

Maxwell–Garnett Estimates of the Effective Properties of a General Class of Discrete Random Composites

BY AKHLESH LAKHTAKIA

*Department of Engineering Science and Mechanics, The Pennsylvania State University,
University Park, PA 16802-1401, USA*

AND WERNER S. WEIGLHOFFER

Department of Mathematics, University of Glasgow, University Gardens, Glasgow G12 8QW, Scotland

(Received 20 March 1992; accepted 8 October 1992)

Abstract

The long-wavelength scattering formalism for an electrically small bianisotropic sphere embedded in a gyroelectromagnetic uniaxial medium is used to obtain the Maxwell–Garnett estimates of the effective properties of a general class of discrete random composites. This work is of relevance to the effective electromagnetic properties of crystals with defects and impurities and also to anisotropic composites.

1. Introduction

Microbubbles, dislocations and chemical impurities are commonly found in natural crystals (García-Ruiz, Lakhtakia & Messier, 1992). These and other defects distort lattices, thereby creating additional electronic energy levels in localized regions (Bube, 1974) as well as residual stress concentrations (Chopra, 1969), which lead to premature performance degradation (Pan, Furman, Dayton & Cross, 1986). These defects are also found in synthetic crystals (Moriya, 1991). Avoiding the formation of defects in artificial crystals is, therefore, a cherished goal of many. Neither are such structural inhomogeneities confined solely to crystalline matter, being found also in pigments, colloids and other amorphous materials of industrial importance (*e.g.* Hall, Benoit, Bordeleau & Rowland, 1988; Chernyi & Sharkov, 1991).

However, having structural inhomogeneities is very desirable in some instances. Thus, the presence of precipitates may be expected to improve the mechanical properties of polycrystalline matter (Tu & Rosenberg, 1982). Extenders are routinely used to space rutile particles in paints (Braun, 1988), while composite electroceramics are especially tailored for hydrophone and ultrasonic applications (Ting, 1986).

Since crystal defects are blessings as well as curses, but generally unavoidable except possibly with great expense, there is great interest in the properties of anisotropic matter impregnated with inhomogeneities (*e.g.* Ward, 1988), the defects being spread only lightly. Such matter can be regarded as a two-phase (or even multiphase) com-

posite, with the defects being thought of as the inclusions in a host medium. Apart from some rather simple mixing rules (Newnham, 1986), there is very little applied analysis available on the effective properties of inhomogeneous crystals. In particular, polycrystalline media are commonly assumed to be macroscopically isotropic (*e.g.* Kröner & Koch, 1976; Bussemer, Hehl, Kassam & Kaganov, 1991) for computational tractability; that tractability has to be a major issue in the field of composite materials becomes clear from even a casual reading of Milton (1990).

In a recent paper (Lakhtakia & Weiglhofer, 1992), a formalism was developed for the scattering of electromagnetic waves by an electrically small bianisotropic sphere embedded in a gyroelectromagnetically uniaxial medium. Bianisotropic materials are the most general spatially local non-diffusive Lorentz-covariant linear electromagnetic substances (Post, 1962; Kong, 1972). Gyroelectromagnetically uniaxial materials also embrace a wide variety of crystalline media. The availability of the long-wavelength scattering analysis provides an opportunity to obtain the Maxwell–Garnett estimates of a very general class of discrete random composites. Using these estimates, one may examine the effective electromagnetic behaviour of crystals containing a random sprinkling of electrically small defects, with possible applications at frequencies in the infrared and the subinfrared ranges. One may also study (artificial) tailored materials in which the point-polarizable inhomogeneities have been deliberately introduced.

2. Scattering by a single sphere

We begin by recapitulating the time-harmonic electromagnetic response of a single bianisotropic sphere embedded in a gyroelectromagnetic host medium. The host medium is characterized by the constitutive relations

$$\mathbf{D} = \bar{\epsilon} \cdot \mathbf{E}, \quad \mathbf{B} = \bar{\mathbf{m}} \cdot \mathbf{H}, \quad (1)$$

where the permittivity dyadic $\bar{\epsilon}$ and the permeability

dyadic \bar{m} are specified by (Weiglhofer, 1990)

$$\bar{e} = \varepsilon_1 \bar{I} + (\varepsilon - \varepsilon_1)cc, \quad \bar{m} = \mu_1 \bar{I} + (\mu - \mu_1)cc. \quad (2)$$

\bar{I} is the identity dyadic and c is a unit vector representing the crystallographic axis (Fedorov, 1975; Chen, 1983). A word about notation: dyadic notation is used throughout the paper; vectors appear in bold face, dyadics are bold and carry an overbar.

