $PbL-143$ (RKD-143) cameras (designed at
the Fiziko-khimicheskiy institut im. L. Ya. Karpova (Physicochemical

Card 1/4

X-ray and electrical analysis...

S/048/62/026/003/007/015
B117/D102

Institute imeni L. Ya. Karpov). The dielectric constant was measured at 450 kcps by a MB-1 (KV-1) Q-meter, electrical conductivity was measured by a MOM-4 (MOM-4) bridge. The results obtained by X-ray analysis agree with those in other publications. The system $\text{PbTiO}_3 - \text{LaFeO}_3$ forms a continuous series of solid solutions which at room temperature occur in three modifications: tetragonal, pseudomonoclinic I, and pseudomonoclinic II. Specimens with an LaFeO_3 content higher than 50% showed a hyperfine structure of the lines whose intensities increased with the LaFeO_3 concentration. The elementary cell volume of solid solutions $(\text{Pb,La})(\text{Ti,Fe})\text{O}_3$ decreased with increasing LaFeO_3 concentration. This became especially distinct in the region of tetragonal modification and can be explained by the specific electrostrictive properties of PbTiO_3 . According to the activation energy determined for PbTiO_3 and LaFeO_3 from their conductivities (with relatively high values), these compounds were classified as semiconductors. The temperature dependences of conductivity of solid solutions as functions $\log \sigma = f(1/T)$ had a complicated course when the LaFeO_3

Card 2/5

X-ray and electrical analysis...

S/048/62/026/003/007/015
B117/B102

content was increased. This indicates a change in the conductivity mechanism of solid solutions according to their composition. At certain temperatures, corresponding to the phase transition points, salient points were observed on these straight lines. A phase diagram (Fig. 5) was set up on the basis of the data obtained. Comparison of the data obtained for $\text{PbTiO}_3 - \text{LaFeO}_3$ with those for $\text{PbTiO}_3 - \text{BiFeO}_3$ showed that in contrast to $\text{PbTiO}_3 - \text{BiFeO}_3$ in which the Curie temperature rises when BiFeO_3 is added, the Curie temperature decreases in $\text{PbTiO}_3 - \text{LaFeO}_3$ when the LaFeO_3 concentration is increased. Probably the main reason thereof is the different polarizability of the La and Bi ions compared with the polarizability of the Pb ion. The different ionic radii of Bi (1.20 Å) and La (1.04 Å) probably do not influence the behavior of the Curie temperature. Presumably they are the main reason of the different sequence of the phases. The relatively high temperature of the magnetic transformation of LaFeO_3 ($\sim 570^\circ\text{C}$) in part of the solid solutions in its neighborhood also suggest magnetic properties. The authors thank Ye. G. Smazhevskaya for her help. There are 5 figures and 13 references: 8 Soviet and 5 non-Soviet.

Card 3/5

X-ray and electrical analysis...

