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主编　钱伟长

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王宽诚教育基金会

学术讲座汇编

（第2集）

主编：钱伟长

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王宽诚教育基金会敬赠

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谨以此书纪念本会创建人、故董事会主席王宽诚先生

王宽诚教育基金会

王宽诚教育基金会简介

王宽诚先生(1907～1986)为香港知名爱国人士，热心祖国教育事业，生前为故乡宁波的教育事业做出积极贡献。1985年独力捐巨资创建王宽诚教育基金会，其宗旨在于为国家培养高级科技人才，为祖国四个现代化效力。

王宽诚先生在世时聘请海内外知名学者担任基金会考选委员会和学务委员会委员，共商大计，确定采用“送出去”和“请进来”的方针，为国家培育各科专门人才，并为提高国内和港澳高等院校的教学水平，资助学术界人士互访，用以促进中外文化交流。在此方针指导下，1985、1986两年，基金会在国家教委支持下，选派学生85名前往英、美、加拿大和西德、瑞士、澳大利亚各国攻读博士学位，并计划资助国内学者赴港澳讲学，资助港澳学者到国内讲学，资助美国学者来国内讲学。正当基金会事业初具规模，蓬勃发展之时，王宽诚先生一病不起，于1986年年底逝世。这是基金会的重大损失，共事同仁，无不深切怀念，不胜惋惜。

王宽诚教育基金会在新任董事会主席张二铭先生和安子介、方善桂、胡百全、李福树等董事的主持下，继承王宽诚先生为国家培育人才的遗愿，继续努力，除按计划执行外，并开发与英国学术机构合作的新项目。王宽诚教育基金会过去和现在的工作态度一贯以王宽诚先生所倡导的“公正”二字为守则，谅今后基金会亦将秉此行事，奉行不缀。借此王宽诚教育基金会《学术讲座汇编》出版之际，特简明介绍如上。

钱　伟　长

一九八九年十二月

Hm0/16/02

前　言

王宽诚教育基金会是由已故全国政协常委、香港著名工商企业家王宽诚先生（1907～1986）出于爱国热忱，出资一亿美元于1985年在香港注册登记创立的。

1987年，基金会开设“学术讲座”项目，此项目由当时的全国政协常委、现任全国政协副主席、著名科学家、中国科学院学部委员、上海工业大学校长、王宽诚教育基金会贷款留学生考选委员会主任委员兼学务委员会主任委员钱伟长教授主持，由钱伟长教授亲自起草设立“学术讲座”的规定，资助国内学者前往香港、澳门讲学，资助美国学者和港澳学者前来国内讲学，用以促进中外学术交流，提高内地及港澳高等院校的教学质量。

本汇编收集的文章，均系各地学者在“学术讲座”活动中的讲稿。文章作者中，有年逾八旬的学术界硕彦，亦有由王宽诚教育基金会考选委员会委员推荐的学者和后起之秀。文章内容有科学技术，有历史文化，有经济专论，有文学，有宗教和中国古籍研究。本汇编涉及的学术领域颇为广泛，而每篇文章都有一定的深度和广度，分期分册以《王宽诚教育基金会学术讲座汇编》的名义出版，并无偿分送港澳和国内部分高等院校、科研机构和图书馆，以广流传。

王宽诚教育基金会除资助“学术讲座”学者进行学术交流之外，在钱伟长教授主持的项目下，还资助由国内有关高等院校推荐的学者前往欧美亚澳参加国际学术会议，出访的学者均向所出席的会议提交论文，这些论文亦颇有水平，本汇编亦将其收入，以供参考。

王宽诚教育基金会学务委员会

凡　例

（一）编排次序

本书所收集的王宽诚教育基金会学术讲座的讲稿及由王宽诚教育基金会资助学者赴欧美亚澳参加国际学术会议的论文均按照收到文稿日期先后编排刊列，不分类别。

（二）分期分册出版并作简明介绍

因文稿较多，为求便于携带，有利阅读与检索，故分期分册出版，每册约 150 页至 200 页不等。为便于读者查考，每篇学术讲座的讲稿均注明作者姓名、学位、职务、讲学日期、地点、访问院校名称。国内及港澳学者到欧、美、澳及亚洲的国家和地区参加国际学术会议的论文均注明学者姓名、参加会议的名称、时间、地点和推荐的单位。上述两类文章均注明由王宽诚教育基金会资助字样。

（三）文字种类

本书为学术性文章汇编，均以学术讲座学者之讲稿原稿或参加国际学术会议学者向会议提交的论文原稿文字为准，即原讲稿或论文是中文的，即以中文刊出，原讲稿或论文是外文的，仍以外文刊出。