Materials exhibiting both electrical anisotropy and magnetic anisotropy include liquid crystals, some nematic liquid crystals having the same principal axes for their permittivity and permeability dyadics (Boulanger & Hayes, 1990). Artificial materials characterized by (2) may also be made possible, recent progress in this direction being in the fabrication of a form-birefringent polarization splitter with a fibre-based composite medium (Shiraishi, Sato & Kawakami, 1991). Another possibility of realizing (2) may be through interleaving magnetically uniaxial layers with electrically uniaxial layers (Reese & Lakhtakia, 1991). Investigations of wave propagation in these materials indicate their considerable engineering potential (Lakhtakia, Varadan & Varadan, 1991*a, b*). Finally, by setting $\mu_1 = \mu$, we can obtain results for uniaxial dielectric hosts; $\varepsilon_1 = \varepsilon$ corresponds to uniaxial magnetic materials; while the isotropic case can be recovered by setting $\varepsilon_1 = \varepsilon$ and $\mu_1 = \mu$.

The sphere of radius a is to be made of the bianisotropic material characterized by the Tellegen equations (Kong, 1972):

$$\mathbf{D} = \bar{e}_i \cdot \mathbf{E} + \bar{a}_i \cdot \mathbf{H}, \quad \mathbf{B} = \bar{m}_i \cdot \mathbf{H} + b_i \cdot \mathbf{E}. \quad (3)$$

Many important materials, including crystals, ferrites, magnetoelectrics, natural optically active materials and magnetoplasmas, are described by specialized versions of (3) (Lakhtakia, 1990).

Since the Green's dyadics for the medium of (2) are known (Weiglhofer, 1990), the boundary-value problem for the embedded sphere can be set up in an integral-equation formalism (Lakhtakia & Weiglhofer, 1992). If the sphere is electrically small with respect to the principal wavelengths in both materials, it can be replaced by an electric dipole moment \mathbf{p} and a magnetic dipole moment \mathbf{m} ; thus,

$$\begin{aligned} \mathbf{p} &= (4\pi a^3/3)(\bar{A}_{ee} \cdot \mathbf{E}_{inc} + \bar{A}_{em} \cdot \mathbf{H}_{inc}), \\ \mathbf{m} &= (4\pi a^3/3)(\bar{A}_{me} \cdot \mathbf{E}_{inc} + \bar{A}_{mm} \cdot \mathbf{H}_{inc}), \end{aligned} \quad (4)$$

where \mathbf{E}_{inc} and \mathbf{H}_{inc} are the values of the actual electric and magnetic fields incident on the electrically small sphere evaluated at the geometric centre of the sphere, while (Lakhtakia & Weiglhofer, 1992)

$$\begin{aligned} \bar{A}_{ee} &= \bar{a}_i \cdot \bar{D}_m^{-1} \cdot \bar{W}_{em}^{-1} \\ &\quad - (\bar{e}_i - \bar{e}) \cdot \bar{D}_e^{-1} \cdot \bar{W}_{me}^{-1} \cdot \bar{W}_{mm} \cdot \bar{W}_{em}^{-1}, \\ \bar{A}_{em} &= (\bar{e}_i - \bar{e}) \cdot \bar{D}_e^{-1} \cdot \bar{W}_{me}^{-1} \\ &\quad - \bar{a}_i \cdot \bar{D}_m^{-1} \cdot \bar{W}_{em}^{-1} \cdot \bar{W}_{ee} \cdot \bar{W}_{me}^{-1}, \end{aligned}$$

