on the surface layers by oxygen molecules will naturally depend on the air pressure. The pressure in the evacuated and sealed tubes in the present experiments was of the order of 10^{-3} mm of Hg. This explains the difference in the luminescence intensity of the two specimens, one heated *in vacuo* and the other in air (Figs. 1 and 2) though both were annealed at at 500 °C for the same duration. It is believed, therefore, that an oxygen molecule-ion O_2^+ or a neutral molecule O_2 situated on a cation site is one of the components of the luminescence centre responsible for 260 nm excitation and 360 nm emission.

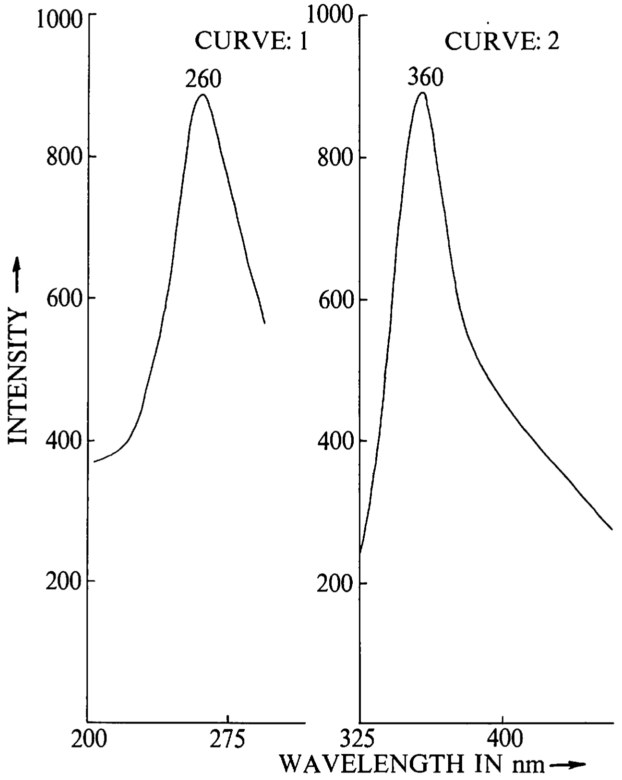

Fig. 3. Excitation (curve 1) and emission (curve 2) spectra of a NaCl:Sr powder specimen prepared from aqueous solution (Sr concentration 10^{-4} *M*). Specimen annealed and quenched in an evacuated and sealed tube at 500 °C for 50 h and quenched rapidly to room temperature.

Comparison of the intensities of the excitation and emission bands displayed by an undoped NaCl specimen, annealed and quenched from 500 °C *in vacuo*, with the intensities of the corresponding bands exhibited by a doped NaCl specimen (Sr concentration 10^{-4} *M*) also annealed and quenched from 500 °C *in vacuo*, clearly demonstrates that the introduction of a trace amount of strontium impurity suppresses the intensities of the luminescence bands by a factor of about 2·5 (compare Figs. 1 and 3). It is known that a major fraction of the divalent impurity ions incorporated in an alkali halide crystal become associated with positive-ion vacancies forming impurity–vacancy dipoles and their higher aggregates (Cook & Dryden, 1960, 1962; Dryden, 1963). It therefore seems plausible that the positive-ion vacancies produced by quenching are used up in the generation of dipoles and this inhibits the formation of 360 nm centres. It is not possible to specify the exact composition of the 360 nm centre. It may involve the O_2 molecule or O_2^+ molecule-ion in association with one or more positive-ion vacancies.

It may be mentioned that oxygen has been suggested as a common impurity of most of the 'pure' alkali halides, though of course, little definitive work has been done with this impurity (Kanzig & Cohen, 1959; Schulman & Compton, 1963). Halperin, Kristianpoller & Ben-zvi (1959) attributed the thermoluminescent emission of undoped alkali halides to centres composed of oxygen impurity and ion vacancies.

