PCP2-1

Observation of surface 1*T* phase on 2*H*-$NbSe_2$ by STM/STS

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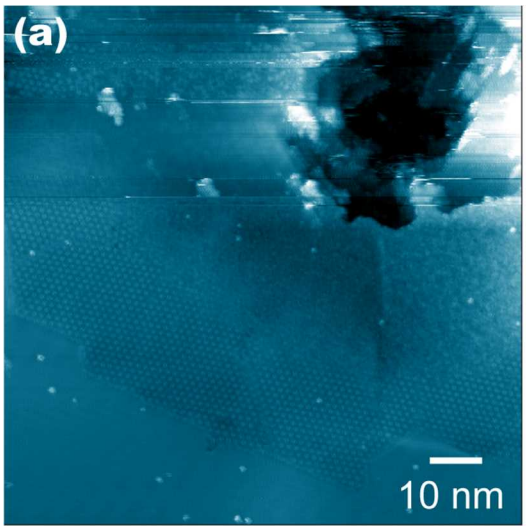
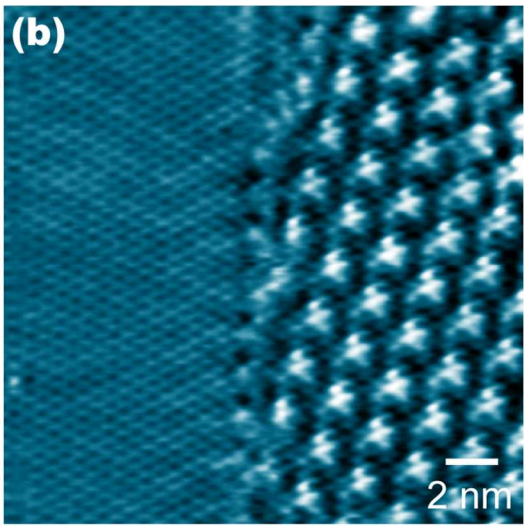
One of the transition metal dichalcogenides, 2*H*-$NbSe_2$ has been studied for a long time because of the existence of charge density wave (CDW) below 33 K and emergence of superconductivity below 7 K. On the other hand, other polytypes, such as 1*T* and 4*H*-$NbSe_2$, have been less studied because of difficulty in single crystal growth. Recently, H. Wang *et al.* reported that a short pulse bias voltage from an STM tip creates 1*T*-$NbSe_2$ on 2*H*-$NbSe_2$ surface. They also revealed that the 1*T*-$NbSe_2$ shows a CDW with $\sqrt{13}\times\sqrt{13}$ periodicity, which is also observed in 1*T*-TaS_2. However, the electronic state is not clarified yet in the study. According to another report by Y. Nakata *et al.*, monolayer 1*T*-$NbSe_2$ also shows the same CDW as that observed by STM and seems to be a Mott insulator with similar gap size to that of 1*T*-TaS_2. Motivated by these studies, we have tried to clarify the electronic states of 1*T*-$NbSe_2$ on the surface of 2*H*-$NbSe_2$ created by application of the pulse bias voltage from the STM tip.
Figure 1(a) shows an STM image that is taken after the application of a pulse voltage on 2*H*-$NbSe_2$ at 4.2 K. This image shows depression of the surface structure. The magnified image near the depression is shown in Fig. 1(b). This image clearly shows the coexistence of the original 3×3 CDW in 2*H*-$NbSe_2$ and the $\sqrt{13}\times\sqrt{13}$ CDW in 1*T*-$NbSe_2$ successfully. We report on not only the structural change but also the change in the electronic states at the conference.





Keywords: 1T-NbSe2, STM, STS

PCP2-2

Effects of the Co-Intercalation of Lithium and Ethylenediamine into 1T-TaS_2 and 2H-TaS_2

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Layered compounds 1T-TaS_2 and 2H-TaS_2 have been studied for more than four decades owing to the discovery of charge density wave (CDW) and superconductivity. A variety of metal atoms and organic molecules have been intercalated into the compounds to elucidate the relationship between CDW and superconductivity [1]. So far, however, there is almost no report on the co-intercalation of metal atoms and organic molecules into 1T-TaS_2 nor 2H-TaS_2.