编 后 记

本书第一集出版后，分送到国内外各大图书馆及各地高等院校和科研机构，引起广泛注意。东至东北鞍山，西至四川渡口，北至郑州，南至广州均有来函表示愿意今后和我们保持联系，希望继续赠阅。有的学校资料室认为内容很好，专业性强，有一定深度和广度，学术水平很高，对学校的教学与科研有一定的参考价值。

我们受到边远地区来函鼓励，倍感亲切，益觉力薄，诚恐失误。第一集第143页脚注中之"香港大学"系"香港中文大学"之误，特此更正。若有其他错误，尚请海内外广大读者批评，勿吝赐教。

王宽诚教育基金会学务委员会

一九九〇年九月

王宽诚教育基金会《学术讲座汇编》

第二集

目　录

王宽诚教育基金会
《学术讲座汇编》第2集，1～105 (1990).

THE TENSOR PROPERTIES OF DIELECTRIC CRYSTALS AND THEIR RELATIONS TO THE CRYSTAL SYMMETRY

CHEN GANG*

INTRODUCTION

The aim of following lectures is to show how to study the subject rather than to serve as a reference work containing all the conclusions, in other words, only the methods but not the results are concerned here, if some results shown up, they just play the role of giving examples of how the methods are used.

Tensors are the majorly used mathematics in these lectures, and the treatment of crystal symmetry is limited to the 32 point groups, since only the macroscopic physical properties are dealt with. Also, only the properties of dielectric crystals are treated here, the conductivity and magnetic properties are excluded because being transport phenomena, they have the complexity of magnetic groups which are beyond our mathematic and symmetry bases used in these lectures.

I should like to give the courses according to the following sequence:

(I) Tensor transformations and definition of tensors.
(II) Elementaries of tensor mathematics.
(III) Symmetry properties of tensors (Intrinsic symmetry of tensors).
(IV) Point groups and crystal classes, crystal systems.
(V) Neumann's Principle.
(VI) Tensor quantities from 1st- to 4th-rank.
1. 1st-rank polar tensor property.
2. 2nd-rank polar tensors.
3. 3rd-rank polar tensor properties.
4. 4th-rank polar tensor properties.
5. 2nd-rank axial tensor property.
6. Fourth-rank axial tensor property.

(VII)Thermodynamics of dielectric crystals.

The attempt at comprehensiveness has been made to include 2 more topics on "Tensor

* 作者陈纲，是北京工业大学教授。1988年10月由王宽诚教育基金会资助，在香港理工学院讲学一个月。

properties in the cyclic axes frames" (Appendix A), and "The group theoretical method for determination of non-zero independent components of tensor properties of crystals" (Appendix B).

NOTES ON THE COURSE

The field of tensor properties of crystals is probably the oldest chapter of solid state physics, it deals with the macroscopic physics of anisotropic solids. This knowledge follows from a purely macroscopic formulation of the physics of anisotropic media. Such a formulation, built on the combined symmetries of physical processes and of crystal structure, effectively establishes the framework within which all microscopic theories must operate. But it is largely bypassed in introductory courses, and is often neglected even in advanced presentations of solid state physics, which nowadays very much emphasizes the microscopic description of phenomena. Of course, crystal physics at the macroscopic level is equally important in its own right in dealing with the great variety of new phenomena.

In recent years, the progresses of science and technology show that more and more macroscopic properties of anisotropic media get in use on the frontiers of different fields, such as laser techniques, electrooptics, acoustooptics, the technique of recording and displaying information, and various new functional devices are being made of crystals to meet the rapid needs of scientific and technological developments.

So, a systematic study of macroscopic properties of crystals will not only help to deepen the microscopic formulation of phenomena, but also will benefit the proceeding of science and technology.

The necessity of introducing tensors to describe the macroscopic physical properties of crystals:

In the traditional theories of physics, the properties of matter are defined by relations between measurable quantities, i.e. the relations between the response quantities of the material to applied forces or fields and the quantities that characterizing the latters. For example, if the relation is linear, we can write

$$B=CA \tag{0.1}$$

where B—the response quantity, A—the applied field quantity, and then C—the physical property of that material.

There may be two cases: The representation of the properties of matter doesn't depend on the direction of measurements, such non-directional physical quantities are called as scalars, and by giving a single number a scalar is completely specified, For example, density is defined from a relation between mass and volume, and mass and volume are measured without reference to direction, so, accordingly, density is a property that does not depend on direction, such a property is taken as an isotropic property. The other case is that the representation of the properties of matter does depend on the direction of measurements. Under this condition, a single number—scalar will not suffice, a set of number is needed instead. When electric field E applies to a crystal, as the response to the field, electric polarization P is induced inside the crystal. Since electric field and electric polarization are all quantities characterized not only by their magnitudes but also by their orientations, the dielectric susceptibility—defined by the relation between E and P, is a property does depend on direction, that is to say, for cryatals, χ is anisotropic.

