Finally, to analyze rocking curves we want analytical expressions for the total derivatives  $dI_0/d\theta$  and  $dI_g/d\theta$ . Consider  $I_0 = |s_{11}|^2$ . Let a superscript asterisk denote the complex conjugate. Then if  $\mathbf{A} = (a_{kl})$ , we have

$$\frac{\mathrm{d}I_0}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}\theta} |s_{11}|^2 = 2 \operatorname{Re}\left(\frac{\mathrm{d}s_{11}}{\mathrm{d}\theta} s_{11}^*\right),$$

where

$$\frac{\mathrm{d}s_{11}}{\mathrm{d}\theta} = \sum_{k=1}^{2} \sum_{l=1}^{2} \frac{\partial s_{11}}{\partial a_{kl}} \frac{\mathrm{d}a_{kl}}{\mathrm{d}\theta} = \frac{\partial s_{11}}{\partial s} \frac{\mathrm{d}s}{\mathrm{d}\theta},$$

since  $s = a_{22}$  is the only element of A which depends on  $\theta$ . Since

$$\frac{\partial s_{11}}{\partial s} = 2\pi i t \exp(\pi i s t) \Psi_{22}^{11} \quad \text{and} \quad \frac{\mathrm{d}s}{\mathrm{d}\theta} = g \cos\theta,$$

we compute immediately

$$\frac{dI_0}{d\theta} = 2 \operatorname{Re} \left( \frac{\partial s_{11}}{\partial s} \frac{ds}{d\theta} s_{11}^* \right)$$
$$= \frac{-2\pi tg \cos \theta}{\xi_g^2 r^2} \left( \frac{s}{r} \right) \sin \left( \pi rt \right)$$
$$\times \left[ \cos \left( \pi rt \right) - \frac{\sin \left( \pi rt \right)}{\pi rt} \right].$$

By an exactly similar computation, we find

$$\frac{\mathrm{d}I_g}{\mathrm{d}\theta} = 2 \operatorname{Re}\left(\frac{\partial s_{21}}{\partial s} \frac{\mathrm{d}s}{\mathrm{d}\theta} s_{21}^*\right) = -\frac{\mathrm{d}I_0}{\mathrm{d}\theta}.$$

The correctness of these expressions may be easily

checked directly from (B3); it is much easier in this case to compute the total derivatives in this manner. When the dimension of the matrices exceeds two, however, it is in general impossible to perform the necessary analytical diagonalization of the structure matrix to obtain expressions for  $I(\theta)$ , so if the derivative is to be computed at all, it must ordinarily be approximated numerically by a difference quotient. In contrast to this, our method allows such derivatives to be calculated directly for matrices of any size.

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## The piezoelectric, elastic, photoelastic and Brillouin tensors for point groups with fivefold rotation

**axes.** By YI-JIAN JIANG, LI-JI LIAO and GANG CHEN, Department of Applied Physics, Beijing Polytechnic University, Beijing, 100022, People's Republic of China, and PENG-XIANG ZHANG, Institute of Physics, Academia Sinica, Beijing, 100080, People's Republic of China

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#### Abstract

### Introduction

The piezoelectric, elastic, photoelastic and Brillouin tensors for the point groups  $5(C_5)$ ,  $\overline{5}(S_{10})$ ,  $\overline{10}(C_{5h})$ ,  $\overline{10}m2(D_{5h})$ ,  $52(D_5)$ ,  $5m(C_{5\nu})$ ,  $52m(D_{5d})$ , 235(I) and  $(2/m)\overline{35}(I_h)$  have been calculated and are tabulated here. Although periodic crystals with pentagonal symmetry in two dimensions and icosahedral symmetry in three dimensions cannot exist, there are both theoretical (Levine & Steinhandt, 1984) and experimental (Shechtmen, Blech,

Table 1. The piezoelectric tensors for point groups with fivefold rotation axes



Table 2. The photoelastic and elastic tensors for point groups with fivefold rotation axes