We have succeeded in synthesizing new co-intercalation compounds of 1T-$Li_x(C_2H_8N_2)_yTaS_2$ with the superconducting transition temperature T_c = 3.2 – 4.0 K via the co-intercalation of Li and ethylenediamine (EDA) $C_2H_8N_2$ into 1T-TaS_2. On the other hand, no superconductivity was observed in the only EDA-intercalated sample of x = 0, while superconductivity with T_c = 3.7 K was observed in 1T-$Li_{0.5}TaS_2$ where EDA was de-intercalated from 1T-$Li_{0.5}(C_2H_8N_2)_yTaS_2$ with T_c = 3.5 K. Moreover, it has been found that the commensurate CDW (CCDW) transition observed in 1T-TaS_2 is suppressed in all the intercalated samples.

We have also succeeded in synthesizing new co-intercalation compounds of 2H-$Li_x(C_2H_8N_2)_yTaS_2$ with T_c = 3.2 – 4.5 K. T_c has been found to be the highest, namely, 4.5 K in the only EDA-intercalated sample of x = 0 and decrease with increasing x. That is, the co-intercalation of Li suppresses the superconductivity in 2H-$(C_2H_8N_2)_yTaS_2$, indicating that the electron doping due to intercalated Li is harmful to the superconductivity. Moreover, it has been found that the incommensurate CDW (ICCDW) transition is suppressed in all the intercalated samples.

The band calculation using WIEN2k has revealed that the density of states at the Fermi level decreases and increases with increasing x in 1T-$Li_x(C_2H_8N_2)_yTaS_2$ and 2H-$Li_x(C_2H_8N_2)_yTaS_2$, respectively.

It has been concluded that both the electron doping due to intercalated Li and the structural disorder due to intercalated EDA suppresses the CCDW and ICCDW transitions, leading to the appearance of superconductivity. Moreover, it has been concluded that T_c roughly increases in correspondence to the increase of the density of states at the Fermi level.

[1] R. A. Klemm, Physica C **514**, 86 (2015).

Keywords: superconductivity, intercalation, transition metal dichalcogenides, lithium

PCP2-3

Effect of non-magnetic rare earth substitution for Zr on mixed anion $Zr(P,Se)_2$ superconductors

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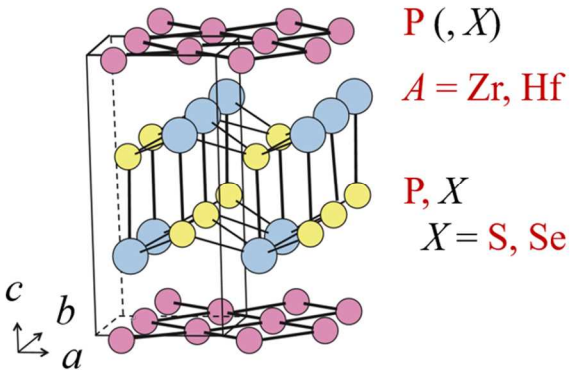
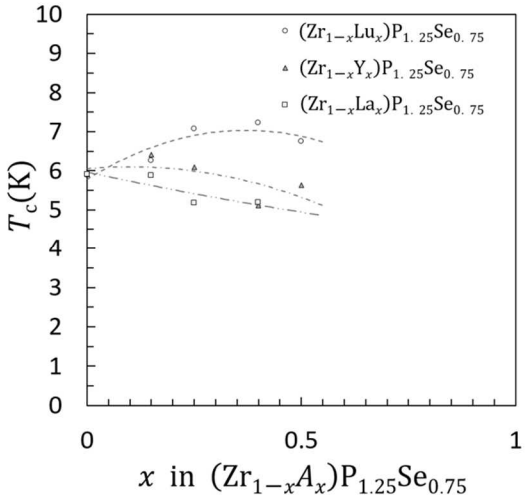
We have reported various physical properties [1] and single crystal growth [2] concerning the group of APX (A = Zr, Hf; X = S, Se) superconductors (Fig. 1) with PbFCl type crystal structure (space group $p4/nmm$) including Zr - P - Se superconductors (the superconducting transition temperature (T_c) ~ 6.3 K). These compounds are layered structures as seen in cuprates and iron-based superconductors. Furthermore, T_c depends on an elemental substitution quantity. Thus T_c is likely to rise even further.
For increasing T_c, we investigated the substitution effect of Zr atoms of $ZrP_{1.25}Se_{0.75}$ by nonmagnetic rare earth atoms. Figure 2 shows T_c as a function of an amount of substitution x by several rare earth atoms. Clearly, the substitution by Lu atoms gives rise to an enhancement of T_c (T_c reaches to 7.22 K when $x \sim 0.4$ and decreases with further substitution). In addition, the lattice constants are proportional to an amount of the substitution as Vegard's law. In the presentation, we report the details and implications of these results [3].