$$\begin{aligned} \bar{A}_{me} &= (\bar{m}_i - \bar{m}) \cdot \bar{D}_m^{-1} \cdot \bar{W}_{em}^{-1} \\ &\quad - \bar{b}_i \cdot \bar{D}_e^{-1} \cdot \bar{W}_{me}^{-1} \cdot \bar{W}_{mm} \cdot \bar{W}_{em}^{-1}, \\ \bar{A}_{mm} &= \bar{b}_i \cdot \bar{D}_e^{-1} \cdot \bar{W}_{me}^{-1} \\ &\quad - (\bar{m}_i - \bar{m}) \cdot \bar{D}_m^{-1} \cdot \bar{W}_{em}^{-1} \cdot \bar{W}_{ee} \cdot \bar{W}_{me}^{-1}, \\ \bar{D}_e &= \bar{I} - \bar{b}_i^{-1} \cdot (2\bar{m} + \bar{m}_i) \cdot \bar{a}_i^{-1} \cdot (2\bar{e} + \bar{e}_i), \\ \bar{D}_m &= \bar{I} - \bar{a}_i^{-1} \cdot (2\bar{e} + \bar{e}_i) \cdot \bar{b}_i^{-1} \cdot (2\bar{m} + \bar{m}_i), \\ \bar{W}_{ee} &= (2\bar{I} + \bar{e}^{-1} \cdot \bar{e}_i)/3, \quad \bar{W}_{em} = \bar{e}^{-1} \cdot \bar{a}_i/3, \\ \bar{W}_{me} &= \bar{m}^{-1} \cdot \bar{b}_i/3, \\ \bar{W}_{mm} &= (2\bar{I} + \bar{m}^{-1} \cdot \bar{m}_i)/3, \end{aligned} \quad (5)$$

a superscript $^{-1}$ indicating the inverse dyadic. We note here that, in view of (4), the quantities $4\pi a^3 \bar{A}_{ee}/3$ etc. may be interpreted as the polarizability dyadics of an electrically small bianisotropic sphere embedded in a gyroelectromagnetic ambient medium.

3. The Maxwell-Garnett model

The developments contained in the previous section may now be utilized to obtain the Maxwell-Garnett estimates of the effective medium. Consider therefore a discrete random medium in which identical bianisotropic spheres are randomly dispersed in a host gyroelectromagnetic uniaxial medium, there being N such inclusion spheres per unit volume. It is assumed that the long-wavelength approximation holds and that the spheres are also identically oriented. In order to obtain the effective properties of this composite, it will be viewed as being effectively homogeneous, with its constitutive equations given as

$$\mathbf{D} = \bar{e}_{eff} \cdot \mathbf{E} + \bar{a}_{eff} \cdot \mathbf{H}, \quad \mathbf{B} = \bar{m}_{eff} \cdot \mathbf{H} + \bar{b}_{eff} \cdot \mathbf{E}. \quad (6)$$

Each inclusion sphere is acted upon by all other inclusions, thereby giving rise to the concept of the local fields, \mathbf{E}_L and \mathbf{H}_L . With this in mind, (4) leads to the relations (Lakhtakia, 1990)

$$\begin{aligned} \mathbf{p} &= (4\pi a^3/3)(\bar{A}_{ee} \cdot \mathbf{E}_L + \bar{A}_{em} \cdot \mathbf{H}_L), \\ \mathbf{m} &= (4\pi a^3/3)(\bar{A}_{me} \cdot \mathbf{E}_L + \bar{A}_{mm} \cdot \mathbf{H}_L). \end{aligned} \quad (7)$$

On a macroscopic basis, these dipole moments are responsible for the polarization field \mathbf{P} and the magnetization field \mathbf{M} . As \mathbf{P} and \mathbf{M} are nothing but the electric and magnetic dipole moments per unit volume, we simply get

$$\begin{aligned} \mathbf{P} &= N\mathbf{p} = c(\bar{A}_{ee} \cdot \mathbf{E}_L + \bar{A}_{em} \cdot \mathbf{H}_L), \\ \mathbf{M} &= N\mathbf{m} = c(\bar{A}_{me} \cdot \mathbf{E}_L + \bar{A}_{mm} \cdot \mathbf{H}_L), \end{aligned} \quad (8)$$

