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## Studies on static and dynamic structures of metallic fluids in the supercritical region

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Liquid Hg is transformed to an insulating state when it is expanded to liquid-vapor critical point (the critical data of Hg [1]:  $T_c=1478^\circ\text{C}$ ,  $p_c=1673\text{bar}$ ,  $d_c=5.8\text{g/cm}^3$ ). To understand the mechanism of the metal-nonmetal transition, it is very important to investigate the dynamical properties. We planned inelastic x-ray scattering experiments to observe the dynamic structure factor of fluid Hg at SPring-8. For the experiments using the multi-analyzer crystals, a new high-pressure vessel with large Be windows for the scattering x-rays was designed. In this report, the results of the first experiment for expanded fluid Hg using the new vessel are presented.

We have made inelastic x-ray scattering measurements for expanded fluid Hg using the spectrometer installed on the BL35XU beamline at SPring-8. The incident x-ray beam of 21.75keV finally monochromatized by Si (11 11) reflection was used and the scattered x-rays were detected by three analyzer crystals with the energy resolution of about 1.8meV. The fluid sample was contained in the specially designed sapphire cell and the experimental conditions of high pressure and high temperature were achieved using a high-pressure vessel containing heating elements.

Figure 1 shows the inelastic x-ray scattering spectra of liquid Hg at 500°C and 100bar detected through a Be window at the scattering angle( $2\theta$ ) of 5 degree. Using the new high-

pressure vessel, the inelastic spectra at three different momenta could be observed at one scan. The spectra include the scattering intensity from the He gas but its contribution was found small by background measurements. A shoulder coming from phonons is observed around 5-10meV in the both sides. The data analysis is now in progress.

[1] W. Götzlaff, PhD Thesis, University of Marburg, 1988.

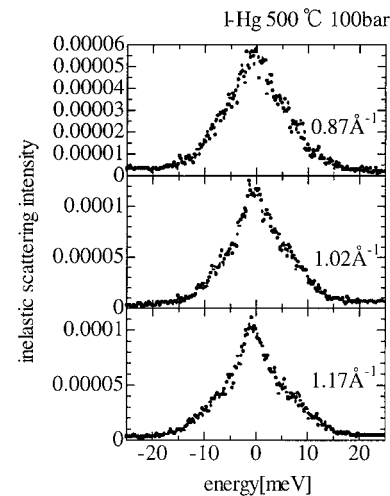


Figure 1

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## X-ray structural analysis of the tetraspanin CD81 Long Extracellular Loop complex with Small Loop.

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### Introduction

Tetraspanins form a widely distributed protein superfamily, structurally characterized by four hydrophobic transmembrane regions (TM1-TM4) and by two extracellular domains, known as large and small extracellular loops (LEL and SEL, respectively). Remarkably, many tetraspanins are being discovered as tumor-associated antigens and appear to be involved in tumor growth and proliferation, in line with an emerging body of evidence indicating their involvement in the regulation of cell adhesion and migration processes

HCV is a positive strand RNA virus of the flaviviridae family chronically infecting about 170 million persons worldwide. Chronic HCV infection results in severe liver diseases in a sizable fraction of cases. It has been recently shown that the HCV envelope E2 glycoprotein binds with nM affinity to the LEL domain (composed of ca. 100 amino acids) of the human hepatocyte tetraspanin CD81, a necessary step for infection and virulence (1).

We have recently reported the crystal structure of human CD81 LEL domain by using MIR method, and showed that this structural key motif is common for the other tetraspanin family (2).

To investigate the detailed structural function of CD81-LEL, we cocrystallized the complexes with SEL domain (30 a.a.) and this cocrystal form different from the native crystal.

### Experiments, Results and Discussions

X-ray diffraction data on CD81-LEL with CD81-SEL cocrystals were collected at 100 K in a nitrogen stream, supplementing the mother liquor solution with 20% glycerol as cryoprotectant using a ADSC-CCD detector system at the beam line of BL38B1 at SPring-8. The X-ray wavelength was 1.00 Å, the angle oscillation range was  $1.0^\circ$  and the crystal-to-detector distance was 170 mm. Analysis of the diffraction pattern and of the systematic absences allowed to assign CD81-LEL/SEL cocrystals to the primitive hexagonal space group C2, with unit-cell parameters  $a = 101.1$ ,  $b = 60.2$ ,  $c = 58.9$  Å,  $\alpha = 90$ ,  $\beta = 120$ ,  $\gamma = 90^\circ$ . A total of 19777 unique reflections were obtained by using the program packages of DENZO and SCALEPACK. The intensity data in the resolution range of 40.0 to 2.00 Å were processed with R-merge of 6.2 %.

Since the intensity data at 100 K were in good quality, the molecular replacement method gives clear solution using native structure of CD81-LEL with R-factor of 0.480. Further crystallographic refinement is now in progress.

### References

1. Pileri, P *et al. Science* 282, 938-941. (1998)
2. Kitadokoro, K *et al. EMBO J* 20, 12-18. (2001)