If all the physical properties of a material are scalars, then we say that the material is

isotropic. Most crystals are anisotropic. For a few properties, such as density, all crystals are isotropic. Cubic crystals happen to be isotropic for a certain number of other properties as well, such as the dielectric constant ε, the dielectric susceptibility χ, and the index of refraction n, etc. But for elasticity, photoelasticity, and certain other properties, cubic crystals are in fact anisotropic. So, cubic crystals are not isotropic media. The lower the crystal symmetry, the fewer number of isotropic properties the crystal can possess.

To represent the isotropic properties of matter, scalars are sufficient. But, in a crystal, for characterizing the anisotropic properties, TENSORS—a finite set of coefficients that obey the transformation laws under the transformations of axes of reference—are to be used, since tensors can describe both the magnitudes and the directions of the anisotropic properties.

Field quantities and matter quantities:

In Equation (0.1), the quantities A,B,C can be of two kinds. One of them we call as field quantities, such as stress, strain, electric field, electric polarization .... They only represent the external influences or the responses induced inside the material, they are also called as field tensors. Field tensors don't represent the properties of matter, they possess only the symmetries of the physical processes which they represent. The other kind of quantities are called as matter quantities, or matter tensors, such as density, dielectric constant, piezoelectric modulus.... They represent the properties of material, and they possess not only the symmetries of physical processes but also symmetries of crystal structures.

The formulation of crystal physics based on these principles of symmetry determines primarily the necessary framework of all possible interactions. It separates allowed and forbidden effects, and it specifies the form of the allowed effects in a crystal of given symmetry. Our approach focuses on the preliminary aspects of determining the classes of crystals to which the search for any particular effect can be restricted, and the form of the response by which this effect is to be identified.

This aspect of crystal physics covers a sufficiently large ground to justify development in its own right. Surprisingly enough, it is not a closed subject. The systematic exploration of highly anistropic crystals is just beginning, and some of the effects predicted in such crystals remain to be discovered experimentally. On the other hand, the recent history of crystal physics includes instances of "forbidden" effects that were found to be "allowed" after more careful examination of the inherent symmetries governing the interaction or of the structure symmetries of crystals. Crystal physics has had its share of "symmetry violations" and of the new worlds opened up by each such discovery. There is good reason to believe that the full intricacy of the interactions possible in crystals is yet to be discovered.

1. Tensop transformations and definition of tensors.

Most of the externally applied influences and the responses of the crystal and the corresponding physical properties of the crystal are represented by quantities that are direction dependent. All such directional aspects are readily described by a mathematical formulation called tensor which is composed of a set of orderly components.

Before an exact definition of tensor can be given, we'll draw some preliminary knowledge of it here:

(1) According to the number of components needed in determining a tensor, tensors can be said to be of zero rank, the 1st rank, the 2nd-rank, ..., and we already know that tensors

of zero rank are scalars which are direction independent, and tensors of the lst rank are vectors which have 3 components in Cartesian coordinate system. As it will be revealed later soon that tensors of the 2nd rank have 9 components, ..., and tensors of the mth rank have 3^m components. So, in this way, we can summarize as following:

Table 1.1

Rank of the tensor m	number of components	examples of quantities
0	$3^0=1$	density, temperature
1	$3^1=3$	electric field, electric polarization, pyroelectric coefficient
2	$3^2=9$	stress, strain, dielectric const.
3	$3^3=27$	piezoelectric modulus, linear electro-optic coefficient
4	$3^4=81$	elastic coeff., photo-elastic coeff.

(2) A proper description of the physical properties of a crystal must be invariant under the operation of the symmetry group of this crystal. In order to assure the above requirement, we must establish how the description itself transforms under the operations relating different coordinate systems. This is the reason why we talk about tensor transformations.

I. 1. Transformations of coordinate axes.

Tensor transformation is closely related to that of the coordinates and makes use of the same basic description quantities.