S/048/62/026/003/007/015
B117/B102

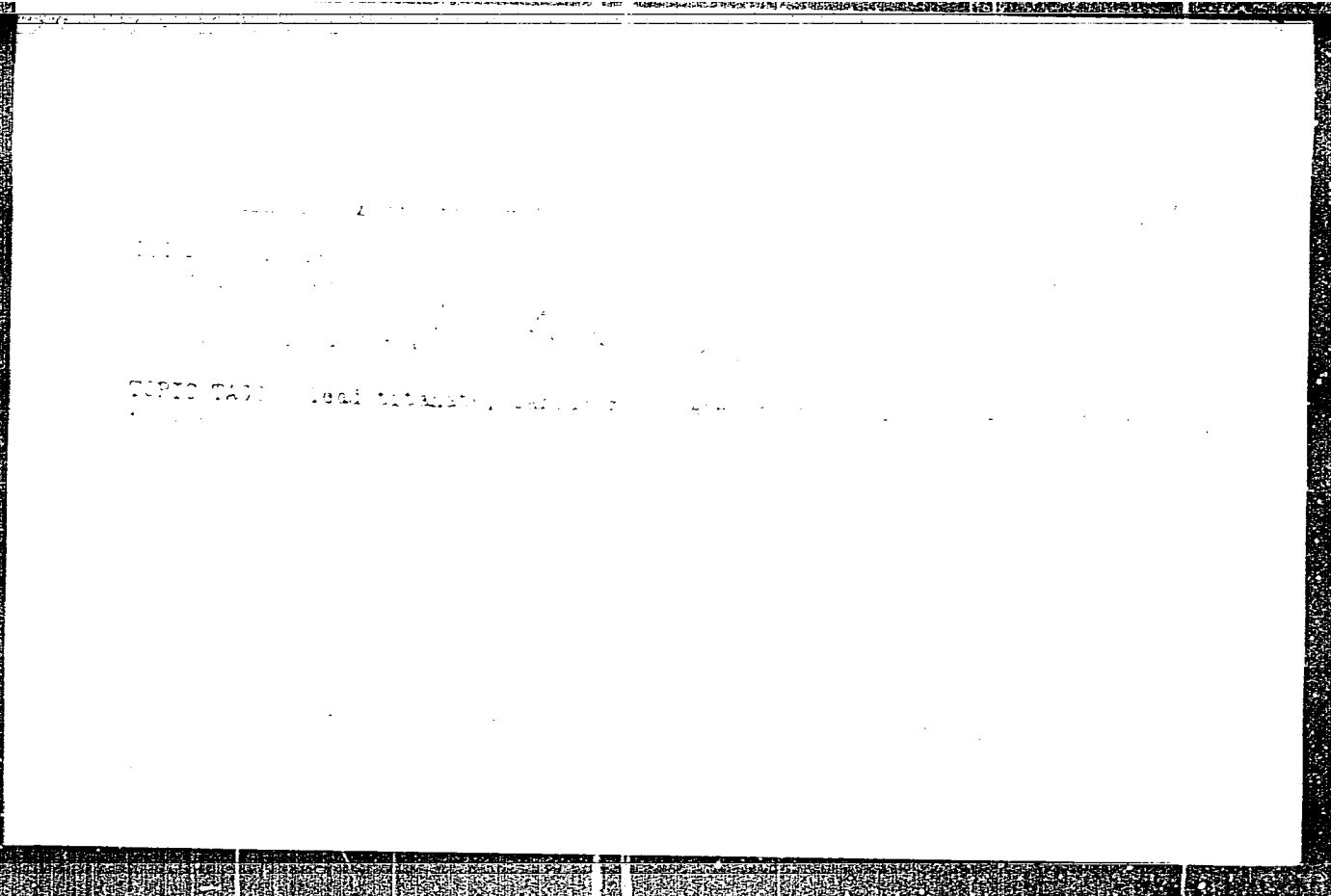
The four references to English-language publications read as follows: N. D. Megaw, Proc. Phys. Soc., 58, 133 (1946); R. Roy, J. Res. Nat. Bur. Standards, 58, 2, 75 (1957); M. H. Francombe, B. Lewis, J. Electronics, 2, 387 (1957); G. Shirane, S. Hoshino, K. Suzuki, Phys. Rev., 80, 6, 1115 (1950). *u*

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova (Physico-chemical Institute imeni L. Ya. Karpov)

Fig. 5. Phase diagram of the system $PbTiO_3 - LaFeO_3$.

Legend: (1) cubic (paraelectric); (2) tetragonal (piezoelectric); (3) pseudomonoclinic I; (4) pseudomonoclinic II.

Card 4/5



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| SUBMITTED: 05JAN68 | DATE REC: 21JAN 68 | ENCL: 00 |
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the $\text{BiFeO}_3\text{-LaFeO}_3$ system

SOURCE: Kristallografiya, v. 8, no. 1, 1963, 610-616

TONIN, TAI. Ferrimagnetic, uniaxial magnet, from ferrite magnet, ferrite-like, ...

... ..

ABSTRACT The $\text{BiFeO}_3\text{-LaFeO}_3$ system

Samples of $\text{BiFeO}_3\text{-LaFeO}_3$ were prepared from reagent-grade Bi_2O_3 , La_2O_3 , and Fe_2O_3 and were fired first at $850\text{--}1000^\circ\text{C}$ for 1.5 hr and then at $850\text{--}1000^\circ\text{C}$ for 1.5 hr.

