Proposal Title: X-ray Crystallographic Study of Novel Protein Folds and Virulence Factors of *Helicobacter pylori*

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Helicobacter pylori is known as a Gram-negative spiral bacterium, colonizes the gastric mucosa of human stomach in half of the world's population and may persist for decades in the absence of eradication therapy It is now known as the only bacterium that survives in the human stomach of extreme acids and is the major causative agent of gastric mucosal inflammation and peptic ulcers. Because of its unique ecological niche and its clinical relevance with the upper digestive tract diseases, *H. pylori* has been a model system for the study of molecular virulence and pathogen-cell interaction at a molecular basis. Multiple factors are believed to participate in different outcomes of the infection: difference degree of virulence from bacterial polymorphisms, the host response itself, and environmental influences.

In this study in SPring-8 beamline 12B2, several crystals of HP1238 proteins were collected using synchrotron radiation source. Several data sets including six native data sets were collected. The crystals diffract well to the resolution of about 1.8 Å with the mosaicity of 0.5 and the overall R_{merge} below 10%. And we collected a set of multiple wavelength anomalous diffraction data. After energy scans we found the signals of Se atom in the proteins, and we are going to solve this structure by using MAD method.

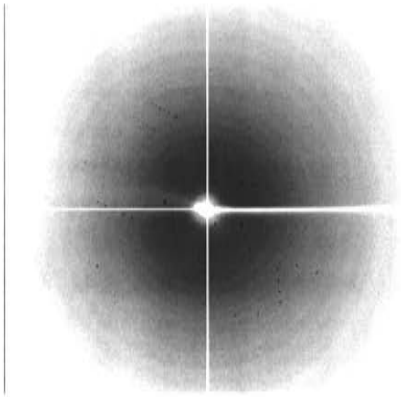

Figure1: diffraction pattern of native crystal with 0.5 degree collected.

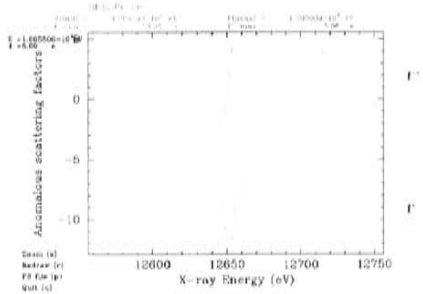

Figure2: Energy scans results.

Dielectric response of high-pressure low-temperature H_2O

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The dynamical behavior of high-pressure phases of ice is of fundamental importance to condensed matter physics and planetary science. We propose to use inelastic x-ray scattering to probe the dielectric response of water, low-density amorphous ice, high-density amorphous ice, and crystalline ices I, II, III, VI, VII and IX at high pressure and low temperatures. The data will reveal rich information on the electronic structure of high-pressure phases of ice and provide important data for comparison with calculations.

Measurements were performed using the IXS spectrometer at BL12XU. The energy resolution of the incident beam was 150 meV at 9884.7eV. The scattered x-ray photons were energy analyzed at a fixed scattering angle of 35 deg using the newly commissioned multiple analyzer system with three 2m radius diced analyzers. The total energy resolution was 179meV at 9884.7eV.

Two Merrill-Bassett diamond-anvil cells with pressure of 0.25GPa and 2.64GPa were used for the experiment, and were cooled with a pulse-tube cryostat that routinely reaches 4K. The combination provides access of the liquid phase, ice II, III, VII, VIII, and IX. For comparison, data were also taken on liquid water under ambient conditions.

Fig.1 shows the data obtained from liquid water, the liquid phase at 0.25GPa, ice II, III, and IX at various temperatures. The data under pressure contain no contribution from the diamond tips, but some scatterings due to the Be gasket used are present and have to be subtracted in order to extract data due only to the sample.

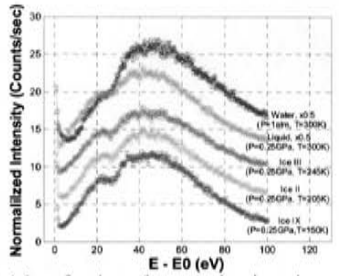

Fig.1 Loss functions of water and various phases of H_2O at 0.25GPa and low temperatures.

The data obtained at 2.64GPa are shown Fig.2. The count rate was much lower due to the smaller sample volume. For all the measured phases, the overall structure of the data is quite similar with small differences over 0 - 40eV. Further analysis is underway.

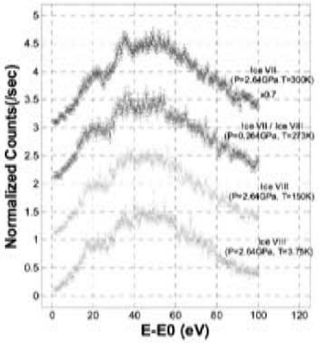

Fig.2 Loss functions of ices VII and VIII at 2.64GPa and various low temperatures.