Let us choose an orthogonal system of axes for the coordinate system O (not necessarily identical with crystal axes of symmetry); O is described by 3 orthogonal basis vectors e_i

$$\begin{cases} e_i \cdot e_j = \delta_{ij} & (1.1a) \\ e_i \times e_j = u_{ijk} e_k \quad \text{(if right-handed)} & (1.1b) \end{cases}$$

where δ_{ij} is the Kronecker delta:

$$\begin{cases} =1, \text{ for } i=j, \\ =0, \text{ for } i \neq j \end{cases} \tag{1.2}$$

and u_{ijk} is the antisymmetric triple product:

$$\begin{cases} =1 \text{ for } i, j, k \text{ in cyclic order;} \\ =-1 \text{ for } i, j, k \text{ in reverse order} \\ =0 \text{ if 2 or more indices are the same} \end{cases} \tag{1.3}$$

Another orthogonal system O', with a set of basis vectors e_i', rotated with respect to O and left the origin and length measuring unit unchanged in the 2 systems, is related linearly to the O system:

$$e_i' = \sum_{j=1}^{3} a_{ij} e_j \qquad (i=1,2,3) \tag{1.4}$$

We now leave out the summation sign:

$$e_i' = a_{ij} e_j \qquad (i\,j=1,2,3) \tag{1.5}$$

and introduce the Einstein summation convention: when a letter suffix occurs twice in the same term, summation with respect to that suffix is to be automatically understood. The coefficients a_{ij} are the direction cosines between the old and new vectors (see Fig. 1. 1)

$$a_{ij} = e_i' \cdot e_j \tag{1.6}$$

If we represent the basis vectors by columns and the nine coefficients a_{ij} as a square array

$$(A)=(a_{ij})=\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}^{*} \tag{1.7}$$

and use the rules of matrix multiplication, Eq. (1.5) can also be expressed in the form

$$\begin{pmatrix} e_1' \\ e_2' \\ e_3' \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} \tag{1.8}$$

The square array of transformation parameters (a_{ij}) is called the transformation matrix be-

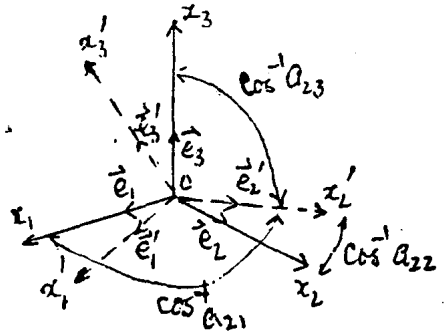

Fig. 1.1 Transformation of axes

tween the two coordinate systems O and O', and has a few well-known properties as following:

$$a_{ik}a_{jk}=\delta_{ij}$$

$$\delta_{ij}=\begin{cases} 1\ (i=j), & \text{normalization,} \\ 0\ (i\neq j), & \text{orthogonality.} \end{cases} \tag{1.9}$$

(1.10)

In general, $a_{ij}\neq a_{ji}$. Because of the above relations, only three of the nine parameters in Eq. (1.7) are truly independent.

The inverse transformation (a_{ji}) has the relation.

$$a_{ij}^{-1}=a_{ji} \tag{1.11}$$

to the former one.

The matrix (a_{ij}) which defines the transformation from O to O' contains information about the sense of the new coordinate system. It is easy to show that there exists two cases. On the one hand, if the transformation is a proper rotation, the determinant $|a_{ij}|$ has the value $+1$, and O and O' have the sense: both are either right-handed or left-handed. On the other hand, if the transformation is an improper rotation (including inversion, reflection and rotation-inversion), $|a_{ij}|=-1$, and the sense of O' is opposite to that of O, that is to say, if O is right-handed, then O' is left-handed, or vice versa.

Note: (*) The relation between the direction cosines of the axes may be shown by drawing up the following table:

New one—O' \ O—old one	e_1	e_2	e_3
e_1'	a_{11}	a_{12}	a_{13}
e_2'	a_{21}	a_{22}	a_{23}
e_3'	a_{31}	a_{32}	a_{33}

If we have another transformation from O' to O'' after the transformation from O to O', and the transformation matrix defining that from O' to O'' is $(B)=(b_{ki})$, then we can say that O transforms directly to O'' with a transformation matrix $(C)=(c_{kj})$ which obeys the multiplication rule of matrix:

$$(C)=(B)\ (A) \tag{1.12a}$$

or, alternatively

$$c_{kj}=b_{ki}a_{ij} \tag{1.12b}$$

Note that the order of the matrices in Eq. (1.12) must not be reversed, since it implies that the transformation from O to O' happens at first and the corresponding matrix (A) is placed behind the matrix (B) that represents the transformation from O' to O'' which happens after that from O to O'. It is easy to show that (C) also satisfies Eq. (1.9) — (1.11), if (A) and (B) both meet the requirement of linear orthogonal rigid transformation.