				Photoelas	tic					Elastic	:	
C5 S10 C5h	$     \begin{array}{r}         P_{11} \\         P_{12} \\         P_{31} \\         \vdots \\         -P_{16}     \end{array} $	$P_{12} P_{11} P_{31} \cdots P_{16}$	$P_{13} P_{13} P_{33} P_{33}$	$ \begin{array}{c} \cdot \\ \cdot \\ P_{44} \\ -P_{45} \\ \cdot \\ \cdot$	P <sub>45</sub> P <sub>44</sub>	$P_{16} - P_{16} \\ . \\ . \\ . \\ \frac{1}{2}(P_{11} - P_{12})$	$C_{11} \\ C_{12} \\ C_{13}$	$C_{12} \\ C_{11} \\ C_{13}$	$C_{13} \\ C_{13} \\ C_{33}$		:	÷
D5 C5v D5d D5h	$P_{11} P_{12} P_{31} P_{31}$	$P_{12} P_{11} P_{31} P_{31}$	$P_{13} P_{13} P_{13} P_{33}$	P <sub>44</sub>		$\frac{1}{2}(P_{11} - P_{12})$				C44 : : (5)	C <sub>44</sub>	$\frac{1}{2}(C_{11}-C_{12})$
I I <sub>h</sub>	$P_{11} P_{12} P_{12} P_{12}$	$P_{12} P_{11} P_{12} \cdots$	$P_{12} P_{12} P_{11} P_{11} .$	$\frac{1}{2}(P_{11} - P_{12})$	$\frac{1}{2}(P_{11}-P_{12})$	$ \frac{1}{2}(P_{11} - P_{12}) $	$C_{11} \\ C_{12} \\ C_{12} \\ . \\ . \\ . \\ . \\ . \\ . \\ . \\ . \\ . \\ $	$C_{12} \\ C_{11} \\ C_{12} \\ \cdot \\ $	$C_{12} \\ C_{12} \\ C_{11} \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot$	$ \frac{1}{2}(C_{11} - C_{12}) \\ \vdots \\ \vdots \\ (2) $	$\frac{1}{2}(C_{11} - C_{12})$	$\frac{1}{2}(C_{11}-C_{12})$

Gratias & Cahn, 1984) reasons to believe that quasicrystals with such symmetries can and do exist. For studying the physical properties of quasicrystals which depend on their symmetries, it is necessary to calculate the property tensors for the quasicrystals' symmetry groups. The Raman and hyper-Raman tensors for groups with fivefold rotation axes have been given by Brandmüller & Claus (1988*a*, *b*), and the mathematical form of the electric susceptibility and piezoelectric tensors have also been discussed in their paper.

Here, with the employment of group theoretical methods, the piezoelectric, elastic and photoelastic tensors corresponding to the point groups  $5(C_5)$ ,  $\overline{5}(S_{10})$ ,  $\overline{10}(C_{5h})$ ,  $\overline{10}m_2(D_{5h})$ ,  $52(D_5)$ ,  $5m(C_{5v})$ ,  $52m(D_{5d})$ , 235(I) and  $(2/m)\overline{35}(I_h)$  are calculated. On the basis of these results, the Brillouin tensors with such symmetries are also derived.

#### Calculation and results

The number, n, of independent non-zero coefficients of piezoelectric, elastic and photoelastic tensors are determined for each point group with fivefold rotation axes using the well known formula

$$n = \frac{1}{N} \sum_{R} \chi(R) \chi_i(R), \qquad (1)$$

where N is the total number of group elements in the given point groups,  $\chi_i(R)$  is the character of the totally symmetric irreducible representation,  $\chi(R)$  is the character of the reducible representation for each tensor mentioned above.

Once the number of non-vanishing independent tensor components have been determined, the tensor components can be identified by the ordinary method (Nye, 1985). Here, the method of direct inspection (Nye, 1985) cannot be used. We have calculated the tensor components by solving the simultaneous equations which arise when imposing the condition that the tensors are invariant under the elements of the point groups. For the sake of brevity, we omit the somewhat lengthy calculations and simply present the results in Tables 1 and 2. Brandmüller & Claus (1988a, b) have calculated the irreducible tensor elements for all point groups including those with fivefold axes. With a little calculation we can see that our results coincide with theirs. From Table 2, one can see that there are only two independent elastic and photoelastic constants for icosahedral point groups, fewer than in any of the 32 crystallographic groups.