Card 1/5

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Card 3/91

L 14282-63

ACCESSION NO. APL 63 63

of a given solid solution. Both properties are dependent upon the same factor, the atomic configuration. "The authors express thanks to A. S. Borovik-Romanov, N. M. Kreynen, and V. I. Smolova for their valuable advice and remarks." Orig. art. has: 5 figures.

ASSOCIATION: Nauchno-issledovatel'skiy fiziko-khimicheskiy institut im. L. Ya. Karpova (Scientific Research Physicochemical Institute)

SUBMITTED: 29 Jan 63

DATE ACQ: 14 Aug 63

ENCL: 1

SUB CODE: PH

NO REF OV: 018

OTHER: 007

Card 4/5.

5 091 03 004 0047 047 044
3111 2135

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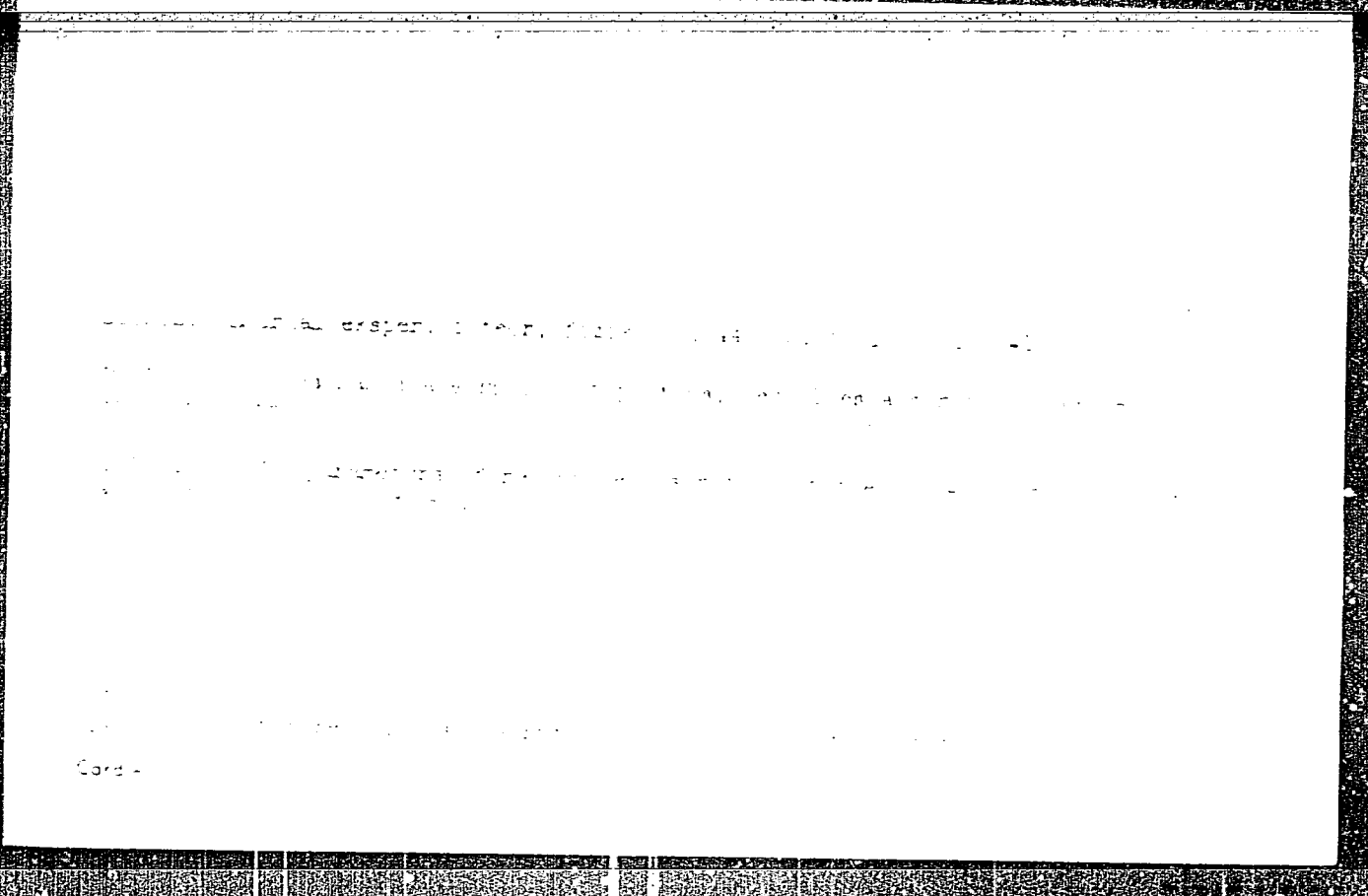
The coexistence of antiferromagnetic

