SPring-8 in JAPAN. Since previous report has shown that the Mn_4Ca-cluster suffer from serious X-ray radiation damage during data collection of PSII crystals [2], we adopted a slide-oscillation method to collect the low-dose X-ray diffraction data using large PSII crystals (length: ~1mm), which allowed us to collect a full data set from nine irradiation points of one single crystal in a range of 180 degree. The X-ray dose irradiated onto each point was estimated to be half of the value determined by the spectroscopic method where the radiation damage begins to occur [2]. In the crystal structure obtained at 1.9 Å resolution, the electron density distributions for each of the 5 metal ions were clearly separated, which were also confirmed by the anomalous difference Fourier map. Five oxygen atoms forming the oxo-bridges between the metal ions were clearly identified by the omitted Fourier map, and several water molecules were found to be associated with the metal cluster, which may function as substrates for the oxygen-evolving reaction. In addition, thousands of water molecules were found in the whole structure of PSII dimer. Some of the water molecules form a network linking the catalytic site and two chloride ion sites identified previously [3]. Including protein subunits and co-factors, we will discuss the atomic resolution structure of PSII complex.

[1] Guskov. A., Kern, J., Gabdulkhakov, A., Broser, M., Zouni, A., Saenger W., Nat. Struct. Mol. Biol., 2009, 16, 334. [2] Yano J., Kern J., Irrgang K.D., Latimer M.J., Bergmann U., Glatzel P., Pushkar Y., Biesiadka J., Loll B., Sauer K., Messinger J., Zouni A., Yachandra V.K., Proc. Natl. Acad. Sci. USA 2005, 102, 12047. [3] Kawakami K., Umena Y., Kamiya N., Shen J.R., Proc. Natl. Acad. Sci. USA, 2009, 106, 8567

Keywords: membrane protein complex, photosynthesis, metal clusters

FA1-MS03-P04

A neutron-diffraction study of the low-cycle fatigue behaviour of an austenitic stainless steel 316.

Adelaide Dubreuil[a,b], Shu Yan Zhang[b], Sophie Eve[a] and Alexander Korsunsky[c], [a]*ENSICAEN, 14000 Caen, France,* [b]*ISIS Facility, STFC, Rutherford Appleton Laborator, Chilton Oxfordshire, OX11 0QX, UK,* [c]*University of Oxford, Oxford, OX1 3PJ, UK*
E-mail: shu-yan.zhang@stfc.ac.uk

Type 316 stainless steel considered to be one of the leading candidate materials for the first wall and blanket structure of future fusion reactors because of its well-characterized properties such as high temperature strength, good compatibility with coolant and irradiation properties for fast breeder reactors.

The present work describes the behavior of this steel under low cycle fatigue at different temperatures.

The in situ neutron diffraction fatigue test was conducted on the ENGIN-X diffractometer at the ISIS spallation neutron source in Chilton, UK. The fatigue tests were performed at room temperature and at 550°C, where the minimum strain and the maximum strains were -1.1% and 1.1%, respectively. Diffraction spectra were acquired at a series of load levels within selected fatigue cycles, enabling measurement of lattice strain parallel and perpendicular to the loading axis.The measurements were used to quantify the evolution of internal microstrain within crystallites as a function of applied macrostress through the fatigue cycles. The measurement has shown that during low cycle fatigue, grain families show different responses to applied stress, i.e. anisotropic behavior is observed. Some grain groups undergo elastic cycling whereas others exhibit plastic deformation characterized by a significant hysteresis fatigue loop.

The cyclic hardening and softening behavior during fatigue are discussed and comparison is made between the experimental results and finite element crystal plasticity modelling.

[1] Introduction to the characterization of residual stress by neutron diffraction MT Hutchings, PJ Withers, TM Holden, T Lorentzen.2005. [2]. MR Daymond, MAM Bourke, RB Von Dreele J Appl Phys, 1997,82(4),1554-62. [3]. AM.Korsunsky, KE James, MR Daymond Engin Fract Mecha, 2004, 71,805-12.

Keywords: Neutron diffraction, Low cycle fatigue, Strain measurement.