atures. This glide will be in {111} planes which are normally not allowed.

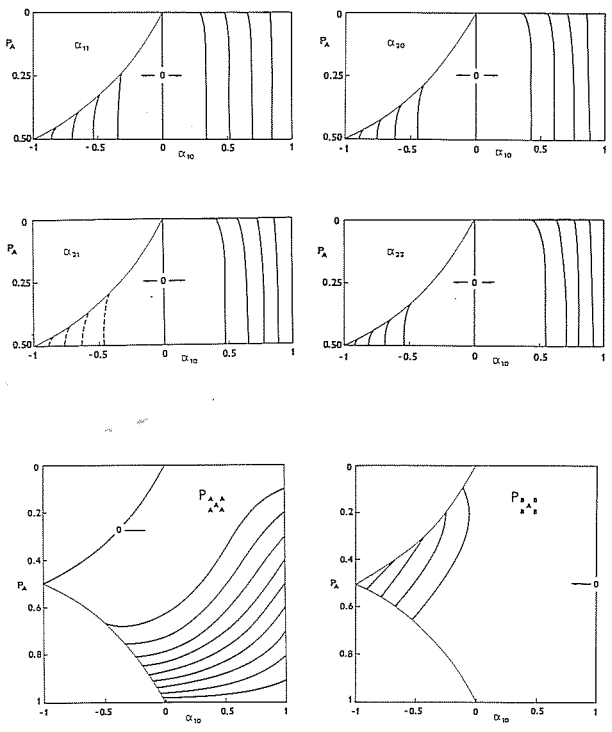
It is further suggested that an individual <112> dislocation in, for example, MgO+Au^{3+} would form an electrostatic dipole together with its ionic atmosphere. Consider a zigzag dislocation lying in $\{1\bar{1}0\}$ and made of alternate <112> and <11$\bar{2}$> segments of separation ℓ. Since Bragg planes around dislocation cores are slightly bent this is equivalent to a chain of dipoles at slight angles δ to one another, alternate dipoles being identically oriented. Now imagine a configuration such that zigs and zags are separated by a distance d parallel to b, each segment retaining its ionic atmosphere. The difference of energy between the "unseparated" and "separated" chains is calculated to be

$$\Delta E = 2\sqrt{2}\ (p^2/\ell^3)\ (d/\ell)\ \sin\delta\ \zeta(4)$$

where p is the macroscopic, averaged dipole moment of a single segment (zig or zag) and ζ is Riemann zeta function. ΔE is positive if $\sin\delta$ is. This implies that the separation due to purely dipole-dipole interaction actually occurs for suitably oriented dipoles. Evidence that certain dislocation configurations observed in MgO+Au^{3+} by microscopy are consistent with this separation occurring has been obtained by G. Kameswara Rao (Thesis (1980) I. I. T. Kanpur; being published).

These ideas may be extended to other structures, *mutatis mutandis*.

Thanks are due to G. Kameswara Rao and J. Mahanty for helpful discussions.



Contour lines: —— positive, ---- negative; in 0.2 steps for α_{uv}, in 0.1 steps for clusters.

11.5-03 EXACT RELATIONS FOR THE STRUCTURE OF SOLID SOLUTIONS FROM DIFFRACTION DATA. M. Simerská and V. Syneček, Institute of Physics, Czechoslovak Academy of Sciences, 180 40 Praha 8, Na Slovance 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. The 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 $\vec{r}_{uv}$ is apparent from the contour maps of several local order parameters $\alpha_{uv}(P_A, \alpha_{10})$, where P_A 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 α's. Such a set permits to calculate all measured α'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 VACANCY IN NbO. By A. Aoki, K. Sato, M. Morinaga, 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(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 $0.1<\sin\theta/\lambda<1.2$ Å^{-1}. 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 peak (2 e/Å^3) was present around a cation site 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 O-O 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.