3/05/67/0247/41/111

... the spontaneous
... with further LaFeO₃ addition
linearly. The temperature

... there are 2 figures.

ASSOCIATION: ...



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SUBMITTED: 28Feb63 DATE ACQ: 12/21/63 ENCL: 00
SUB CODE: 00 NO REF SOV: 01S OTHER: 006

Card 2 2

VEHEVTSEV, Yu. N.; ZHDANOV, G. S.; ROGINSKAYA, Yu. Ye.; FEDULOV, S. A.;
IVANOVA, V. V.; CHKALOVA, V. V.; VISOV, A. S.; KAPYSHEV, A. G.;
BONDARENKO, V. S.; LADYZHINSKIY, P. B.

Some solid solutions on the basis of the ferroelectric-
antiferromagnetic BiFeO_3 . Izv. AN SSSR. Ser. fiz. 28 no. 4:
683-690 Ap '64. (MIRA 17:5)

FAM ZUI KHIYEN; VISKOV, A.S.; SHPINEL', V.S.; ~~VENEVTSSEV, Yu.N.~~

Abrupt change of the probability of the Mossbauer effect during a phase transition in ferroelectric substances. Zhur. eksp. i teor. fiz. 44 no.6:2182-2183 Je '63. (MIRA 16:6)

1. Institut yadernoy fiziki Moskovskogo gosudarstvennogo universiteta i Fiziko-khimicheskiy institut im. L.Ya. Karpova.
(Mossbauer effect)

FEDULOV, S.A.; VENEVTSEV, Yu.N.

Study of the systems $PbTiO_3 - CaSnO_3$ and $PbTiO_3 - CaZrO_3$.
Kristallografiia 9 no.3:358-362 My-Je '64. (MIRA 17:c)

1. Vsesoyuznyy nauchno-issledovatel'skiy institut khimicheskikh reaktivov.

ACCESSION NR: AP4043189

S/0070/64/009/004/0516/0520

AUTHORS: Fedulov, S. A.; Lady*zhenskiy, P. B.; Venevtsev, Yu. N.

TITLE: Investigation of the system $\text{BiFeO}_3\text{-LaAlO}_3$

SOURCE: Kristallografiya, v. 9, no. 4, 1964, 516-520

TOPIC TAGS: bismuth inorganic compound, lanthanum compound, ferroelectric property, perovskite structure, solid solution, dielectric constant

ABSTRACT: Both investigated compounds have a perovskite structure and were expected to form solid solutions. It was also assumed that addition of LaAlO_3 to BiFeO_3 would lead to a decrease of the conductivity which would facilitate the study of the temperature dependence of the dielectric constant in a wide range of temperatures. It was assumed that the results of these measurements would further confirm the presence of ferroelectric properties in bismuth ferrite. The in-