with $c = N(4\pi a^3/3)$ being the volumetric proportion of the inclusion phase ($0 \leq c \leq 1$). Since \mathbf{P} and \mathbf{M} are due to the presence of the inclusions in the host medium, we

may write for the composite

$$\begin{aligned} \mathbf{D} &= \bar{\mathbf{e}} \cdot \mathbf{E} + \mathbf{P} = \bar{\mathbf{e}}_{\text{eff}} \cdot \mathbf{E} + \bar{\mathbf{a}}_{\text{eff}} \cdot \mathbf{H}, \\ \mathbf{B} &= \bar{\mathbf{m}} \cdot \mathbf{H} + \mathbf{M} = \bar{\mathbf{m}}_{\text{eff}} \cdot \mathbf{H} + \bar{\mathbf{b}}_{\text{eff}} \cdot \mathbf{E}. \end{aligned} \quad (9)$$

To find the local fields, the interaction among the inclusion spheres is assumed to be Lorentzian; therefore (Lakhtakia, 1992),

$$\mathbf{E} = \mathbf{E}_L - (1/3)\bar{\mathbf{e}}^{-1} \cdot \mathbf{P}, \quad \mathbf{H} = \mathbf{H}_L - (1/3)\bar{\mathbf{m}}^{-1} \cdot \mathbf{M}. \quad (10)$$

Now, from (8) and (10), we obtain

$$\begin{aligned} \mathbf{E}_L &= \bar{\mathbf{N}}_{ee}^{-1} \cdot (-\bar{\mathbf{B}}_{em}^{-1} \cdot \mathbf{E} + \bar{\mathbf{B}}_{mm}^{-1} \cdot \mathbf{H}), \\ \mathbf{H}_L &= \bar{\mathbf{N}}_{mm}^{-1} \cdot (\bar{\mathbf{B}}_{ee}^{-1} \cdot \mathbf{E} - \bar{\mathbf{B}}_{me}^{-1} \cdot \mathbf{H}), \end{aligned} \quad (11)$$

where

$$\begin{aligned} \bar{\mathbf{B}}_{ee} &= \bar{\mathbf{I}} - (c/3)\bar{\mathbf{e}}^{-1} \cdot \bar{\mathbf{A}}_{ee}, \\ \bar{\mathbf{B}}_{em} &= -(c/3)\bar{\mathbf{e}}^{-1} \cdot \bar{\mathbf{A}}_{em}, \\ \bar{\mathbf{B}}_{me} &= -(c/3)\bar{\mathbf{m}}^{-1} \cdot \bar{\mathbf{A}}_{me}, \\ \bar{\mathbf{B}}_{mm} &= \bar{\mathbf{I}} - (c/3)\bar{\mathbf{m}}^{-1} \cdot \bar{\mathbf{A}}_{mm}, \\ \bar{\mathbf{N}}_{ee} &= \bar{\mathbf{B}}_{mm}^{-1} \cdot \bar{\mathbf{B}}_{me} - \bar{\mathbf{B}}_{em}^{-1} \cdot \bar{\mathbf{B}}_{ee}, \\ \bar{\mathbf{N}}_{mm} &= \bar{\mathbf{B}}_{ee}^{-1} \cdot \bar{\mathbf{B}}_{em} - \bar{\mathbf{B}}_{me}^{-1} \cdot \bar{\mathbf{B}}_{mm}. \end{aligned} \quad (12)$$

Finally, from (8), (9) and (11), the Maxwell-Garnett estimates of the effective properties of the composite medium are obtained as

