and satisfy ahmm point symmetry, the superstructure was assumed to have the highest degree of freedom for convenience of crystallographic calculations. The actual structure was examined as a superstructure having a face-centered cubic lattice with a lattice constant of a = \(13a_{0}\text{nm}\).

Through analysis of the partial Patterson function, the superstructure was found to be basically defined by clusters of Bi and 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 CuB\(_{1-x}\)S\(_2\), which also has a non-integral type superstructure (Ohmae, Tomoaki & 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 phase, the crystal can be represented as a combination of a disordered subcell structure and a periodic, modulated structure at greater concentrations in which atom positions are influenced by the phase transition. This cubic phase and CuB\(_{1-x}\)S\(_2\) are stable under conditions when Bi and Cu are present.

The crystallographic structure has shed considerable light on the geometrical structure of these defects and high resolution electron microscopy. This allows us to identify which facial directions may indeed be of apparent space group symmetry. We present the results of a detailed atomistic computer simulation study of extended defect formation in Re\(_0\)\(_3\)(D\(_0\)\(_9\)) structured nonstoichiometric oxides. The phenomenon of crystallographic shear (CS) planes 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). During quenching, however, the metal atoms aggregate 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 established 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.

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20.4-04 THE ENERGY OF FORMATION AND ORDERING OF CRYSTALLOGRAPHIC SHEAR PLANES IN ReO\(_3\) STRUCTURED NONSTOICHIOMETRIC OXIDES

We present the results of a detailed atomistic computer simulation study of extended defect formation in Re\(_0\)\(_3\)(D\(_0\)\(_9\)) structured nonstoichiometric oxides. The phenomenon of crystallographic shear (CS) planes 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). During quenching, however, the metal atoms aggregate 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.

The absences \(F(hkl) = 0\), \(h + 2k + 3l = 2n + 1\) and \(F(hhk') = 0\), \(h = 2n + 1\) do not correspond to symmetry elements of any primitive space group of 4/mm 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 \(m\) 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 \(4/m\) Laue symmetry. Systematic absences of \(F(hkk') = 0\) for \(k = 2l\) correspond to an allowed symmetry element for this disordered subcell structure. Twinning must be a condition for \((hkl)\) data with \(h + k = 2n\) to also have \(4/m\) Laue symmetry. Systematic absences of the subcell be obtained. Two structures based upon spacegroup \(Pm\_mm\_mm\) have been refined, one of true spacegroup \(P_{6}2/m\), the other of true spacegroup \(Pb\_mm\_mm\). Both showed \(|F(hkl)| = |F(hk\bar{l})|\) for all data. Constrained refinement is essential when twinning occurs. Fourier analysis methods identify which combinations of parameters are poorly defined.