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A different best rigid-body molecular fit routine*.

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A different algorithm which gives a least-squares fit between two sets of atoms is described [*cf.* Nyburg (1974). *Acta Cryst.* B**30**, 251–253]. With this algorithm the coordinates of the moving set of atoms are changed only once.

Rigid-body least-squares best molecular fit programs have recently been described by Nyburg (1974) and by Gavuzzo, Pagliuca, Pavel & Quagliata (1972). We routinely use a different method for obtaining the best fit. This method has been incorporated into the system of programs *REFINE*2 developed in this laboratory for model building (= idealization, if desired with nonbonded energy constraints) and conformational analysis primarily of protein molecules (Hermans & McQueen, 1974; Hermans, Ferro, McQueen & Wei, 1976: these Fortran programs are available upon re-

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quest). The most frequent use that we make of the least-squares fit is to evaluate the discrepancies between different models of a protein molecule obtained by various refinement procedures.

In order to optimize the least-squares fit between the two structures, one of these is subjected to rigid-body translation and rotation. The problem therefore consists of finding a particular axis-rotation matrix **M** which is a function of three independent variables, *e.g.* the three Euler angles, and a translation vector **t**. This problem has a linear solution for the components of **t**. The best choice for **t**, the vector connecting the centroids of the two structures, is readily calculated.

The solution of the optimization is nonlinear in terms of the Euler angles or other independent parameters that have been considered, and is found by iteration. The following describes how the iteration to approximate **M** can be performed without changing the coordinates, in fact using the two sets of coordinates but once. There are two advantages to the use of this method. (1) After the salient information has been extracted from the coordinates, the effort spent on approximating **M** is the same for a very large structure as for a three-atom structure, and (2) the coordinates are not changed, hence no special measures have to be taken to prevent loss of significance of the last digit(s) of the *coordinates.* These advantages are particularly important when using a slow computer with a short wordlength.

Analysis

Given two sets of coordinates $\mathbf{X}'$ and $\mathbf{Y}'$, it is asked to change $\mathbf{Y}'$ to $\mathbf{Y}'''$ by rotation and translation in order to minimize

$$F=\sum_i |\mathbf{x}_i'-\mathbf{y}_i'''|^2\,. \tag{1}$$

The matrices $\mathbf{X}'$, $\mathbf{Y}'$ and $\mathbf{Y}'''$ have dimension $3\times n$ (n is the number of atoms), and each vector $\mathbf{x}$ and $\mathbf{y}$ represents the coordinates of a single atom. The notation $|\mathbf{u}|$ is used to denote the magnitude of the vector $\mathbf{u}$. As is well known, one rewrites this

$$F=\sum_i |(\mathbf{x}_i'-\mathbf{t}_x)-\mathbf{M}(\mathbf{y}_i'-\mathbf{t}_y)|^2=\sum_i |\mathbf{x}_i-\mathbf{M}\mathbf{y}_i|^2\,. \tag{2}$$

Here $\mathbf{t}_x$ and $\mathbf{t}_y$ are the coordinates of the centroids of $\mathbf{X}'$ and $\mathbf{Y}'$, and $\mathbf{X}$ and $\mathbf{Y}$ represent these coordinates when centered at the origin by translation.

We define

$$\mathbf{Y}''=\mathbf{M}\mathbf{Y} \tag{3}$$

then

$$\mathbf{y}_i'''=\mathbf{y}_i''+\mathbf{t}_x\,. \tag{4}$$

The problem is then to find the elements of the 3 × 3 axis-rotation matrix **M** that minimize the function F expressed by equation (2). This equation can be rewritten

$$F=\sum_{i=1}^{n}\sum_{j=1}^{3}\Big(x_{ji}^2+\sum_{k=1}^{3} m_{jk}^2y_{ki}^2-2\sum_{k=1}^{3} m_{jk}x_{ji}y_{ki} + \sum_{\substack{k=1\\k\neq l}}^{3}\sum_{l=1}^{3} m_{jk}m_{jl}y_{ki}y_{li}\Big)\,. \tag{5}$$