The Christoffel matrices of the point groups with fivefold axes can be calculated and the velocities of sound waves are obtained by solving the secular equations (Auld, 1973). Based upon these results, the Brillouin tensors for point groups with fivefold rotation axes can be derived following Cummius & Schoen (1972). The results are presented in Table 3.

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### Table 3. Brillouin tensors for point groups with fivefold rotation axes

 $C_5 \quad S_{10} \quad C_{5h}$ 1. x phonon q = (1, 0, 0) $\rho v^2 = C_{11}$  $\mathbf{u} = (1, 0, 0)$  (L)  $\varepsilon_0^2 P_{11} - \varepsilon_0^2 P_{16} \qquad .$  $-\varepsilon_0^2 P_{16} \quad \varepsilon_0^2 P_{12} \quad .$  $\varepsilon_e^2 P_{31}$ . .  $\rho v^2 = C_{66}$ u(0, 1, 0) (T<sub>1</sub>)  $\varepsilon_0^2 P_{16} \quad \varepsilon_0^2 P_{66}$  .  $\varepsilon_0^2 P_{66} - \varepsilon_0^2 P_{16}$ . .  $\rho v^2 = C_{44}$  $\mathbf{u} = (0, 0, 1) \quad (T_2)$  $| . . P_{44} |$  $\varepsilon_2 \varepsilon_e$  . .  $P_{45}$ P<sub>44</sub> P<sub>45</sub> 2. y phonon q = (0, 1, 0) $\rho v^2 = C_{11}$  $\mathbf{u} = (0, 1, 0)$  (*L*)  $\varepsilon_0^2 P_{12} \quad \varepsilon_0^2 P_{16} \qquad .$  $\varepsilon_0^2 P_{16} \quad \varepsilon_0^2 P_{11} \quad .$  $\cdot \cdot \cdot \varepsilon_e^2 P_{31}$  $\rho v^2 = C_{44}$  $\mathbf{u} = (0, 0, 1) \quad (T_1)$ . . -P<sub>45</sub>  $\varepsilon_0 \varepsilon_e \begin{vmatrix} \cdot & \cdot & P_{44} \\ -P_{45} & P_{44} & \cdot \end{vmatrix}$  $\rho v^2 = C_{66}$  $\mathbf{u} = (1, 0, 0) \quad (T_2)$  $P_{16} P_{66}$ .  $\varepsilon_0^2 | P_{66} - P_{16}$  . 3. z phonon q = (0, 0, 1) $\rho v^2 = C_{33}$  $\mathbf{u} = (0, 0, 1)$  (L)  $|\varepsilon_0^2 P_{13}$  . .  $. \varepsilon_0^2 P_{13}$  .  $\varepsilon_e^2 P_{33}$ | . .  $\rho v^2 = C_{44}$  $\mathbf{u} = (1, 0, 0) \quad (T_1)$ | . . P<sub>44</sub>  $\varepsilon_0 \varepsilon_e$  . .  $P_{45}$  $P_{44} P_{45}$  .  $\rho v^2 = C_{44}$  $\mathbf{u} = (0, 1, 0) \quad (T_2)$ . . – P<sub>45</sub>  $\varepsilon_0 \varepsilon_e$  . .  $P_{44}$ -P45 P44

