

**s7.m1.p1** **Complementarity of Ultra-High Resolution SR X-Ray and Neutron Protein Crystallography.** J.R. Helliwell\*, *Department of Chemistry, University of Manchester, M13 9PL.*

Keywords: instrumentation, neutron diffraction.

The combination of SR X-ray protein crystallography and neutron protein crystallography is effecting a renaissance of the importance of hydrogen atoms in a protein's structure and function and in the detailed structure of the bound solvent (as D<sub>2</sub>O). Indeed the molecular recognition of a ligand for a protein at a receptor site involves bonding (H bonds and van der Waals) and entropic effects especially displacement of bound waters. The study of the molecular relationship between structure and thermodynamics is important. Highly resolved crystal structures of protein molecules can be obtained now using X-ray crystallographic data measured at synchrotron radiation sources with high performance detectors and cryoprotected samples. Details of the mobility of the atoms is also available from their 'thermal parameters' in the refined molecular model. In this way we have now studied the sugar binding plant protein concanavalin A to 0.94 Å resolution using the Cornell CHESS synchrotron, USA. The ease of exchange of particular protons for deuterium in the protein has then been studied using neutron Laue diffraction data measured at the ILL in Grenoble. In addition, most recently, we have determined the D<sub>2</sub>O bound solvent structure of concanavalin A using a combined Cu K $\alpha$  X-ray refinement at 1.8 Å and neutron at 2.4 Å refinement approach, and then compared the results with the bound solvent in the 0.94 Å SR X-ray structure. Many more bound water molecule deuteriums can be located this way rather than the ultra-high resolution X-ray approach alone. However the latter does deliver a few very detailed water molecule hydrogen atoms. The two approaches are thus complementary. In another aspect improvements in the diffraction resolution for room temperature protein X-ray crystallography are important because this is closer to physiological temperature. There are significant differences between cryo and room temperature protein structures involving changes in the multiple occupancies of side chains. Moreover the extra mobility of bound waters at room temperature makes their study via X-rays yet more challenging, which increases the utility of the combined SR X-ray and neutron approaches.

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**s7.m1.p2** **Small-Angle Neutron Scattering and Mossbauer Effect in Austenitic N- and C-containing steels.** V.M. Nadutov<sup>1</sup>, V.M. Garamus<sup>2</sup>, <sup>1</sup>G.V. Kurdyumov *Institute for Metal Physics of the NAS of Ukraine, Kyiv, Ukraine,* <sup>2</sup>GKSS Research Centre, *Geesthacht, Germany.*

Keywords: austenite, SANS, NGR.

An attention is focused on the study of chemical and structural inhomogeneities in austenitic nitrogen-containing Fe-18%Cr-10%Mn-16%Ni-0.5%N and carbon-containing Fe-20-21%Cr-10-11%Mn-17%Ni-0.5%C steels after solution treatment at high temperature. All samples were single phase. Nuclear gamma-resonance (Mossbauer spectroscopy) and small-angle neutron scattering (SANS) were used as effective methods for this purpose.

The hyperfine parameters of Mossbauer spectra of the austenitic steels were analyzed taking into account the parameters derived from Mossbauer spectra of binary Fe-i and ternary Fe-s-i alloys (i = C,N; s = Ni,Mn,Cr). Several subspectra with different isomeric shifts and quadrupole splitting were revealed and attributed to iron atoms in different local surroundings with interstitial and/or substitutional atoms.

More details on inhomogeneous atomic distribution were obtained from the SANS measurements. SANS was observed in all samples and attributed to the chemical inhomogeneities that was consistent with the inelastic neutron scattering data obtained previously. The Guinier and Porod laws were considered for approximation of the SANS curves. The different cross-section of neutron scattering in N-containing and C-containing steels was revealed.

It was established that the inhomogeneities in the N-containing and C-containing austenites were characterized by the same order of the size whereas their structure was different. Unlike the carbon austenite the inhomogeneities in the N-containing steel were characterized by a fractal-like structure. The nature of the fractal properties of the inhomogeneities in the steels was analyzed.