11. REAL AND IDEAL CRYSTALS

11.5-03 EXACT RELATIONS FOR THE STRUCTURE OF SOLID SOLUTIONS FROM DIFFRACTION DATA. M. Símerská and V. Syneček, Institute of Physics, Czechoslovak Academy of Sciences, 180 40 Freho 5, Na Slovence 2, Czechoslovakia.

Exact mathematical relations have been established revealing the structure of binary substitutional solid solutions in terms of local order parameters accessible directly from measured intensities of diffuse scattering. The relations are deduced from a general physical principle of the existence of the finite ranges of many-atom site interactions governing the interrelations of local order parameters. Figures present the results obtained for the case of A and B atoms arranged on a square lattice with the nearest-neighbour site interactions only. The decrease of site correlations with the increase of interatomic vectors \( r_{ij} \) is apparent from the contour maps of several local order parameters \( \alpha_{ij} \) (\( \alpha_{AA}, \alpha_{AB}, \alpha_{BB} \)), where \( \alpha \) is the fraction of A atoms. The contour maps of densities are given for clusters comprising an A atom with all like and with all unlike nearest neighbours. We can generally get the densities of clusters from a limited set of \( \alpha \)'s. Such a set permits to calculate all measured \( \alpha \)'s from relations corresponding to the existing ranges of site interactions. This allows to solve the many-body problem irrespective of the nature of atomic interactions. Similar calculations for bcc, fcc, and hcp lattices as well as for the solid solution separation into coherent phases are in progress. The aim is to provide a real structure basis for the quantitative studies of physical properties of materials based on realistic many-body atomic interactions.

11.5-04 DETERMINATION OF CHARGE DISTRIBUTIONS NEAR VACANT IN NbO. By A. Aoki, K. Sato, M. Morlaza, Toyohashi University of Technology, Toyohashi 440 Japan J. Harada, Department of Applied Physics, Nagoya University, Chikusa-ku, Nagoya 464 Japan.

NbO has a defective structure, derived from the NaCl type cell by the ordered omission of 25% of the ions on both cation and anion sublattices. These ordered vacancies affect charge distributions in NbO. In the present study integrated X-ray intensities of Bragg reflections were obtained from a single crystal of NbO. In this crystal was grown by the arc-Czochralski method. The X-ray measurements were carried out at 188 K and 296 K, employing the monochromatic Mo Kα radiation. About one hundred and thirty independent \( h k l \)'s were measured in the range of 0.1<\( \sin \theta/\lambda <1.2 \). The measured data was compared with those of an ordered NbO-\( \alpha \) by the arc-Czochralski method. The X-ray measurements were carried out at 188 K and 296 K, employing the monochromatic Mo Kα radiation. About one hundred and thirty independent \( h k l \)'s were measured in the range of 0.1<\( \sin \theta/\lambda <1.2 \). Both standard least-squares refinements and difference electron density synthesis techniques were used to examine the structure in detail. Extinction was remarkable. The \( R \) values after refinements were 1.3% for the result at 188 K and 2.0% for 296 K. In both temperatures the anisotropy of electron density at cation and anion sites near a vacancy was clearly observed. For instance, large positive electron density peaks (2 e/\( \alpha^3 \)) near cation sites near an anion vacancy. There was no indication that direct coupling between cation- and anion-vacancy exists in charge distributions. Also, broad electron distribution was found mainly in the Nb-Nb direction, whereas this trend was scarcely observed in the 0-0 direction. This may imply that the cation-cation overlapping bands are important for considering band scheme in NbO. These experimental results will be compared with the theoretical calculations by the DV-Xα cluster method.