D5 C5v D5d D5h 1. x phonon q = (1, 0, 0) $\rho v^2 = C_{11}$  $\mathbf{u} = (1, 0, 0)$  (L)  $|\varepsilon_0^2 P_{11}$  .  $\varepsilon_0^2 P_{12}$  .  $\varepsilon_e^2 P_{31}$ . .  $\rho v^2 = C_{66}$  $\mathbf{u} = (0, 1, 0) \quad (T_1)$  $| . \epsilon_0^2 P_{66} .|$  $\varepsilon_0^2 P_{66}$  . . .  $\rho v^2 = C_{44}$  $\mathbf{u} = (0, 0, 1) \quad (T_2)$ . . P<sub>44</sub>  $\varepsilon_0 \varepsilon_e$  . . . P44 . . 2. y phonon q = (0, 1, 0) $\rho v^2 = C_{11}$  $\mathbf{u} = (0, 1, 0)$  (L)  $|\varepsilon_0^2 P_{12}$  .  $\varepsilon_0^2 P_{11}$  .  $\varepsilon_e^2 P_{31}$ .  $\rho v^2 = C_{44}$  $\mathbf{u} = (0, 0, 1) \quad (T_1)$  $\varepsilon_0 \varepsilon_e$  . .  $P_{44}$ . P<sub>44</sub>  $\rho v^2 = C_{66}$  $\mathbf{u} = (1, 0, 0) \quad (T_2)$ . P<sub>66</sub>  $\varepsilon_0^2 | P_{66}$  . 3. z phonon q = (0, 0, 1) $\rho v^2 = C_{33}$  $\mathbf{u} = (0, 0, 1)$  (L)  $|\varepsilon_0^2 P_{13}$  . .  $. \varepsilon_0^2 P_{13}$  $\cdot \cdot \cdot \varepsilon_e^2 P_{33}$  $\rho v^2 = C_{44}$  $\mathbf{u} = (1, 0, 0) \quad (T_1)$ . . P<sub>44</sub>  $\varepsilon_0 \varepsilon_e$  . . P44 .  $\rho v^2 = C_{44}$  $\mathbf{u} = (0, 1, 0) \quad (T_2)$  $\varepsilon_0 \varepsilon_e$  . .  $P_{44}$ P<sub>44</sub>

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Table 3 (cont.)