With the order of summation changed this becomes

$$F=\sum_i\sum_j x_{ji}^2+\sum_k\sum_i y_{ki}^2\sum_j m_{jk}^2-2\sum_k\sum_j m_{jk}\sum_i x_{ji}y_{ki} + \sum_{k\neq l}\sum_l\sum_i y_{ki}y_{li}\sum_j m_{jk}m_{jl}\,. \tag{6}$$

The first two terms are independent of the elements of $\mathbf{M}(\sum_j m_{jk}^2=1)$ and the last term is zero ($\sum_j m_{jk}m_{jl}=0$ if $k\neq l$). In order to minimize F we must therefore maximize

$$G=\sum_k\sum_j m_{jk}\sum_i x_{ji}y_{ki}\,. \tag{7}$$

If we define 3×3 correlation matrices $\mathbf{C}$ and $\mathbf{C}''$ with

$$c_{kj}=\sum_i x_{ji}y_{ki} \text{ and } c_{kj}''=\sum_i x_{ji}y_{ki}'' \tag{8}$$

we can express equation (7) in matrix form:

$$G=\sum_k\sum_j m_{jk}c_{kj}=\operatorname{tr}(\mathbf{MC})=\operatorname{tr}(\mathbf{C}'')\,, \tag{9}$$

which states that the best fitting coordinates $\mathbf{Y}''$ are those for which the trace of the correlation matrix is a maximum.

The double sum in equation (7) is a linear combination of the elements of **M** with constant coefficients. The coefficients can be calculated by considering each atom just twice: once to calculate the centroids and again to calculate the nine terms $\sum_i x_{ji}y_{ki}$. In order to maximize G one may change **M** iteratively by applying the best rotation about each Cartesian axis in turn. This means that after s iterations have been performed, new matrices **M** and $\mathbf{C}''$ are obtained with:

$$\begin{aligned}\mathbf{M}^{(s+1)}&=\mathbf{R}\mathbf{M}^{(s)}\\ \mathbf{C}''^{(s+1)}&=\mathbf{R}\mathbf{C}''^{(s)}\end{aligned} \tag{10}$$

where **R** is of the form

$$\begin{bmatrix}1 & 0 & 0\\ 0 & \cos\phi_s & \sin\phi_s\\ 0 & -\sin\phi_s & \cos\phi_s\end{bmatrix}$$

or a suitable permutation thereof. By imposing zero first derivative and negative second derivative of G with respect to ϕ_s it may be shown that

$$\phi_s=\tan^{-1}(\sigma/\gamma)$$

where

$$\begin{aligned}\sigma&=c_{rq}''^{(s)}-c_{qr}''^{(s)}\\ \gamma&=c_{qq}''^{(s)}+c_{rr}''^{(s)}\,,\end{aligned}$$

p,q,r being any cyclic permutation of 1, 2, 3. As a consequence one has

$$\begin{aligned}m_{pk}^{(s+1)}&=m_{pk}^{(s)}\\ m_{qk}^{(s+1)}&=(\gamma m_{qk}^{(s)}+\sigma m_{rk}^{(s)})/(\gamma^2+\sigma^2)^{1/2}\\ m_{rk}^{(s+1)}&=(-\sigma m_{qk}^{(s)}+\gamma m_{rk}^{(s)})/(\gamma^2+\sigma^2)^{1/2}\end{aligned}$$

for $k=1,2,3$ and similar equations for the components of $\mathbf{C}''$. The iteration described by these equations is carried out changing the index p each time until the absolute value of ϕ_s for each p has become less than a preset tolerance. The identity matrix is a suitable initial choice for **M**.