Cord 1/5

ACCESSION NR: AP4043189

Investigation of the system was also aimed at studying the effect of various factors on the magnetic properties of similar compounds, and to determine regions in which they possess special dielectric and magnetic properties. The starting materials were Bi_2O_3 , Fe_2O_3 , Al_2O_3 (analytical purity), and La_2O_3 (technical purity). The x-ray analysis was carried out with $\text{CuK}\alpha$ and $\text{CoK}\alpha$ radiation. The lattice parameters were determined to within 0.0015 \AA , the volume to within 0.07 \AA^3 , and the angle to within $2'$. The magnetic measurements were carried out by a method described in *Kristallografiya* v. 8, no. 4, p. 610, 1963. X-ray analysis of samples with intermediate compositions showed that one-phase perovskite solid solutions occurred only up to 37.5 mole % LaAlO_3 . Samples with 25--35 mole % LaAlO_3 exhibit the clear maxima of the dielectric constant typical of ferroelectrics. With increasing LaAlO_3 content the maxima shift towards lower temperatures. The temperature dependence of the specific magnetization for samples of the homogeneous region was obtained at $H = 7600 \text{ Oe}$.

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ACCESSION NR: AP4043189

All solid solutions were found to be antiferromagnetic with weak ferromagnetism. For samples with 35 mole % LaAlO_3 the specific spontaneous magnetization reaches 0.15. The Curie temperature of BiFeO_3 is estimated by extrapolation to be about 850°C . The data make it possible to construct a part of the phase diagram of the system BiFeO_3 -- LaAlO_3 on the side of BiFeO_3 (Encl. 01). The decrease of the ferroelectric Curie temperature with increasing LaAlO_3 content is due, in the opinion of the authors, to the considerably weaker electron polarizability of the Li^{3+} ion compared with that of Bi^{3+} . Most interesting is the rather strong increase of the Neel temperature on the introduction of LaAlO_3 . This is due mainly to the somewhat smaller lattice constant of LaAlO_3 . "The authors thank Prof. G. S. Zhdanov and Yu. E. Roginskaya for valuable advice and remarks." Orig. art. has: 7 figures.

Card 3/5

ACCESSION NR: AP4043189

ASSOCIATION: VNII khimicheskikh reaktivov i osobo chisty*kh veshchestv Fiziko-khimicheskii institut im. L. Ya. Karpova (All-Union Institute of Chemical Reagents and Ultrapure Materials, Physico-chemical Institute)

SUBMITTED: 25Sep63

ENCL: 01

SUB CODE: SS

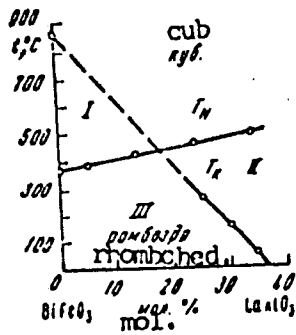
NR REF SOV: 014

OTHER: 002

Card 4/5

ACCESSION NR: AP4043189

ENCLOSURE: 01



Part of the phase diagram of the BiFeO₃-LaAlO₃ system on the BiFeO₃ side.

T_K - ferroelectric Curie temperature, T_N - antiferromagnetic Neel temperature
I - ferroelectric region
II - region of weak ferromagnetism
III - region with combined properties

Card 5/5

ACCESSION NR: AP4030644

S/0048/64/028/004/0683/0690

AUTHOR: Venevtsov, Yu.N.; Zhdanov, G.S.; Roginskaya, Yu.Ye.; Fedulov, S.A.; Ivanova, V.V.; Chkalova, V.V.; Viskov, A.S.; Kapy*shev, A.G.; Bondarenko, V.S.; Lady*zhinskiy, P.B.

TITLE: Investigation of some solid solutions based on the ferroelectric-ferromagnet bismuth ferrite [Report, Symposium on Ferromagnetism and Ferroelectricity held in Leningrad 30 May to 5 June 1963]

SOURCE: AN SSSR. Izv. Ser.fiz., v.28, no.4, 1964, 683-690

TOPIC TAGS: ferromagnetism, ferroelectricity, bismuth ferrite, bismuth ferrite solid solution

ABSTRACT: By investigating solid solutions of $\text{Bi}_2\text{O}_3 \cdot \text{Fe}_2\text{O}_3$ in PbTiO_3 , some of the authors, together with others, were able to show the existence of the compound Bi-FeO_3 with the perovskite structure and strong ferroelectric properties. This work is reviewed, and later investigations are reported of the electric and magnetic properties of solid solutions containing BiFeO_3 . The solutions discussed are the two-component systems in which one component is BiFeO_3 and the other is LaFeO_3 , LaCrO_3 ,