$C_{5}  S_{10}  C_{5h}$ 4. $x \pm y$ phonon $\mathbf{q} = (1, \pm 1, 0)/\sqrt{2}$ $\rho v^{2} = (C_{11} - C_{12})/2$ $\mathbf{u} = (1, \pm 1, 0)/\sqrt{2}$ (L) $\left  \frac{1}{2} \varepsilon_{0}^{2} (P_{11} + P_{12} \pm 2P_{16}) + \varepsilon_{0}^{2} P_{66} + \varepsilon_{0}^{2} P_{6} + \varepsilon_{0}^{2} P_{6$	$\begin{array}{c} \cdot \\ \cdot \\ 2\varepsilon_e^2 P_{31} \end{array}$	$D_{5}  C_{5v}  D_{5d}  D_{5h}$ 4. $x \pm y$ phonon $\mathbf{q} = (1, \pm 1, 0)/\sqrt{2}$ $\rho v^{2} = (C_{11} - C_{12})/2$ $\mathbf{u} = (1, \pm 1, 0)/\sqrt{2}$ (L) $\left  \frac{1}{2} \varepsilon_{0}^{2} (P_{11} + P_{12}) \pm \varepsilon_{0}^{2} P_{66} + \varepsilon_{0}^{2} P_{6} +$	P <sub>31</sub>
$\rho v^{2} = C_{11}$ $\mathbf{u} = (1, \mp 1, 0) / \sqrt{2}  (T_{1})$ $\varepsilon_{0}^{2} \begin{vmatrix} P_{66} & -P_{16} & \cdot \\ -P_{16} & -P_{66} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$		$\rho v^{2} = C_{11}$ $\mathbf{u} = (1, \mp 1, 0) / \sqrt{2}  (T_{1})$ $\epsilon_{0}^{2} \begin{vmatrix} P_{66} & \cdot & \cdot \\ \cdot & -P_{66} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$	
$\rho v^{2} = C_{44}$ $\mathbf{u} = (0, 0, 1)  (T_{2})$ $\frac{\varepsilon_{e} \varepsilon_{0}}{\sqrt{2}} \begin{vmatrix} \cdot & \cdot & \mp P_{45} + P_{44} \\ \cdot & \cdot & \pm P_{44} + P_{45} \\ \mp P_{45} + P_{44} & \pm P_{44} + P_{45} \\ \cdot & \cdot & \cdot \end{vmatrix}$		$\rho v^{2} = C_{44}$ $\mathbf{u} = (0, 0, 1)  (T_{2})$ $\frac{\varepsilon_{e} \varepsilon_{0}}{\sqrt{2}} \begin{vmatrix} \cdot & \cdot & P_{44} \\ \cdot & \cdot & \pm P_{44} \\ P_{44} & \pm P_{44} & \cdot \end{vmatrix}$	
5. $x \pm z$ phonon $\mathbf{q} = (1, 0, \pm 1)/\sqrt{2}$ $\rho v^2 = (C_{44} + C_{66})/2$ $\mathbf{u} = (0, 1, 0)  (T)$ $\begin{vmatrix} \varepsilon_0^2 P_{16} & \varepsilon_0^2 P_{66} & \mp \varepsilon_0 \varepsilon_e P_{45} \\ \varepsilon_0^2 P_{66} & -\varepsilon_0^2 P_{16} & \pm \varepsilon_0 \varepsilon_e P_{44} \\ \mp \varepsilon_o \varepsilon_0 P_{45} & \pm \varepsilon_e \varepsilon_0 P_{44} & . \end{vmatrix}$	:	5. $x \pm z$ phonon $\mathbf{q} = (1, 0, \pm 1)/\sqrt{2}$ $\rho v^2 = (C_{44} + C_{66})/2$ $\mathbf{u} = (0, 1, 0)  (T)$ $\begin{vmatrix} \cdot & \varepsilon_0 P_{66} & \cdot \\ \varepsilon_0^2 P_{66} & \cdot & \pm \varepsilon_0 \varepsilon_e P_{44} \\ \cdot & \pm \varepsilon_0 \varepsilon_e P_{44} & \cdot \end{vmatrix}$	
6. $y \pm z$ phonon $\mathbf{q} = (0, 1, \pm 1)/\sqrt{2}$ $\rho v^2 = (C_{44} + C_{66})/2$ $\mathbf{u} = (1, 0, 0)  (T)$ $\begin{vmatrix} \varepsilon_0^2 P_{16} & \varepsilon_0^2 P_{66} & \pm \varepsilon_0 \varepsilon_e P_{44} \\ \varepsilon_0^2 P_{66} & -\varepsilon_0^2 P_{16} & \pm \varepsilon_0 \varepsilon_e P_{45} \\ \pm \varepsilon_0 \varepsilon_e P_{44} & \pm \varepsilon_0 \varepsilon_e P_{45} & . \end{vmatrix}$		5. $y \pm z$ phonon $\mathbf{q} = (0, 1, \pm 1)/\sqrt{2}$ $\rho v^2 = (C_{44} + C_{66})/2$ $\mathbf{u} = (1, 0, 0)  (T)$ $\begin{vmatrix} & \varepsilon_0^2 P_{66} & \pm \varepsilon_0 \varepsilon_e P_{44} \\ & \varepsilon_0^2 P_{66} & \cdot & \cdot \\ & \pm \varepsilon_0 \varepsilon_e P_{44} & \cdot & \cdot \end{vmatrix}$	
$\rho v^{2} = C_{11}$ $\mathbf{u} = (1, 0, 0)  (L)$ $\varepsilon_{0}^{2} \begin{vmatrix} P_{11} & \cdots \\ P_{12} & \cdots \\ \vdots & P_{12} \\ \vdots & \vdots & P_{12} \end{vmatrix}$	1. x phonon $\mathbf{q} = (1, 0, 0)$ $\rho v^2 = (C_{11} - C_{12})/2$ $\mathbf{u} = (0, 1, 0)  (T_1)$ $\varepsilon_0^2 \begin{vmatrix} \cdot & P_{66} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$	$\rho v^{2} = (C_{11} - C_{12})$ $\mathbf{u} = (0, 0, 1)  (T_{2})$ $\varepsilon_{0}^{2} \begin{vmatrix} \cdot & \cdot & P_{66} \\ \cdot & \cdot & P_{66} \\ \cdot & \cdot & \cdot \\ P_{66} & \cdot & \cdot \end{vmatrix}$	)
$\rho v^{2} = C_{11}$ $\mathbf{u} = (1, 1, 0)/\sqrt{2}  (L)$ $\frac{\varepsilon_{0}^{2}}{2} \begin{vmatrix} P_{11} + P_{12} & 2P_{66} & \cdot \\ 2P_{66} & P_{11} + P_{12} & \cdot \\ \cdot & \cdot & 2P_{12} \end{vmatrix}$	xy phonon $\mathbf{q} = (1, 1, 0)/\sqrt{2}$ $\rho v^2 = (C_{11} - C_{12})/2$ $\mathbf{u} = (1, -1, 0)/\sqrt{2}$ (T <sub>1</sub> ) $\varepsilon_0^2 \begin{vmatrix} P_{66} & \cdot & \cdot \\ \cdot & -P_{66} & \cdot \\ \cdot & \cdot & \cdot \end{vmatrix}$	$\rho v^{2} = (C_{11} - C_{12})$ $\mathbf{u} = (0, 0, 1)  (T_{2})$ $\frac{\varepsilon_{0}^{2}}{\sqrt{2}} \begin{vmatrix} \cdot & \cdot & P_{1} \\ \cdot & \cdot & P_{2} \\ \cdot & \cdot & P_{2} \\ P_{66} & P_{66} \end{vmatrix}$	/2 ) 66
$\rho v^{2} = C_{11}$ $\mathbf{u} = (1, 1, 1)/\sqrt{3}  (L)$ $\frac{\varepsilon_{0}^{2}}{\sqrt{3}} \begin{vmatrix} P_{11} + 2P_{12} & 2P_{66} & 2P_{66} \\ 2P_{66} & P_{11} + 2P_{12} & 2P_{66} \\ 2P_{66} & 2P_{66} & P_{11} + 2P_{12} \end{vmatrix}$	3. xyz phonon $\mathbf{q} = (1, 1, 1)/3$ $\rho v^2 = (C_{11} - C_{12})/2$ $\mathbf{u} = (-1, 1, 0)/\sqrt{2}$ (T <sub>1</sub> ) $\frac{\varepsilon_0^2}{\sqrt{6}} \begin{vmatrix} -2P_{66} & & -P_{66} \\ & -2P_{66} & P_{66} \\ -P_{66} & P_{66} & \cdot \end{vmatrix}$	$\rho v^{2} = (C_{11} - C_{12})$ $\mathbf{u} = (1, 1, -2)/\sqrt{6}$ $\frac{\varepsilon_{0}^{2}}{3\sqrt{2}} \begin{vmatrix} 2P_{66} & 2P_{66} \\ 2P_{66} & 2P_{66} \\ -P_{66} & -P_{6} \end{vmatrix}$	$\frac{1}{2}$ (T <sub>2</sub> ) (T <sub>2</sub> ) (T)) (T)) (T)) (T)) (T)) (T)) (T)) (T