$$\begin{aligned} \bar{\mathbf{e}}_{\text{eff}} &= \bar{\mathbf{e}} + c(\bar{\mathbf{A}}_{em} \cdot \bar{\mathbf{N}}_{mm}^{-1} \cdot \bar{\mathbf{B}}_{ee}^{-1} \\ &\quad - \bar{\mathbf{A}}_{ee} \cdot \bar{\mathbf{N}}_{ee}^{-1} \cdot \bar{\mathbf{B}}_{em}^{-1}), \\ \bar{\mathbf{a}}_{\text{eff}} &= c(\bar{\mathbf{A}}_{ee} \cdot \bar{\mathbf{N}}_{ee}^{-1} \cdot \bar{\mathbf{B}}_{mm}^{-1} \\ &\quad - \bar{\mathbf{A}}_{em} \cdot \bar{\mathbf{N}}_{mm}^{-1} \cdot \bar{\mathbf{B}}_{me}^{-1}), \\ \bar{\mathbf{b}}_{\text{eff}} &= c(\bar{\mathbf{A}}_{mm} \cdot \bar{\mathbf{N}}_{mm}^{-1} \cdot \bar{\mathbf{B}}_{ee}^{-1} \\ &\quad - \bar{\mathbf{A}}_{me} \cdot \bar{\mathbf{N}}_{ee}^{-1} \cdot \bar{\mathbf{B}}_{em}^{-1}), \\ \bar{\mathbf{m}}_{\text{eff}} &= \bar{\mathbf{m}} + c(\bar{\mathbf{A}}_{me} \cdot \bar{\mathbf{N}}_{ee}^{-1} \cdot \bar{\mathbf{B}}_{mm}^{-1} \\ &\quad - \bar{\mathbf{A}}_{mm} \cdot \bar{\mathbf{N}}_{mm}^{-1} \cdot \bar{\mathbf{B}}_{me}^{-1}). \end{aligned} \quad (13)$$

Expressions (13) constitute the chief result of this paper. The effect of varying the concentration c of the inclusions may be easily studied, as may also the effect of having different inclusion types. The formulation is straightforward to implement on a digital computer since dyadics, being second-rank Cartesian tensors, can be very easily interpreted as 3×3 matrices and are very convenient to handle (Chen, 1983). As the procedure given is so general, we have not felt it necessary to provide numerical results and are content to give the expressions for a few special cases in what follows.

4. Special applications

4.1. Isotropic dielectric spheres in vacuum

As a test case, let the host medium be free space, *i.e.* $\bar{\mathbf{e}} = \epsilon_0 \bar{\mathbf{I}}$, $\bar{\mathbf{m}} = \mu_0 \bar{\mathbf{I}}$, while the inclusions be made of an isotropic dielectric material, $\bar{\mathbf{e}}_i = \epsilon_r \epsilon_0 \bar{\mathbf{I}}$, $\bar{\mathbf{m}}_i = \mu_0 \bar{\mathbf{I}}$, $\bar{\mathbf{a}}_i = \bar{\mathbf{b}}_i = 0$; in this case, the only non-zero normalized polarizability is given by $\bar{\mathbf{A}}_{ee} = 3\epsilon_0[(\epsilon_r - 1)/(\epsilon_r + 2)]\bar{\mathbf{I}}$, so that

$$\begin{aligned} \bar{\mathbf{e}}_{\text{eff}} &= \epsilon_0 \frac{\epsilon_r + 2 + 2c(\epsilon_r - 1)}{\epsilon_r + 2 - c(\epsilon_r - 1)} \bar{\mathbf{I}}, \\ \bar{\mathbf{m}}_{\text{eff}} &= \mu_0 \bar{\mathbf{I}}, \quad \bar{\mathbf{a}}_{\text{eff}} = \bar{\mathbf{b}}_{\text{eff}} = 0, \end{aligned} \quad (14)$$

as expected (Ward, 1988).

4.2. Anisotropic inclusions

A case of wide applicability concerns anisotropic (as opposed to bianisotropic) spheres, where $\bar{\mathbf{a}}_i = \bar{\mathbf{b}}_i = 0$. Then,