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ACCESSION NR: AP4030644

$PbTiO_3$, $BaTiO_3$, $PbZrO_3$, $LaAlO_3$, or $SrSnO_3$. Of these solutes, two are ferromagnetic, two are ferroelectric, one is antiferroelectric and two are perovskites with normal magnetic and electric properties. Phase diagrams are given for the $PbTiO_3$, $LaCrO_3$, and $BaTiO_3$ solutions. Curves of magnetization versus temperature are given for various compositions of the $LaCrO_3$ and $PbZrO_3$ solutions, and curves of dielectric constant versus temperature for the $LaAlO_3$, $PbZrO_3$ and $BaTiO_3$ solutions. The Neel point is plotted against composition for all the solutions except those containing $SrSnO_3$, which could not be obtained as a single phase. Extrapolation of the Curie points of the $LaAlO_3$ and $PbZrO_3$ solutions to zero concentration confirmed the high ferroelectric Curie point (about $350^\circ C$) of $BiFeO_3$. The weak ferromagnetic properties of $BiFeO_3$ persisted in solutions containing high concentrations of materials without peculiar magnetic properties. Particularly interesting is the concentration dependence of the spontaneous magnetization of the $LaCrO_3$ solutions; the magnetization increased discontinuously as the system crossed the boundary from the ferroelectric to the antiferroelectric state. The $LaFeO_3$ solutions are said to have behaved similarly, but as these solutions have been discussed in detail elsewhere (Yu.B. Roganskaya, Yu. N. Venevtsev, G.S. Zhdanov and S.A. Fedulov, *Kristallografiya*, 8, 1963), the data are not given. An anomaly in the Mossbauer spectrum of the $SrSnO_3$ solutions that was pro-

Card 2/3

ACCESSION NR: AP4030644

Previously ascribed to a ferroelectric transition (Fam Zui Khiyen, A.S. Viskov, V.C. Shpinel' and Yu.N. Vonevtsev, Zhur. eksp. i teor. fiz., 44, 1963) is now believed to be due to antiferromagnetic ordering. Orig.art.has: 10 figures.

ASSOCIATION: none

SUBMITTED: 00

DATE ACQ: 30Apr64

ENCL: 00

SUB CODE: EM

NR REF SOV: 016

OTHER: 006

Card 3/3

TOMASHPOL'SKIY, Yu.Ya.; VENEVTSEV, Yu.N.; ZHDANOV, G.S.

Interrelation of specific dielectric and magnetic properties
in "ferromagnetics." Zhur. eksp. i teor. fiz. 46 no.5:1921-
1923 My '64. (MIRA 17:6)

1. Fiziko- khimicheskiy institut imeni Karpova.

ACCESSION NR: AP4030634

S/0048/64/028/004/0630/0635

AUTHOR: Venevtsev, Yu.N.; Lyubimov, V.N.; Solov'yev, S.P.; Zhdanov, G.S.

TITLE: Calculation of the internal electric fields and their gradients in perovskite compounds with distinctive dielectric properties [Report, Symposium on Ferromagnetism and Ferroelectricity held in Leningrad 30 May to 5 June 1963]

SOURCE: AN SSSR. Izv.Ser.fiz., v.28, no.4, 1964, 630-635

TOPIC TAGS: internal field, crystal internal field, perovskite structure, ferroelectricity, ionic ferroelectricity model, ferroelectric compound

ABSTRACT: For a number of years the authors have been engaged in calculating the internal electric fields in compounds having the perovskite structure and peculiar dielectric properties. The methods of calculation and the results have been reported in a series of papers appearing in Kristallografiy (Crystallography) and Fizika tverdogo tela (Solid State Physics) from 1958 to 1962. The results of these calculations are discussed in the present paper. The calculations were based on the ionic model of a crystal with known or assumed structure. The charges and polarizabilities of the point ions were treated as given quantities, but the induced dipole moments