### Discussion

The significance of the results in Table 2 goes beyond the mere purpose of providing the elastic and photoelastic tensors for the given groups. From Table 2, any polar time-reversal invariant tensor of rank 4, such as the second electro-optic or electrostriction tensor can be easily obtained by considering its intrinsic symmetry.

We expect the Raman and Brillouin scattering technique to be useful in the study of quasicrystals. But, so far as we know, there is no experimental work involving Raman and Brillouin scattering by quasicrystals (Brandmüller, 1989, private communication).

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## Notes and News

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## The Dorothy Hodgkin Prize of the British Crystallographic Association

In celebration of Professor Dorothy Hodgkin's 80th birthday, the British Crystallographic Association (BCA) is pleased to announce the creation of the Dorothy Hodgkin Prize, in recognition of her great contribution to crystallography and to science in general.

Nominations for this prize are welcomed from any part of the crystallographic community and the award will be made at the time of the BCA Spring Meeting. Periodically the award will recognize specifically the achievements of young crystallographers. The BCA is counting on the generosity of Dorothy's many friends and colleagues to make the prize financially worthwhile as well as prestigious. All donors will be named within the prize scroll and it is hoped that you will wish to be associated with this splendid and permanent tribute to Dorothy's scientific achievements. In order that the first award may be closely associated with Dorothy's 80th birthday, we wish to make the first presentation of the prize at the Sheffield Meeting of the BCA in March 1991. It is expected that Dorothy herself will be there to present the award at this time.

Please forward your contributions as early as possible to the Treasurer, Dr Ian Langford, Department of Physics, The University, Birmingham B15 2TT, England. (Cheques payable to 'The Dorothy Hodgkin Prize/BCA'.) Further details concerning the nominations for the award will appear in subsequent BCA Newsletters this year, or can be obtained from the BCA Secretary, Dr Judith Howard.