11.4-05 ANHARMONIC CONTRIBUTION TO DEBYE-WALLER FACTORS OF SOME HCP METALS. By P.D. Pathak, Physics Department, University School of Sciences, Ahmedabad 380 009, India, and R.J. Desai, Nanavati Hospital, Ville Parle (West), Bombay 400 056, India.

Debye- Waller factors of zinc, cadmium and magnesium are determined from room temperature up to about their melting points by X-ray diffraction using a specially designed furnace. For all the three metals, the Debye-Waller factor B is found to rise rapidly at higher temperatures. It is assumed that the deviations ΔB from the extrapolated initial part of the curve is due to the contribution of higher order anharmonic terms in the potential energy function of the metals. It is shown for the first time that ΔB or B(anh) varies exponentially with 1/T. When reduced values of B are plotted against reduced temperature, the points corresponding to all the three metals fall approximately on the same curve. Thus, the metals obey a "law of corresponding states". A common relation, applicable to all the three metals, between the total anharmonic contribution to B and the melting temperature is established.

11.4-06 TEMPERATURE DEPENDENCE OF THERMAL MOTION IN CRYSTALLINE NAPHTHALENE AND ANTHRACENE. By C. P. Brock* and J. D. Dunitz, Lab. für Organische Chemie, ETH-Zentrum, 8092 Zürich, Switzerland.

Although Cruickshank's classic study (Acta Cryst., 9, 1005 (1956)) of the thermal motion in crystalline naphthalene and anthracene was based on what are by present standards poor experimental data, the conclusions are still widely quoted. In the present study we attempt to provide better results for comparison with theoretical calculations.

Single-crystal data for naphthalene have been measured at five temperatures between 90 and 240°K. Positional and thermal parameters for C and H atoms at each temperature were refined by conventional least-squares techniques. The effect of varying the weighting scheme was examined. Contributions of internal molecular modes to the motions of the C atoms turn out to be important. They were estimated at each temperature from a standard force field and subtracted from the experimental Uij values. The corrected Uij's were then analyzed to determine rigid-body translational and librational tensors for the naphthalene molecule. The absolute magnitudes and temperature dependence of these quantities have been compared with values calculated from atom-atom potentials and from spectroscopic data.

An analogous study of the thermal motion in anthracene between 90 and 300°K is in progress.

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11.5-01 ANALYSIS OF ERRORS IN QUANTITATIVE STUDIES OF DIFFUSE X-RAY SCATTERING. By T. B. Wu, E. Matsubara, and V. A. Kramb, Department of Material Science and Engineering, Technological Institute, Northwestern University, Evanston, IL 60201, USA.

Errors in separating the contributions of the diffuse x-ray scattering for binary solid solutions have been examined. The Georgopoulos-Cohen procedure was employed which divides the intensity due to displacements into several terms each involving a different atomic pair, as well as the short-range order intensity. A linear least-squares analysis was adopted to solve the intensity equations, from which an optimized solution and a standard deviation of each intensity component can be obtained. An error equation was derived and the standard deviations and the expected errors in the corresponding Fourier coefficients were evaluated. It was found that a large variation in the ratio of the scattering factors across the volume measured in reciprocal space improved the accuracy of the separation of the individual displacement intensity terms. For the case where one is concerned with the goodness of the separated displacement intensities, a shorter wavelength radiation, say molybdenum K_α radiation, is thus suggested. It was also found that weighting the intensity equation with respect to the counting error improved the separation. Although uncertian errors from Compton scattering and other sources still induce a significant error in the separated short-range order intensity, after Fourier inversion, error in the Warren SRO coefficients is quite low. Typical results will be shown. An attempt to extend this approach to ternary systems will be described.

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11.5-02 ELECTROSTATIC INTERACTIONS INVOLVING CHARGED DISLOCATIONS AND IMPURITY IONS IN IONIC CRYSTALS. By A. S. Pârasnis, Department of Physics, Indian Institute of Technology, Kanpur 208 016, India

We deal only with configurationally charged dislocations. Examples are: type A or C dislocation, b = (a/2)<1$\bar{1}$0>, lying along <11$\bar{2}$> in crystals of NaCl structure; type A or C dislocation, b = (a/2)<1$\bar{1}$0>, lying along <110> in crystals of CaF_2 structure. Due to the excess electric energy thus acquired normally they do not exist. Some sort of neutralizing factors are required. For NaCl structure Pârasnis *et al* (Phil. Mag. (1963) 8, 1053) proposed, and found evidence for, substitutional replacement of alternate cations along the core of type A dislocation by aliovalent impurity ions; for CaF_2 structure Evans and Pratt (Phil. Mag. (1969) 20, 1213) proposed removal of alternate cations at the core of type C or of a row of anions at the core of type A dislocation.

Dislocations thus neutralized are more or less immobilized due to pinning by impurity ions or because of the need for indigenous ions to move along the core during glide. They participate in ordinary deformation not at all or with difficulty. It is suggested that there is a way for type A (or C) dislocation in NaCl structure to neutralize but still be mobile to some extent if the aliovalent impurity ions form an interstitial atmosphere around the charged core rather than go into substitutional sites at it. Appropriately small ions, e.g. Au^{3+} in MgO, could move along with the dislocation more easily now, especially at high enough temper-