I. 2. Tensor transformations:

(1) Transformation of scalars (tensors of zero-rank):

As is already known, scalars are quantities that are direction independent, and only one number is needed to specify a scalar. Under the transformation of coordinate system, the value of a scalar will remain unchanged, but its sign will be different according to whether the transformation is a proper or an improper rotation. When it is a proper rotation, the sign of the scalar doesn't change, while for improper rotation the sign changes. We express as

$$\phi'=\pm\phi \tag{1.13}$$

where the quantity with a (') is corresponding to the scalar after the coordinate axes transformation.

Among the physical quantities of dielectric crystals we'll deal with later, the rotatory power which describes the optical activity of crystal is an example of that kind of scalar which will change its sign under an improper rotation.

The scalars that do not change sign under any kind of transformation are called "true scalars", and those changing signs under improper rotations are called "pseudo scalars", or "axial scalars".

(2) Transformation of vectors (tensors of the first-rank), or, more precisely, transformation of vector components.

Suppose now there is a vector r connecting the origin of the coordinate system O and a fixed point P in a certain crystal. If the point P has the coordinates (x_1,x_2,x_3) in O, they are given by the relation to the vector r:

$$r=x_1e_1+x_2e_2+x_3e_3 \tag{1.14}$$

so, the coordinates of point P are also the components of vector r. We now want to ask how do the x_is transform into a new set of x_i's when the coordinate system transforms from O to O'? If the transformation from O to O' leaves the crystal and the point P unmoved, then in O', it must be the same vector r but with a new set of coordinates (x_1',x_2',x_3'):

$$r=x_1'e_1'+x_2'e_2'\times x_3'e_3' \tag{1.15}$$

Take the scalar product of e_1' with (1.14) and (1.15), and we obtain

$$e_i'\cdot(x_je_j)=e_i'\cdot(x_k'e_k')$$

and make use of Eq. (1.1) and (1.6), we arrive at the final result

$$x_i'=a_{ij}x_j \qquad (i,j=1,2,3) \tag{1.16}$$

Hence we have shown that the coordinates of a point or the components of a vector

transform exactly like basis vectors of the coordinate systems.

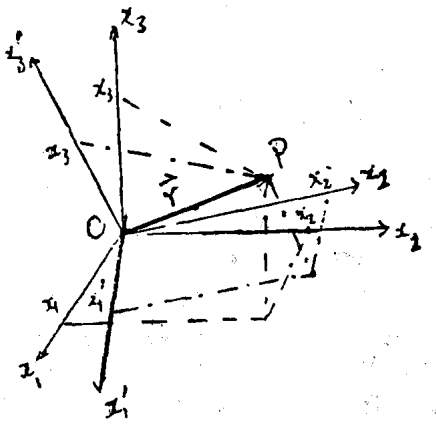

Fig. 1.2 Transformation of vector components (coordinates of a point).

For the reverse transformation and by referring again to Eq. (1.6), we have

$$x_i = a_{ji} x_j' \qquad (i,j=1,2,3) \tag{1.17}$$

Note that in the O to O' transformation, 'new' (with's) in terms of 'old' (without's), the dummy suffices occur in neighbouring places. In the reverse transformation, they are separated.

Up to this point we have not made any distinction among vectors, but in fact we can divide the vectors into two kinds: The one which transforms exactly according to Eq. (1.16) under any kind of transformation of coordinate system and can be represented without ambiguity by an arrow pointing in a certain direction like that shown in Fig. 1. 2 is called polar vector or true vector. The examples of this kind are forces, lineary velocity, the strength of electric field and many other polar vectors.

Another kind of vectors such as angular velocity, angular momentum, mechanical torque, etc., which are represented by straight lines with definite orientation and screw motion attached to them as shown in Fig. 1. 3b, the length of the line is in proportion to the magnitude of the vector and the direction of the vector is given by the orientation of the line and the sense of the screw motion. If the axes are right-handed, then a positive sense of rotation will attach to the line given by a right-handed screw motion, and the same for left-handed axes. These vectors are called axial vectors (or pseudo-vectors). From Fig. 1. 3, we see that there is a difference between polar and axial vectors. In a plane perpendicular to the line, reflection of polar vector reverses its direction but that of axial vector remains unchanged. On the other hand, reflection in a plane parallel to the line has the opposite effect.

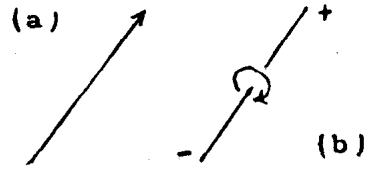

Fig. 1.3 Symbolic representation of vectors. (a) a polar vector, (b) an axial vector

As for the transformation of vector components, there is also a little different between them.