

## 【Grant-in-Aid for Specially Promoted Research】

### Science and Engineering (Mathematics/Physics)



#### Title of Project : Material Sciences at Very High Pressure: Frontier of Mbar Chemistry

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Research Area : Material Science

Keyword : High Pressure, Superconductivity, Metals, Magnetism

#### 【Purpose and Background of the Research】

To explore material science at extreme condition of ultra-high pressure exceeding megabar (100 GPa), original designed high-pressure technique will be investigated. The pressure-induced superconductivity in simple systems such as elemental material, organic and inorganic molecular crystals were found at high pressure, and it was recently found that some of them show complete different phenomena at megabar pressures. This project forms following 3 parts. A: Materials science at very high pressure on simple systems. B: High-pressure synthesis of functional materials. C: Developments of multi-megabar technique and theoretical calculations.

#### 【Research Methods】

A: The most attractive among various elements is hydrogen in the condensed phase as solid metallic hydrogen is expected to be a room-temperature superconductor. Also, fluid metallic hydrogen under high pressure and at high temperature may provide important information about the interior of giant planets. Light halogen elements and metal hydrides are also subject of the research.

B: High efficiency needs in materials such as thermoelectric, multiferroic, magnetoresistive, carbon system, nano materials, and hydrogen storage materials. The physical properties of these materials will be clarified, and new functions and chemical reaction will be tested.

C: Technical development: To exceeding 4 megabar that is known as the generating limit of a diamond anvil cell. The precise structural analysis of the submicron size will be performed using a synchrotron X-ray with simultaneous physical measurements in the range of large temperature and pressure by developing of so called megabar platform. The computer simulation using ab-initio calculation is a powerful technique at the prediction and analysis under ultra-high pressure. The precise theoretical calculation will be performed in physical properties, such as pressure-induced phase transition, structural stability, and pressure-induced superconductivity in A and B.

#### 【Expected Research Achievements and Scientific Significance】

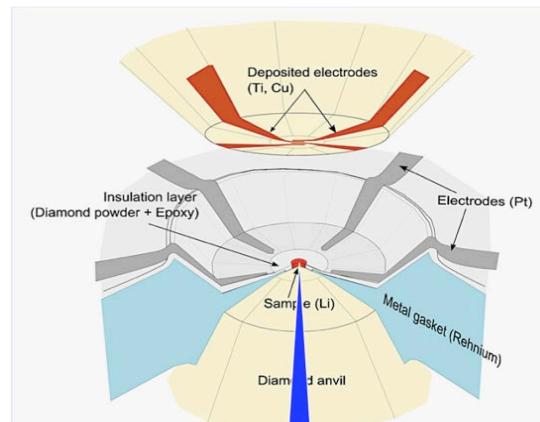


Figure 1. "megabar" platform

The impact of the realization of the RTS (Room Temperature Superconductivity) of the metallic hydrogen is immeasurable. Not only RTS but also developing new functions of materials must be great influence in our energy, electronics, and communications system in our human beings. The establishment of a synthetic method by the megabar pressure can be a breakthrough of the limit of materials developments by substitution and doping method, etc.

#### 【Publications Relevant to the Project】

K. Shimizu, "Elemental Superconductors" 100 years of Superconductivity 4-8, 278-282, CRC Press, Taylor & Francis (2011).

T. Matsuoka and K. Shimizu, Direct observation of a pressure-induced metal-to-semiconductor transition in lithium, Nature 458, 186-189 (2009).

#### 【Term of Project】 FY2014-2018

#### 【Budget Allocation】 395,500 Thousand Yen

#### 【Homepage Address and Other Contact Information】

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