and satisfy m3m point symmetry, the superstructure was assumed to have the highest space group Fm3m for convenience of crystallographic calculations. The actual structure was examined as a superstructure having a face-centered cubic lattice with a lattice constant of $\underline{a}'=13\underline{a}=72.32Å$.

Through analysis of the partial Patterson function, the superstructure was found to be basically defined by clusters of Bi and of Cu. These two kinds of metal clusters occur alternately and are arranged in a face-centered cubic lattice mode. Such local clustering of the atoms is interpreted to be a combination of two different kinds of modulation factors: the periodic substitution between Bi and Cu and the periodic positional displacement of the atoms. Structure factor calculations, based on the clustering structure, gave substantial agreement with observed intensities.

The problems of the clustering structure can be attributed to the process of cooling from high temperature. This cubic phase and $Cu_3Bi_5S_9$, which also has a non-integral type superstructure(Ohmasa, Tomeoka & Sadanaga, 1979, AIP Conf. Proc., 53, 355), are stable only at temperature higher than 400°C and metastable at room temperature. In their stable high temperature phases, the crystals exist with random replacement between Bi and Cu and have structures approximating the substructures as defined in our studies (Ohmasa, 1973, Neues Jahrb. Miner. Monatsh., 227; Tomeoka, Ohmasa & Sadanaga, 1980, Mineralogical Journ., 10, 57.) During quenching, however, the metal atoms segregate into two kinds of clusters. The long-range repeat distances are directly influenced by these metal clusters and seem to be independent of the period of the subcell.

departure from stoichiometry. We also establish that at very low deviations from stoichiometry, dissociation of CS planes into anion vacancies may be possible due to the closeness in energy of the point defect mode of reduction with the extended defect mode. From our simulations we have thus been able to rationalise the apparently complex relationship between structure and composition in these nonstoichiometric oxides.

20.4-04   THE ENERGETICS OF FORMATION AND ORDERING OF CRYSTALLOGRAPHIC SHEAR PLANES IN ReO$_3$ STRUCTURED OXIDES. By A.N. Cormack, C.R.A. Catlow, University College London, and P.W. Tasker, AERE, Harwell.

We present the results of a detailed atomistic computer simulation study of extended defect formation in ReO_3 (DO$_9$) structured nonstoichiometric oxides. The phenomenon of crystallographic shear (CS) planes, as extended defects, in such compounds as WO_{3-x} and MoO_{3-x} has been extensively studied by both X-ray diffraction and high resolution electron microscopy. This combination of Reciprocal Space and Real Space crystallography has shed considerable light on the geometrical structure of these defects which may be considered as perturbations of a periodic, modulated structure (Proc. Int. Conf. on 'Modulated Structures', Hawaii 1979. American Institute of Physics conf. proc. No. 53, Plenum Press, New York.). At the same time, however, several fundamental problems have been raised concerning the preferred orientation for the formation of isolated CS planes, and their long range ordering into regular, or nearly regular, arrays at greater concentrations in the crystal. Our model correctly establishes that (102) CS planes are the most energetically favoured isolated CS planes in ReO$_3$ type structures and we also show that lattice relaxations play an essential part in stabilising this orientation over others such as (001) and (103). However, the energies of these defects are sufficiently close, so that the difference between them in the isolated case becomes outweighed by terms arising from their interaction at larger concentrations with increasing

20.4-05   IMPLICATIONS OF PSEUDO SYSTEMATIC ABSENCES IN APPARENT TETRAGONAL 4/MMM DIFFRACTION SYMMETRY. By A.D. Rae, School of Chemistry, University of New South Wales, Kensington, 2033, N.S.W. Australia.

The absences $F(hh\ell) = 0$, $h + \ell = 2n + 1$ and $F(hh\ell) = 0$, $h = 2n + 1$ do not correspond to symmetry elements of any primitive space group of 4/mmm Laue symmetry. When either systematic absence occurs in data of apparent 4/mmm diffraction symmetry, it may imply that the true crystal structure is not 4/mmm Laue symmetry but is of either mmm or 4/m Laue symmetry. Diffraction data with {hkℓ} strong only for h + k = 2n may be described as arising from a disordered structure in a subcell of axial lengths a/$\sqrt{2}$. a/$\sqrt{2}$, c which may indeed be of 4/mmm Laue symmetry. Systematic absences of $F(0k'\ell') = 0$ for k' + ℓ' = 2n + 1 or $F(0k'\ell')$ for k' = 2n + 1 correspond to an allowed symmetry element for this disordered subcell structure. Twinning must be a condition for {hkℓ} data with h + k = 2n + 1 to also have 4/mmm diffraction symmetry, should a satisfactory disordered structure consistent with the systematic absences of the subcell be obtained. Two structures based upon spacegroup $P4_2/mmm$ have been refined, one of true spacegroup $P4_2/n$, the other of true spacegroup Pbam. Both showed $|F(hk\ell)| = |F(kh\ell)|$ for all data. Constrained refinement is essential when twinning occurs. Fourier analysis methods identify which combinations of parameters are poorly defined.