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ACCESSION NR: AP4030634

were calculated. Calculations were performed for several values of the charge, polarizability, and radius of the ions; reasonable variations of these parameters did not alter the qualitative picture of the fields in the six compounds investigated (lead, barium, calcium and cadmium titanates, sodium tantalate, and lead zirconate). Good agreement was obtained between observed and calculated values of the spontaneous polarization with the value 0.5 for the ionic charge factor. The results of the calculations indicate that NaTaO_3 and CdTiO_3 are ferroelectric materials and that PbZrO_3 is a ferroelectric material with nearly antiferroelectric properties. The internal field at the position of the Ti ion was found to vanish in CaTiO_3 but to be large in BaTiO_3 and PbTiO_3 . This difference in the fields accounts for the different dielectric behavior of these materials. Because of the strong field at the Ti ion, the conclusion of H.D. Megaw (*Acta crystallogr.*, 5, 739, 1952; *Ibid.*, 7, 167, 1954) that the principal factor in ferroelectric transitions of ABO_3 type materials must be a sharp increase in the covalent character of the B-O bond is regarded as inadequately grounded. It is concluded that further theoretical and experimental investigation of the possibilities of the ionic model is desirable, and improved calculations of field gradients are promised for the near future. Orig.art.has: 1 table.

Card 2/3

ACCESSION NR: APL039396

S/0070/64/009/003/0358/0362

AUTHORS: Fedulov, S. A.; Venevtsev, Yu. N.

TITLE: Investigating the system $PbTiO_3$ - $CaSnO_3$ and $PbTiO_3$ - $CaZrO_3$

SOURCE: Kristallografiya, v. 9, no. 3, 1964, 358-362

TOPIC TAGS: ceramic technology, x ray analysis, electric property/ RKU 114 x ray camera, RKD 143 x ray camera

ABSTRACT: Samples of the indicated systems were prepared by ordinary ceramic technology. X-ray analyses were made with CuK_{α} , FeK_{α} , and CrK_{α} radiation in RKU-114 and RKD-143 cameras. The results show a continuous series of solid solutions in the $PbTiO_3$ - $CaSnO_3$ system. The solid solutions form at room temperature in three modifications: tetragonal I, tetragonal II, and pseudomonoclinic. In the field of tetragonal I, the lattice constant c decreases sharply and increases with increase in $CaSnO_3$ content. When the $CaSnO_3$ content reaches ~22% (by weight), the tetragonal II field is reached. With further increase in $CaSnO_3$ content, the change in c is negligible, but it diminishes appreciably. At ~55% $CaSnO_3$ the

Card 1/3

ACCESSION NR: AP4039396

pseudomonoclinic field is reached. Here $a = c$ and the two increase slightly with increase in CaSnO_3 , but b remains almost unchanged. The $\text{PbTiO}_3\text{-CaZrO}_3$ system displays no continuous series of solid solutions. Here there is a broad two-phase region consisting of two perovskite modifications. The dielectric constant shows a sharp maximum for each system when the concentration of the second constituent (stannate or zirconate) is 20% or less. The absolute value is higher for $\text{PbTiO}_3\text{-CaZrO}_3$ (~ 3000) than for $\text{PbTiO}_3\text{-CaSnO}_3$ (~ 2000). In both systems the values decrease appreciably with increase in content of the second constituent. Conductivity and dielectric loss diminish markedly with increase in these second constituents. The decrease in conductivity was found to be on the order of a thousandfold for a content of 15% CaSnO_3 over pure PbTiO_3 at 100C. The authors conclude that no anomalous effects were noted that might be associated with transitions of "crumpling." The authors thank Professor G. S. Zhdanov for his interest in the work and his discussions of the results. Orig. art. has: 3 figures.

