

regions of low scattering power (defect clusters) and compensating expansion in other parts of the structure.

We further evolve this physical picture of the defect structure of wüstite by presenting a step by step description of how the diffuse diffraction patterns arise and are influenced by various possible real-space variables such as defect distribution, defect cluster size, number of interstitials and lattice strain. The *motif* of diffuse incommensurate superlattice peaks around each main Bragg peak position is indicative of the presence of a paracrystal-like distribution of defects. The most significant result of the present work is that in order to explain the presence of the asymmetric central peak within this diffraction *motif* it is necessary that the lattice is inhomogeneous. That is, there exist regions containing the paracrystal array of defect clusters interspersed with regions containing no defects. Of all the possible single cluster types the  $V_{13}T_4$  (Koch-Cohen) clusters appear to us to give diffraction patterns most similar in detail to the observed patterns, but there is also evidence for the presence of a proportion of larger clusters, such as  $V_{16}T_5$  clusters.

**PS10.12.09 THE METHOD FOR ACCURATE CALCULATIONS OF BINARY CORRELATION FUNCTIONS IN TWO-COMPONENT CRYSTAL STRUCTURES.** Roman V. Chepulsii, Vladimir N. Bugaev, Dept. of Solid State Theory, Inst. for Metal Physics NAS of Ukraine, Kiev-142, 252180, Ukraine

By use of fluctuation wave method within the framework of thermodynamic theory of perturbations in the grand canonical ensemble the regular procedure is developed for calculations of the binary correlation functions as well as their Fourier components for two-component crystal structures with an arbitrary Bravais crystal lattice. Therewith, the analytical expressions are derived without *a priori* limitations on the range of both interparticle interactions and correlations. The high accuracy of the method is demonstrated by comparing its results with those of Monte Carlo simulations and cluster-variation method calculations.

**PS10.12.10 X-RAY SCATTERING FROM MICRODEFECTS.** E. Gartstein and D. Mogilyanski Inst. for Appl. Research, Ben-Gurion University, POB 653, BeerSheva, 84105, Israel

Knowledge of structure perfection in single crystal materials used for fabrication of devices, allows better control of their electronic properties. Microdefects resulting from clustering of point defects or dislocation loops, are common in these materials. X-ray scattering is very sensitive to the presence of these defects, particularly in transmission mode, when the concentration is low. Analysis can be performed to obtain information on the nature, size and concentration of the defects. Triple-crystal diffractometry was employed to measure anomalously transmitted X-ray scattering in InP. Metallographic studies of InP crystals showed the presence of the dislocation loops with the uncertainty regarding their system type:  $\{111\} <110>$  or  $\{110\} <110>$ . Simulation of the Huang scattering and comparison with the symmetric intensity component  $1/2[I(\bar{q}) + I(-\bar{q})]$  obtained from the measurements, indicated that -dislocation loop system is consistent with  $\{111\} <110>$  interstitial model. However, the measured antisymmetric intensity component  $1/2[I(\bar{q}) - I(-\bar{q})]$  where  $\bar{q}$  is the momentum transfer near to the peak (022), was about  $90^\circ$  rotated as shown in Fig. 1a, while the theory predicts the positive (solid lines) and negative (dashed lines) intensity contours to be located along the reciprocal lattice vector as is shown in Fig. 1b. This feature could be explained by including into simulation of the diffuse scattering its asymptotic part and considering the possibility of the vacancy loops to be present as well. The rotation of the antisymmetric intensity resulted when vacancy loops occupy the (111) plane and the rest of the  $\{111\}$  planes are occupied by interstitial loops as is shown in Fig. 1c

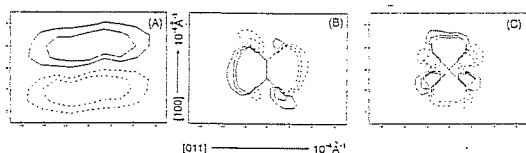


Fig. 1

**PS10.12.11 THE INFLUENCE OF THE VACANCIES INDUCED BY INTERSTITIAL IMPURITY ON STRUCTURAL STABILITY OF CRYSTAL STRUCTURES.** V. G. Gavriljuk, V. N. Bugaev, A. V. Tarasenko, B. Z. Yanchickii, Inst. for Metal Physics NAS of Ukraine, Kiev-142, 252180, Ukraine

Statistical-thermodynamic analysis of a possibility for a significant increase of the concentration of the site vacancies with the concentration of interstitial impurity in crystal structures is performed. The influence of such impurity-induced vacancies on diffusivity of matrix atoms and structural stability of crystal is studied. The vacancy contribution into martensitic transformations of the stainless austenitic hydrogenated steels is studied by using of the X-ray and TEM techniques.

The factors assisting the formation of the impurity-induced vacancies are: (1) sufficiently high repulsion of interstitial and substitutional atoms, (2) sufficiently high solubility of interstitial atoms (or clustering in interstitial subsystem), (3) atomic ordering in interstitial subsystem.

**PS10.12.12 RECOVERY OF STATIC ATOMIC DISPLACEMENTS IN Fe-Ni SOLID SOLUTIONS WITH THE 3 $\lambda$  TECHNIQUE.** G. E. Ice, X. Jiang, L. Robertson, C. J. Sparks, P. Zschack, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6118, USA

The use of resonant-scattering techniques to recover local pair displacements and local chemical order has brought new and useful information to our understanding of crystalline solid solutions. It has been long recognized that "atom size differences" move the atoms off the sites of the average lattice and play an important role in alloy properties and in phase stability. Most of the information about atomic size differences comes from the change in lattice parameter with elemental concentration. The success of Vegard's law in fitting this mostly straight line relationship of lattice parameter versus concentration is found to be fortuitous in the Fe-Ni system. Neither the like pair distance (AA and BB pairs) is independent of concentration nor is the AB pair separation the mean between the pure elements as predicted by Vegard's law. Mathematical treatment of the data is discussed and both the systematic and statistical errors are assessed. Concern with the inelastic processes such as resonant Raman, Compton and plasmon scattering contributions to the diffuse scatter is important to the recovery of the weak elastic scattering. Resonant (anomalous) x-ray scattering near absorption edges is used to effect contrast changes in the Laue scattering needed to unravel the individual pair displacements.

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**PS10.12.13 X-RAY DIFFRACTION STUDY OF DIAMOND CONTAINING PLATELETS.** G. Kowalski, J. Gronkowski, Institute of Experimental Physics, University of Warsaw, 00681, Poland and Moreton Moore Royal Holloway University of London, Egham, TW20 0EX, England

Reciprocal space maps of a natural Type Ia diamond containing impurity platelets have been measured in a four-crystal six-reflexion geometry employing a Bartels-type beam conditioner and single-bounce analyzer. The platelets lie on  $\{100\}$  planes: they are about 10 nm across, are a few atoms thick and, even after decades of study, excite interest because their precise composition is still unknown. [They are akin to the Guinier- Preston zones in Al-5%Cu.] Platelets are found in natural diamonds (Type Ia) which contain nitrogen; but recent studies suggest that they are not composed of nitrogen; at least, not entirely [1]. They were first directly observed by transmission electron microscopy [2]; but their presence had already been deduced from  $<100>$  spikes extending from certain reciprocal lattice points (relps) in x-ray diffraction photographs [3]. X-ray spike topography has been made quantitative: by recording intensity at angles slightly off-set from the 111 reflexion [4,5]. Studies of the 331 relp have been made by