Notice that new coordinates $\mathbf{Y}'''$ need not be calculated if one is only interested in knowing the minimized sum of the squares of the differences. This is given by the sum of the first three terms in equation (6); the summation of x_{ji}^2 and of y_{ki}^2 can be done simultaneously with the summation of the coefficients $x_{ji}y_{ki}$.

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International Union of Crystallography

Deposition of Tables of Anisotropic Thermal Parameters

In its report to the IUCr Executive Committee and Tenth General Assembly of the Union which was held in Amsterdam, 7–15 August 1975, the Working Party on Information Services proposed that tables of anisotropic thermal parameters should, in general, be deposited together with structure factor tables.

With the agreement of the Executive Committee and the Chairman of the Commission on Journals, this proposal has now been implemented. All tables of anisotropic thermal parameters (except for very short tables) will be deposited, unless the Co-editor accepting the paper specifically requires that they be published. If a table gives both positional and thermal parameters both will be deposited but the positional parameters will also be published.

Two copies of the tables will be required. They should be in typescript, and not reduced photographically. They should be headed descriptively on the first page, with column headings recurring on each page, and pages should be numbered clearly to ensure the correct sequence. The optimum page size is up to 30 cm × 21 cm, whilst the limiting page size is 33 cm high × 24 cm wide. Each set of material to be deposited should be accompanied by the title, the authors' names and addresses and the abstract from the parent paper.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

The solid state. By H. M. ROSENBERG. Pp. 235. Oxford: Clarendon Press, 1975. Price £2.75 (paper).

In this paperback H. M. Rosenberg approaches the subject in a refreshingly practical and down-to-earth way. The student beginner is introduced to dislocations, vacancies, interstitials, *etc.* in some detail before learning about Bloch waves and electron band structure. The applied, almost do-it-yourself approach is maintained throughout the book, with emphasis on advanced experimental techniques, such as electron and field-ion microscopy, ESCA, metallography (to name just a few), and with little importance attached to abstract ideas. In those few cases where difficult concepts are treated, very illuminating figures (such as the one illustrating *Umklapp*) are provided.

Devices are treated in great detail. While most texts may at most treat the *p–n* junction and the transistor, in this volume a wide variety of devices, such as the bipolar transistor, FET's, LED's and many others are treated.

The treatment of electron band theory and phonons is short and may even be regarded as weak, however, this may be justified for an introductory book of this kind, as is the courageous omission of superconductivity. This attitude is reminiscent of that of Pauli at the ETH, who treated in his courses classical physics in great detail and thoroughness, at the expense of omitting quantum mechanics. His reasoning was, that if students are taught advanced subjects, necessarily in a superficial way (in an undergraduate course), they may end up feeling that they understand everything; while the judicious omission of some of the most exciting subjects leaves them in a state of curiosity when they graduate, a curiosity that may be preserved throughout their lives.

I feel that the exercise problems in the book are somewhat of a routine nature, and that a few more difficult and stimulating ones (perhaps requiring some further reading) for advanced students would be very desirable.

In addition to engineering students (and perhaps chemistry, biology, and even humanity students) I would strongly recommend the book as required reading for advanced graduate courses in the theory of solids. Many students graduate nowadays from such courses with some technical competence in the handling of Green functions, Feynman diagrams, and even renormalization groups, without the faintest understanding how a transistor works and what a dislocation is. A compulsory examination on the material of this book can add perspective and also some genuine understanding to students of this type.

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Introduzione alla fisica dei materiali. By G. CAGLIOTI. Pp. xvi + 381. Bologna: Zanichelli, 1974. Price 11.800 Lire.

Despite its title ('Introduction to the Physics of Engineering Materials' according to the English synopsis provided on p. XIII), this is a very fundamental book on the basic physical principles needed in the development of a scientifically sound interpretation of the properties of materials. Caglioti's concept is to develop a unified picture starting from quantum mechanics and arriving at macroscopic properties of materials. The first three chapters deal with atoms, molecules, and