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 <u>inhomogeneous</u>. 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. Chepulskii, 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 $1/2[I(\vec{q}) + I(-\vec{q})]$ obtained from the measurements, indicated that - dislocation loop system is consistent with {111}< 110 > interstitial model. However, the measured antisymmetric intensity component $1/2[I(\vec{q}) - I(-\vec{q})]$ where $\vec{q}$ is the momentum transfer near to the peak (022), was about 90° 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 antysymmetric 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
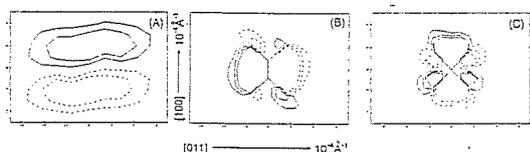

Fig.1

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 3λ 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.

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

synchrotron double-crystal diffractometry and we also report here the high-resolution reciprocal space mapping around the 220 and 111 relps.

[1] G.S.Woods, in Properties & Growth of Diamond (ed. G.Davies) London: INSPEC, Inst.Elec.Eng. (1994) 94.
[2] T.Evans and C.Phaal, Proc.R.Soc.London A270 (1962) 538.
[3] K.Lonsdale, Proc.R.Soc.London A179 (1942) 315.
[4] M.Moore & A.R.Lang, J.Applied Cryst. 10 (1977) 422.
[5] S.G.Clackson, M.Moore, et al., Phil. Mag. B62 (1990) 115.

PS10.12.14 LOCALLY MODULATED STRUCTURES OF THE Y$_2$O$_3$-Nb$_2$O$_5$ SOLID SOLUTIONS. R.Miida, *F.Satoh, *M.Tanaka,**H.Naito and **H.Arashi Sci. Univ. of Tokyo Suwa Coll. Chino Nagano Japan, *Res. Inst. Sci. Meas., **Fac. of Eng. Tohoku Univ. Sendai Japan

Modulated structures formed in the defect fluorite type $(Y_2O_3)_{1-x}(Nb_2O_5)_x$ $(0.21 \leqq X \leqq 0.27)$ solid solutions have been investigated by electron microscopy. The [1 1 0] diffraction pattern showed a pair of diffuse spots in the [1 1 2] direction at both sides of the $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ reciprocal lattice point. The distance between the diffuse spots decreased from 0.064Å^{-1} to 0.045Å^{-1} with increasing x from 0.21 to 0.27. The HREM images revealed the existence of small domains with an antiphase structure (APS). The two-dimensional APS (x=0.21) projected on the (1 $\bar{1}$ 0) plane is described by compositional waves of Y/Nb and O/vac and displacement waves along the [1 1 $\bar{2}$] direction, as shown in Fig.1. The composition at cation-sites is expressed by a sinusoidal wave, whose amplitude changes between Y and 0.58Y+0.42Nb. The occupation probability of O at anion-sites is expressed to change between 0.806 and 0.904 in the form of a sinusoidal function. Amplitudes of the displacement waves for anions and cations were estimated to be about 0.3Å and 0.02Å, respectively.
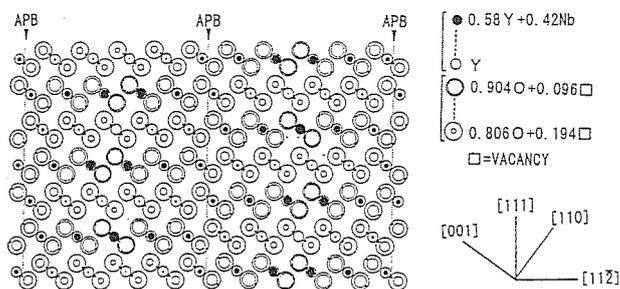

Fig.1 Two-dimensional APS model   APB = antiphase boundary

PS10.12.15   REVERSE MONTE CARLO SIMULATIONS OF THE NEUTRON- AND X-RAY DIFFUSE SCATTERING OF CUBIC STABILIZED ZIRCONIAS. Th. Proffen[1], T.R. Welberry[1], R.B. Neder[2], [1]Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia, [2]Insitut für Kristallographie und Mineralogie, Universität München, Theresienstr. 41, 80333 München, Germany

A new approach to analyse the diffuse scattering of cubic stabilized zirconia is made by Reverse-Monte-Carlo (RMC) simulations. The RMC method applies random changes to a model structure and tries to optimize the agreement between the resulting diffraction pattern and the experimental data. The main features of the defect structure are given by oxygen vacancies introduced by the dopant material (e.g. CaO, Y$_2$O$_3$, MgO) and the relaxation of the oxygens and metals neighbouring these vacancies. Subsequently the simulations are carried out in four separate steps: ordering of the oxygen vacancies, ordering of the Zr and dopant metal ions and relaxation of the metal and metal ions. Calculations are still in progress. The RMC routines which allow to model occupational as well as displacive disorder were integrated in the program DISCUS [1]. They allow a simultaneous refinement of neutron- and x-ray data.

A successful RMC run will lead to one structure which produces a diffraction pattern in good agreement with the experimental data. The resulting structural features have to be discussed from a chemical point of view and are compared to the results of a recent study using the "modulated wave approach"and Monte Carlo simulations [2].

[1] DISCUS, © R.B.Neder & Th. Proffen, see http://rschp2.anu.edu.au:8080/proffen/discus/discus.html
[2] T.R. WELBERRY, R.L. WITHERS & S.C. MAYO (1995). J. Solid State Chem. 115, 43-54

PS10.12.16 DEFECT STRUCTURE OF ZrO$_2$-Y$_2$O$_3$ (Y$_2$O$_3$ -3,12,30 MOL%) SINGLE CRYSTALS. NEUTRON AND X-RAY INVESTIGATION. V.A. Sarin[1], E.E. Rider[1], D. Hohlwein[2], W. Depmeier[3], H. Bessert[3], F. Frey[4], K. Hroudil[4]. [1]FLNP, JINR, Dubna, Russia; [2]Institute fur Kristallographie, Uni Tubingen, BRD; [3]Institute fur Mineralogie, Uni Kiel, BRD; [4]Institute fur Kristallographie, Uni Munchen, BFD

Statistic defect structures of tetragonal and cubic yttria stabilized zirconia were investigated by X-ray and neutron methods using Bragg diffraction and diffuse scattering.

ZrO$_2$+3 mol% Y$_2$O$_3$. Space group P42$_1$/nmc. Crystallographic relations between components of twins are proposed to be two 90° rotation axes a and b (a). There are diffuse scattering in reciprocal space in directions between splitted spots from different components of twins. These data are interpreted as due to domain microstructure and the internal stresses resulting from cubic-tetragonal transformation and differences between the fluorite cubic and tetragonal structures.

ZrO$_2$+12 and 30 mol% Y$_2$O$_3$. Space group Fm3m. From neutron diffuse scattering there were found the very similar experimental pictures. There are some satellite diffuse maxima with a wave vector (0.4, 0.4, (0.8)) and broad diffuse bands. But their integrated intensities are different for 12 and 30 mol% Y$_2$O$_3$. There is no such diffuse scattering for 3 mol% Y$_2$O$_3$.

For interpretation of defect structures of yttria stabilized zirconia two approaches connected with Bragg diffraction data and diffuse scattering will be compared and opportunities of neutron steady beam (flat cone diffractometer E2, BENSC, Berlin) and time of flight methods (DN2 & HRFD, IBR-2, FLNP, Dubna) will be discussed. [s1]