MS10.12.04 RESIDUAL SHORT-RANGE ORDER IN A HEAVY FERMION COMPOUND $CeInCu_2$. Isao Takahashi, Tomoko Kagayama†, Gendo Oomi†, Yoshichika Onuki††, and Takemi Komatsubara†††, School of Science, Kwansei Gakuin University Uegahara, Nishinomiya 662, Japan, †Department of Physics, Kumamoto University, Kumamoto 860, Japan, ††Department of Physics, Osaka University, Toyonaka 560, Japan, †††Department of Physics, Touhoku University, Sendai 980, Japan

$CeInCu_2$ is a heavy fermion compound which is known to have a cubic, Heusler-type structure. Disorder between Ce and In sites has been investigated by an X-ray diffuse scattering measurement with use of synchrotron radiation (beam line 4C, Photon factory, KEK Japan). Rod-shaped diffuse scattering emanating from the 002 Bragg point along [111] and other equivalent directions in reciprocal space was clearly observed at room temperature. The diffuse scattering is an evidence of residual short-range order which would be an origin of the large residual resistivity and a small T^2-term in the resistivity.

In the present study, an analysis of the diffuse scattering has been performed under the assumption of structural disorder in a linear -Ce-In-Ce-In- chain along the [111] direction. For the Ce-site next to the disordered In-site, i.e. Ce atom occupied, obtained order parameters indicate more than 85% occupancy by In atom. In addition, such a disordered cluster tends to form a one-dimensional lattice with an approximate period of 5 - 6 nm. The relationship between the disorder and the large resistivity will be discussed in detail.

MS10.12.05 NEUTRON AND X-RAY SCATTERING STUDIES OF NEUTRON IRRADIATED IRON CRYSTALS. J. L. Robertson and R. E. Stoller. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Results on the structure of defect cascades produced by fast neutron irradiation of Fe single crystals will be presented. Diffuse neutron and x-ray scattering methods are used to study correlations of the interstitial Fe atoms introduced by the irradiation. Because the irradiation is done at ~300K there is significant recombination of defects (interstitials with vacancies). Consequently, the defect concentration is quite low, less than 1 ppm, however, the response of the lattice to the presence of the defects (displacement field) is quite large. The interpretation of the scattering data benefits significantly from the results of recent efforts to construct computer models of the defect cascades. These models follow the time evolution of the defect cascades and show that the surviving interstitials aggregate while the vacancies do not appear to be mobile. Interpretation of these results with regard to radiation hardening in pure metals will be discussed.

MS10.12.06 DEFECT STRUCTURE AND DISORDER IN LITHIUM NIOBATE. By H. Boysen, F. Frey and N. Zotov*, Institut für Kristallographie, Universität München, Theresienstr. 41, 80333, München, Germany.

The defect structures of congruent ([Li]:[Nb]=0.947) and, for comparison, stoichiometric $LiNbO_3$ (space group R3c) have been investigated by Bragg and diffuse scattering of X-rays and neutrons between 38 K and 1515 K. Because the physical properties of Lithium Niobate depend strongly on the non-stoichiometry, a large number of different models for the defect structure has been proposed and discussed in the literature. From the Bragg data the average disorder is characterized by excess Nb^{5+} atoms and charge compensating vacancies on the regular Li-sites (Zotov et al. (1994), *J.Phys.Chem.Solids* **55**, 145). With increasing temperature the mobility of Li increases strongly. The para-ferroelectric phase transition (R3c | 3- Rc) at $T_c \approx 1430$ K is of the order-disorder type (of Li) with some displacive components (Boysen and Altorfer (1994), *Acta Cryst.* B**51**, 405).

The diffuse scattering is concentrated in three planes perpendicular to the ´pseudo-cubic´ directions $[2\bar{2}1]$, [241] and $[\bar{4}21]$ (Zotov et al. (1995), *Acta Cryst.* B**51**, 961). It is attributed to 1-dim displacive and substitutional disorder along Li-O-Li...-chains running along these directions. The chemical component includes Nb_{Li} atoms and vacancies. From the observed correlation length the various cluster models discussed are restricted to four atoms. At room temperature 3-dim short-range order correlations are observed. At low temperatures longer range correlations between the (1-dim) defect clusters set in. With increasing temperature the diffuse scattering intensity increases and becomes more homogeneous. This is interpreted either by a temperature dependent variation of the static defect clusters or by dynamical fluctuations similar to those observed in other perovskite structures.

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MS10.12.07 THE DEFECT STRUCTURE OF NON-STOICHIOMETRIC FERROUS OXIDE. W. Schweika, Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

The defect structure in non-stoichiometric wüstite $Fe_{1-x}O$ has been investigated as a function of temperature and oxygen partial pressure by means of diffuse elastic neutron scattering of a single crystal at thermal equilibrium.

Various methods for analyzing the diffuse scattering data are discussed. The observations that (i) diffuse peaks evolved and (ii) the Huang scattering decreased with increasing non-stoichimetry can be reproduced qualitatively by a Kanzaki force model of the long range displacement fields which is going beyond the usual single defect approximation. Based on Coulomb-like forces and independent phonon data, therefore, it has been assumed that the defects are arranged in so called 4:1 cluster of vacancies and interstitials, which are surrounded preferentially by regular cations for charge compensation.

Furthermore, a Fourier analysis of the (3-dim) data measured at T = 1423 K and x = 0.08 yielded short range order - and lattice displacement parameters as well as the ratio of the numbers of vacancies to interstitials, = 4.0± 0.5. Indeed, a strong correlation between nearest interstitials and vacancies was found. All measured short range order parameters were simulated in a computer model. Further analysis yielded the size distribution of the vacancy-interstitial defect clusters exhibiting a large fraction of 30% of free vacancies, while further 15% of the defects are bound in isolated 4:1 defect clusters. [1]

[1] W. Schweika, A. Hoser, M. Martin, and A.E. Carlsson, Phys. Rev. B **51**, 15771-15788 (1995).

MS10.12.08 A PARACRYSTALLINE DESCRIPTION OF DEFECT DISTRIBUTIONS IN WÜSTITE, $Fe_{1-x}O$. T.R. Welberry & A.G. Christy Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia

Diffuse X-ray scattering data from a crystal of wüstite, $Fe_{0.943}O$, have been recorded. Satellite reflections corresponding to an incommensurate repeat distance of ~2.7Å in all three cubic directions were observed (the P' phase). The incommensurate satellites were diffuse, anisotropically elongated, interconnected by weaker continuous streaks and negligible in intensity beyond first order. Monte Carlo computer simulations have been carried out which demonstrate that this diffraction behaviour is consistent with defect clusters forming a paracrystalline (or highly distorted) lattice. The paracrystalline distribution which best fits the observations is such that the spacing between defects tends to be maintained fairly constant, but relative lateral translations may occur more variably.

The diffuse satellites are systematically more intense on the low-angle side of a Bragg reflection than on the high-angle side. This behaviour may be understood in terms of the well known atomic size effect and is consistent with there being a local contraction of the structure around

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. 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 $1/2[I(\bar{q}) + I(-\bar{q})]$ 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° rotated as shown in Fig. la, 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. lb. 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

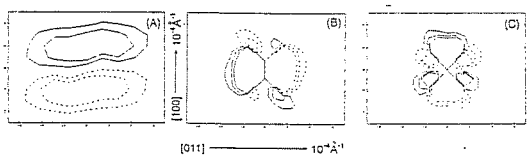

Fig.1

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.

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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