$$\begin{aligned} \bar{\mathbf{e}}_{\text{eff}} &= \bar{\mathbf{e}} + 3c(\bar{\mathbf{e}}_i - \bar{\mathbf{e}}) \cdot (\bar{\mathbf{e}}_i + 2\bar{\mathbf{e}})^{-1} \cdot \bar{\mathbf{e}} \\ &\quad \cdot [\bar{\mathbf{I}} - c\bar{\mathbf{e}}^{-1} \cdot (\bar{\mathbf{e}}_i - \bar{\mathbf{e}}) \cdot (\bar{\mathbf{e}}_i + 2\bar{\mathbf{e}})^{-1} \cdot \bar{\mathbf{e}}]^{-1}, \\ \bar{\mathbf{m}}_{\text{eff}} &= \bar{\mathbf{m}} + 3c(\bar{\mathbf{m}}_i - \bar{\mathbf{m}}) \cdot (\bar{\mathbf{m}}_i + 2\bar{\mathbf{m}})^{-1} \cdot \bar{\mathbf{m}} \\ &\quad \cdot [\bar{\mathbf{I}} - c\bar{\mathbf{m}}^{-1} \cdot (\bar{\mathbf{m}}_i - \bar{\mathbf{m}}) \cdot (\bar{\mathbf{m}}_i + 2\bar{\mathbf{m}})^{-1} \cdot \bar{\mathbf{m}}]^{-1}, \end{aligned} \quad (15)$$

while $\bar{\mathbf{a}}_{\text{eff}} = \bar{\mathbf{b}}_{\text{eff}} = 0$.

4.3. Perfect conductors

For perfectly conducting inclusions we need to set $\bar{\mathbf{e}}_i = \bar{\mathbf{e}}\nu$, $\bar{\mathbf{m}}_i = \bar{\mathbf{m}}/\nu$, $\bar{\mathbf{a}}_i = \bar{\mathbf{b}}_i = 0$. If the inclusion spheres are perfect *electric* conductors (PEC), *i.e.* in the limit $\nu \rightarrow 0$, one obtains

$$\begin{aligned} \bar{\mathbf{e}}_{\text{eff}} &= (1 + 2c)/(1 - c)\bar{\mathbf{e}}, \\ \bar{\mathbf{m}}_{\text{eff}} &= 2(1 - c)/(2 + c)\bar{\mathbf{m}}, \\ \bar{\mathbf{a}}_{\text{eff}} &= \bar{\mathbf{b}}_{\text{eff}} = 0; \end{aligned} \quad (16)$$

whereas for perfect *magnetic* conductors (PMC), which correspond to $\nu \rightarrow \infty$,

$$\begin{aligned} \bar{\mathbf{e}}_{\text{eff}} &= 2(1 - c)/(2 + c)\bar{\mathbf{e}}, \\ \bar{\mathbf{m}}_{\text{eff}} &= (1 + 2c)/(1 - c)\bar{\mathbf{m}}, \\ \bar{\mathbf{a}}_{\text{eff}} &= \bar{\mathbf{b}}_{\text{eff}} = 0. \end{aligned} \quad (17)$$

Many other cases of interest may be similarly worked out using the long-wavelength scattering formalism presented.

References

- BOULANGER, P. & HAYES, M. (1990). *Philos. Trans. R. Soc. London Ser. A*, **330**, 335–393.
BRAUN, J. H. (1988). *J. Coatings Technol.* **60**, 67–71.

