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