[1] H.Kitô *et al.* : J.Phys.Soc.Jpn. 83 (2014) 074713.
[2] H.Kitô *et al.* : The Physical Society of Japan(Fall 2014 meeting) 9aPS-13.
[3] K. Iwakiri : Tokyo Univ. of Science Graduation thesis(2016)





Keywords: Mixed anion superconductor, APX (A = Zr, Hf; X = S, Se), substitution effect

PCP2-4

Single Crystal growth of mixed anion Zr(P, Se)$_2$ superconductor and related materials

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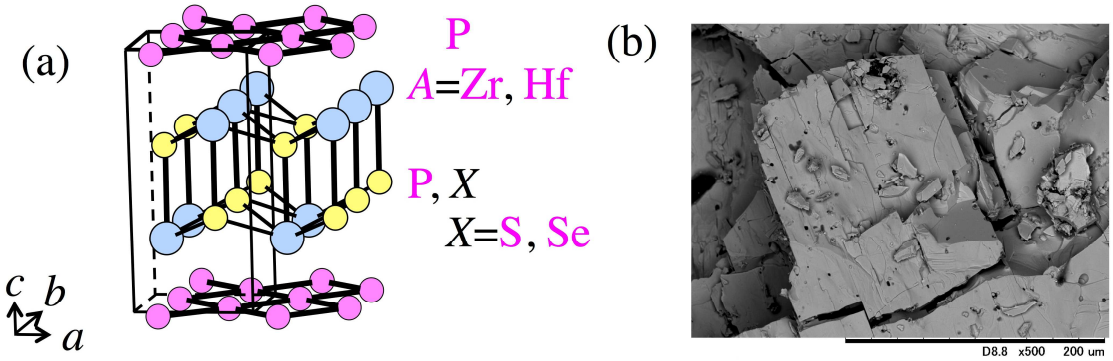
A new method to grow single crystals of PbFCl-type mixed anion $AP_{2-x}X_x$ (A=Zr, Hf, X=S, Se) superconductor [1] are examined. Using a wedge-type, cubic-anvil, high- pressure apparatus, single crystals of $ZrP_{1.25}Se_{0.75}$ (A=Zr, X=Se) were grain grown from nominal composition melts under a pressure of 2.0 GPa. Plate-like obtained single crystal with approximate edge sizes of 200×200×10 micron^3 was measured on electron probe microanalysis and X-ray diffraction indicate that the as-grown boules are a single phase $ZrP_{1.25}Se_{0.75}$. Superconducting transition temperature (T_c) is 6.31 K for $ZrP_{1.25}Se_{0.75}$ single crystal. Single crystal growth of the substitution of non-magnetic rare earth ions for A (A=Zr) site were from the nominal composition $(Zr_{0.60}Lu_{0.40})PSe$ also successful and T_c is reached at 7.50 K for these single crystals [2]. In the presentation, we will also discuss the crystal growth of these compounds.

[1] H. Kitô *et al.* J. Phys. Soc. Jpn. 83 (2014) 074713.
[2] H. Kitô *et al.*, private communication.



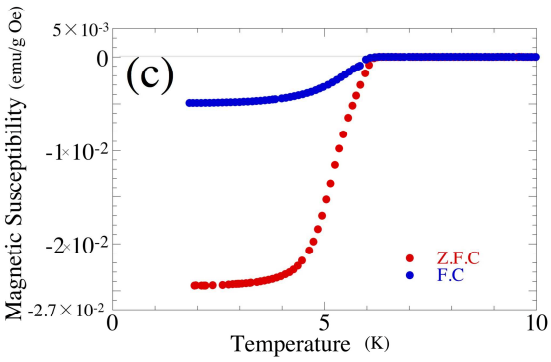


Fig.(a) The crystal structure for PbFCl-type $AP_{2-x}X_x$ (A=Zr, Hf; X=S, Se).
Fig.(b) SEM image of the obtained typical $AP_{2-x}X_x$ (A=Zr, X=Se) crystal
Fig.(c) The temperature dependence of the magnetic susceptibility under H=20 Oe for the obtained typical $AP_{2-x}X_x$ (A=Zr, X=Se) crystal.