ASSOCIATION: Vsesoyuznyy nauchno-issledovatel'skiy institut khimicheskikh reaktivov (All Union Scientific Research Institute of Chemical Reagents)

Card 2/3

ACCESSION NR: AP4039396

ENCL: 00

SUBMITTED: 25Sep63

OTHER: 005

SUB CODE: SS, EC, MT

NO REF SOV: 004

Card 3/3

ACCESSION NR: AP4037617

meters, the dielectric constant, and the specific magnetization, with special care in the region of the antiferromagnetic transition. The details of the experiment are described. The noticeable anomalies in the curves of these parameters in the region of the Neel point offer evidence of the existence of a connection between the magnetic, electric, and atomic structures. It is precisely by virtue of this connection that the sharp change in the magnetic structure at the point of antiferromagnetic transition leads to noticeable changes in the electric and atomic structures, as reflected in the anomalies of the corresponding parameters near the Neel point. The observation of one of the manifestations of such an interaction in BiFeO_3 indicates that this connection is experimentally detectable and can be observed and investigated in a comprehensive fashion, by studying the changes in the magnetic and electric characteristics of the parameters of the atomic lattice as functions of several extraneous factors (temperature, pressure, fields, etc.). The connection can be regarded both on a unit-cell scale, as well as on a scale

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ACCESSION NR: AP4037617

of multidomain formations in the case of single crystals or polycrystals. Orig. art. has: 1 figure.

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova (Physicochemical Institute)

SUBMITTED: 04Mar64

DATE ACQ: 09Jun64

ENCL: 01

SUB CODE: SS

NR REF SOV: 011

OTHER: 000

Card 3/4

L 15328-66 EWT(d)/EWT(m)/EWP(v)/EWP(k)/EWP(h)/EWP(l)/ETC(m)-6 DIAAP
ACC NR: AP6001001 SOURCE CODE: UR/0285/65/000/022/0067/0067

AUTHORS: Mitrofanov, K. P.; Viskov, A. S.; Venevtsev, Yu. N.; Shpinel', V. S.;
Plotnikova, H. V.

44

ORG: none

TITLE: Method for measuring temperature.^{qm} Class 42, No. 176442

SOURCE: Byulleten' izobreteniy i tovarnykh znakov, no. 22, 1965, 67

TOPIC TAGS: temperature measurement, gamma ray absorption

ABSTRACT: This Author Certificate presents a method for measuring temperature, based on the discontinuous change of the effect of resonance gamma-ray absorption with a phase transition in the absorber. To increase the accuracy of measurements, a series of absorbers with different phase transition temperatures is placed in direct thermal contact with the investigated sample. The absorbers are exposed to radiation from a resonance source of gamma-rays and the absorption effect is recorded with detectors.

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SUB CODE: 20/

SUBM DATE: 14Apr64

SB
Card 1/1

UDC: 536.51 615.84

L 22121-66 EWT(1)/EWT(m)/EWP(w)/EFP(n)-2/T/EP(t) IJP(c) JD/JG/3G

ACC NR: AP6004921

SOURCE CODE: UR/0056/66/050/001/0069/0075

AUTHOR: Roginskaya, Yu. Ye.; Tomashpol'skiy, Yu. Ya.; Venevtsev, Yu. N.; Petrov, V. M.; Zhdanov, G. S.

ORG: Physicochemical Institute im. L. Ya. Karpov (Fiziko-khimicheskiy institut)

TITLE: On the character of dielectric and magnetic properties of BiFeO₃

SOURCE: Zhurnal eksperimental'noy i teoreticheskoy fiziki. v. 50, no. 1, 1966, 69-75

TOPIC TAGS: bismuth compound, ferroelectric material, dielectric property, solid solution, Curie point, Neel temperature, magnetic property

ABSTRACT: This is a continuation of earlier work by the authors on BiFeO₃ (ZhETF v. 46, 1921, 1964). In view of the contradictory reports on the properties of BiFeO₃, especially with respect to its ferroelectric properties, the authors analyze the published data and in addition carried out a more detailed investigation of the dielectric properties and the structure of BiFeO₃ in a broad range of temperatures, as well as of solid solutions of this substance with PbFe_{1/2}Nb_{1/2}O₃. Particular attention is paid to the 400--500C region, and to the solid solution. The polycrystalline samples for the investigation were prepared by the usual ceramic techniques. The dielectric constant and the loss angle were measured at

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