- BUBE, R. H. (1974). *Electronic Properties of Crystalline Solids*. Orlando, Florida: Academic Press.
- BUSSEMER, P., HEHL, K., KASSAM, S. & KAGANOV, M. I. (1991). *Waves Random Media*, **2**, 113–131.
- CHEN, H. C. (1983). *Theory of Electromagnetic Waves*. New York: McGraw-Hill.
- CHERNYI, I. V. & SHARKOV, E. A. (1991). *Sov. Tech. Phys. Lett.* **17**, 107–108.
- CHOPRA, K. L. (1969). *Thin Film Phenomena*. New York: McGraw-Hill.
- FEDOROV, F. I. (1975). *Theory of Gyrotropy*. Minsk: Nauka i Tekhnika. (In Russian.)
- GARCÍA-RUIZ, J.-M., LAKHTAKIA, A. & MESSIER, R. (1992). *Speculat. Sci. Technol.* **15**, 60–71.
- HALL, J. E., BENOIT, R., BORDELEAU, R. & ROWLAND, R. (1988). *J. Coatings Technol.* **60**, 49–61.
- KONG, J. A. (1972). *Proc. IEEE*, **60**, 1036–1046.
- KRÖNER, E. & KOCH, H. (1976). *Solid Mech. Arch.* **1**, 183–238.
- LAKHTAKIA, A. (1990). *J. Phys. (Paris)*, **51**, 2235–2242.
- LAKHTAKIA, A. (1992). *Adv. Chem. Phys.* **83**. In the press.
- LAKHTAKIA, A., VARADAN, V. K. & VARADAN, V. V. (1991a). *J. Mod. Opt.* **38**, 649–657.
- LAKHTAKIA, A., VARADAN, V. K. & VARADAN, V. V. (1991b). *Int. J. Electron.* **71**, 853–861.
- LAKHTAKIA, A. & WEIGLHOFER, W. S. (1992). *Proc. IEE-H*, **139**, 217–220.
- MILTON, G. W. (1990). *Commun. Pure Appl. Math.* **43**, 63–125.
- MORIYA, K. (1991). *Philos. Mag.* **B64**, 425–445.
- NEWNHAM, R. E. (1986). *Annu. Rev. Mater. Sci.* **16**, 47–68.
- PAN, W., FURMAN, E., DAYTON, G. O. & CROSS, L. E. (1986). *J. Mater. Sci. Lett.* **5**, 647–649.
- POST, E. J. (1962). *Formal Structure of Electromagnetics*. Amsterdam: North-Holland.
- REESE, P. S. & LAKHTAKIA, A. (1991). *Z. Naturforsch. Teil A*, **43**, 384–388.
- SHIRAIISHI, K., SATO, T. & KAWAKAMI, S. (1991). *Appl. Phys. Lett.* **58**, 211–213.
- TING, R. Y. (1986). *Ferroelectrics*, **67**, 143–157.
- TU, K. N. & ROSENBERG, R. (1982). *Preparation and Properties of Thin Films*. New York: Academic Press.
- WARD, L. (1988). *The Optical Constants of Bulk Materials and Films*, ch 8. Bristol: Adam Hilger.
- WEIGLHOFER, W. S. (1990). *Proc. IEE-H*, **137**, 5–10.

Acta Cryst. (1993). **A49**, 269–280

Layer and Rod Classes of Reducible Space Groups. I. Z-Decomposable Cases

BY VOJTĚCH KOPSKÝ*

Department of Physics, University of the South Pacific, PO Box 1168 Suva, Fiji

(Received 1 June 1990; accepted 19 June 1992)

Abstract

Reducible plane groups are classified into pairs of frieze-group classes; reducible space groups are classified into pairs of layer and rod classes with respect to all possible Z decompositions. Firstly, all reductions of translation groups to the form of a direct sum (Z decomposition) or of a subdirect sum (Z reduction) of two G -invariant translation groups of lower dimensions are determined according to Bravais types. A practical way to determine layer and rod classes with the use of standard space-group diagrams is described and a geometric interpretation of symmorphic representatives of these classes is explained. Tables of the distribution of plane groups into pairs of frieze classes and of space groups into layer and rod classes with respect to possible Z decompositions are given. A notation for layer and rod groups compatible with Hermann–Mauguin symbols for space groups is used; compatibility is achieved on the basis of the factorization procedure.

* On leave of absence from Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, PO Box 24, 18040 Praha 8, Czechoslovakia.

1. Introduction

This is the first part of a two-paper series [paper II: Fuksa & Kopský (1993)] in which we apply the results of dimension-independent analysis of the factorization of reducible space groups by their partial translation subgroups (Kopský, 1989*a, b*) to plane groups and to space groups in three dimensions. We start with a brief review of the factorization procedure to make the reader familiar with symbols and terms used in the papers by Kopský (1989*a, b*), which will be referred to as papers *A* and *B*. According to the definition of a reducible space group, the plane groups of oblique and rectangular systems and all space groups, with the exception of cubic ones, are reducible. The translation subgroup T_G of a reducible space group \mathbb{G} contains ‘partial translation subgroups’ that are maximal in the sense that they are equivalent to intersections of T_G with the rational (or real) space they themselves generate and invariant under the point group G and hence normal in \mathbb{G} .

According to the ‘factorization theorem’ (paper *A*, theorem 2), the factor groups of reducible space groups over partial translation subgroups have the structure of subperiodic groups. The whole T_G is