Keywords: Single crystal Growth, Mixed anion superconductor, AP2-xXx (A=Zr, Hf; X=S, Se)

PCP2-5

Synthesis and Superconductivity of a Strontium Digermanide $SrGe_{2-\delta}$ with $ThSi_2$ Structure

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We have succeeded in crystallizing a new strontium digermanide (SrGe2-δ) with the ThSi2-type structure (tetragonal $SrGe_2$) [1], which is theoretically predicted to compete with the EuGe2-type one (trigonal SrGe2) under pressure [2]. The tetragonal SrGe2 appeared as a metastable phase in samples at approximately 900°C under a pressure of 2 GPa. X-ray diffraction studies show that the tetragonal SrGe2 is formed by the reaction between trigonal SrGe2 and excess Sr. The composition of the tetragonal SrGe2 was analyzed to be $SrGe_{1.66(4)}$. Lattice parameters for the tetragonal SrGe2 are determined to be a = 4.559(4) Å and c = 14.42(1) Å. The tetragonal SrGe2 shows metallic resistivity behavior and exhibits superconductivity with a critical temperature (T_c) of 7.3 K, which is the highest among compounds with the ThSi2-type structure. Superconducting properties of the tetragonal SrGe2, such as the upper critical field, and the effect of pressure on T_c, are presented and superconductivity is discussed on the basis of electronic band structure calculations.

[1] A. Iyo, I. Hase, K. Kawashima, S. Ishida, H. Kito, N. Takeshita, K. Oka, H. Fujihisa, Y. Gotoh, Y. Yoshida and H. Eisaki, Inorg. Chem. **56** (2017) 8590.
[2] J. T. Wang, C. Chen and Y. Kawazoe, Phys. Rev. B **91** (2015) 054107.

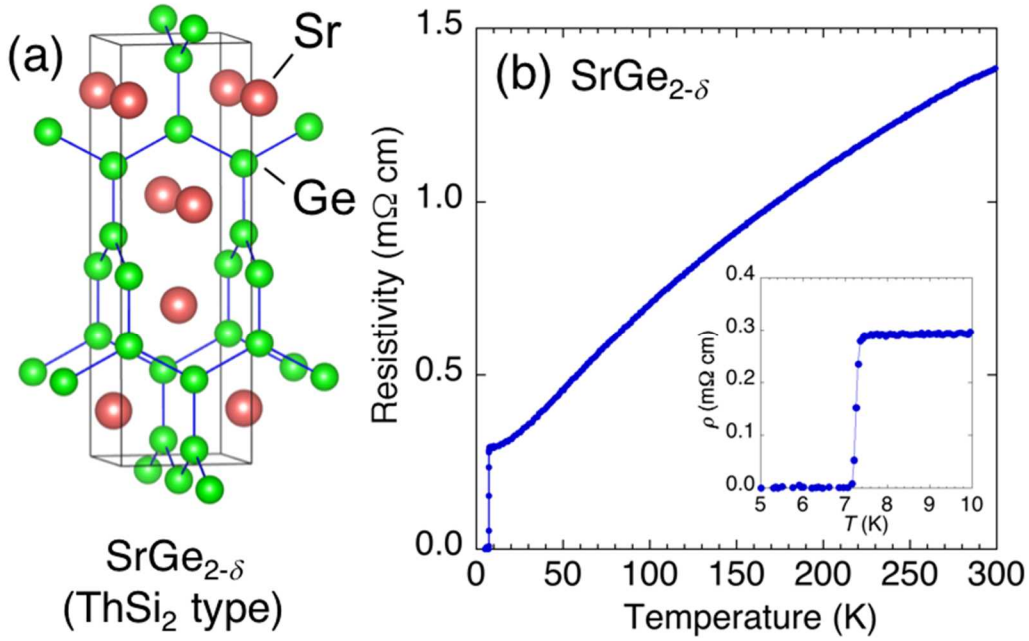

Fig. (a) Crystal structure and (b) temperature dependence of resistivity for a new strontium digermanide (SrGe2-δ)

Keywords: New superconductor, ThSi2-type structure, High-pressure synthesis, Band structure calculations

PCP2-6

Electronic Structure of Novel Binary Superconductor $SrGe_2$: A First-principle study

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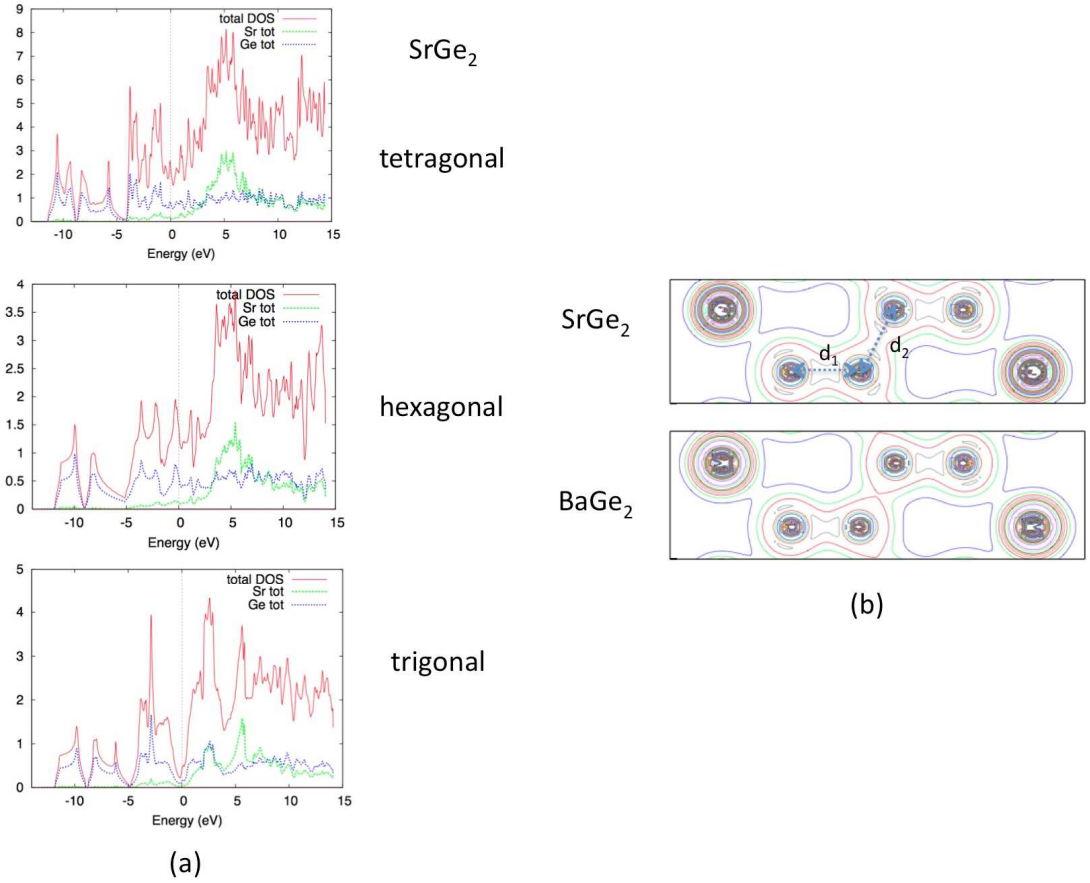
Due to the simplicity of its composition, many binary superconductors have been developed so far. Some are practically used like Nb_3Ge, and others have high T_c like MgB_2 or single layer FeSe. Recently we discovered that tetragonal $SrGe_{2-x}$ shows superconductivity by high pressure synthesis[1]. This compound attracts our attention because it has the highest T_c among AGe_2 series (A: alkaline-earth or rare-earth element).

In this paper we investigated the electronic structure of $SrGe_2$ from first principles. There are several polymorphs of $SrGe_2$, and the obtained density of states at the Fermi level (=$D(E_F)$) per $SrGe_2$ is 5.5, 20.3, 16.3 Ry^{-1} for trigonal, hexagonal and tetragonal structure, respectively. $D(E_F)$ of tetragonal $SrGe_2$ is not more than the isostructural and isovalent compound $BaGe_2$, which has lower T_c than $SrGe_2$. Electron density map suggests that the valence electrons in $SrGe_2$ form a three-dimensional network, while in $BaGe_2$ they form a dimer.

[1] A. Iyo *et al.* Inorg. Chem. **56** (2017) 8590.



Keywords: binary superconductor, electronic structure, SrGe2, ThSi2-type structure

PCP2-7

The electrical resistance of gold-capped chromium thin films

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From the point of view not only of pure research but also of applied and practical one, there are many examples of superconducting thin films. But almost all of them were those in which superconductivity disappears when the film thickness is made thin. It is likely to make a superconducting electron pair when it becomes thinner than the mean free path of electrons. On the other hand, Schmidt et al. reported that thin films of chromium (Cr) metal suppress the antiferromagnetic ordering and become superconductive at T_C ~1.5 K (P. H. Schmidt et al., Physics Letters, **41A**, 367 (1972)). Taking account that the bulk Cr is an antiferromagnet below T_N = 311 K and does not show superconductivity, the relationship between film thickness and existence of superconductivity of Cr is opposite to the other examples of superconducting thin films. Recently, we have studied the electrical resistance of Cr thin films (M.Ohashi et al., Physics Letters, A, **380**, 3133 (2016)), and found a sudden decrease in resistance at T_C = 1.5K. However, the electric resistivity did not drop to zero below T_C and the resistivity drop ratio was very small in all film. Talking account that aluminum wires were bonded as electrodes on the film plane because chromium oxide layer is uncongenial to the gold wires, such behavior may come from superconductivity of aluminum wires. In the present work, we prepared polycrystalline Cr thin films capped by gold layer in order to prevent the oxidation. Several thickness polycrystalline Cr thin films were deposited on silicon substrate using ion beam sputtering. The gold layer were deposited 5nm on Cr film surface. Gold wires were bonded as electrodes on the film plane. The electrical resistance was measured using the Quantum-Design PPMS between 0.5 and 350K. The X-ray measurement was performed using Rigaku SmartLab. The details of the results will be reported in the presentation.

Keywords: Cr film, Electric resistivity, Superconductivity

PCP2-8

Diamond Anvil Cell with Boron-doped Diamond Electrodes and Undoped Diamond Insulating Layer

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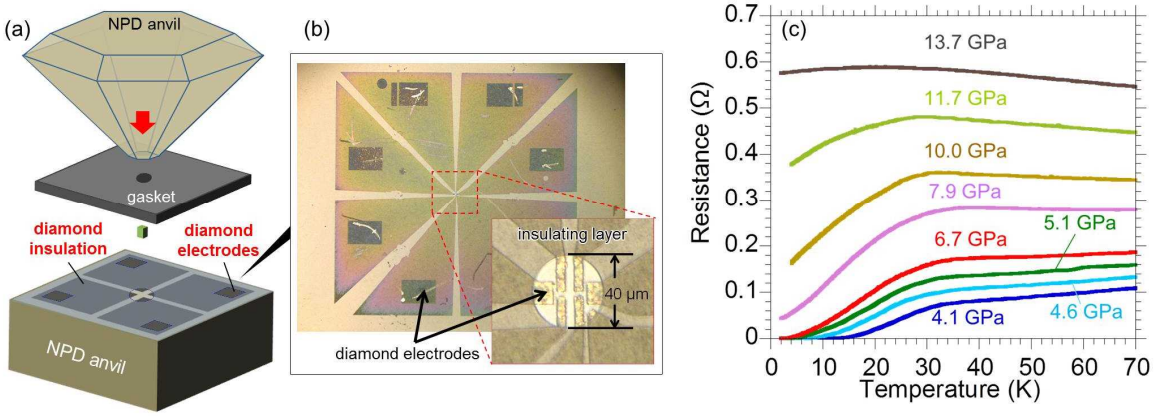
NIT, Yonago College[4]

The great discovery of 200 K superconductivity in H_3S under 150 GPa has recently reported by resistivity measurements using a diamond anvil cell (DAC) [1]. It is interesting that if we can measure the resistivity under extremely higher pressure above 300 GPa, superconductivity at room temperature in hydrogen could be observed [2]. However, resistivity measurement using DAC is difficult because it requires the small sample sizes (< 100 μm) and the hard electrodes. Moreover, an insulating layer should be inserted between the electrodes and a metal gasket which is also broken by applying pressure. In this study, we focused on the boron-doped metallic diamond [3,4] and undoped diamond as a very hard electrode and an insulating layer, respectively. The diamond electrodes and insulating layer have been designed on the bottom diamond anvil as presented in Fig (a). As shown in Fig (b), the resistivity measurements of single crystal FeSe have been demonstrated using the developed device under various pressures, and then the pressure effect for T_c was clearly observed.

[1] A. P. Drozdov et al., *Nature* **525**, 73(2015).
[2] N. W. Ashcroft, *Phys. Rev. Lett.* **21**, 1748 (1968).
[3] R. Matsumoto et al., *Rev. Sci. Instrum.* **87**, 076103 (2016).
[4] R. Matsumoto et al., *Jpn. J. Appl. Phys.* **56**, 05FC01 (2017).



Keywords: Diamond anvil cell, High pressure