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Hydrostatic pressure effects on severely-strained Nb

Masaki MITO[1,*], Takayuki TAJIRI[2], Terukazu NISHIZAKI[3], Kaveh EDALATI[4,5], and Zenji HORITA[4,5]

[1] Graduate School of Engineering, Kyushu Institute of Technology, Kitakyushu 804-8550, Japan
[2] Faculty of Science, Fukuoka University, Fukuoka 814-0180, Japan
[3] Department of Electrical Engineering, Kyushu Sangyo University, Fukuoka 813-8503, Japan
[4] Department of Materials Science and Engineering, Faculty of Engineering, Kyushu University, Fukuoka 819-0395, Japan
[5] International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Fukuoka 819-0395, Japan

We investigated the effects of hydrostatic pressure (HP) on the crystal structure of severely strained Nb samples, in which severe plastic deformation by high-pressure torsion (HPT) treatment brought about strain at the unit-cell level as well as reduction in the grain size. The HP effects on non-strained Nb have already been investigated in the pressure regime over 100 GPa by Struzhkin *et al*. [Phys. Rev. Lett. **79**, 4262 (1997)], and T_c reportedly exhibited an increase from 9.2 to 9.9 K at approximately 10 GPa. In the present study, the pressure scale of the pressure response observed by Struzhkin *et al*. was reduced down to approximately one-fifth at maximum: In a Nb sample subjected to HPT (6 GPa, 10 revolutions), T_c exceeds 9.9 K at HP of approximately 2 GPa. We observed pronounced anisotropic change of the unit cell there. According to our first-principle calculations, the reduction in structural symmetry affords an increase in the density of states at the Fermi energy, thereby yielding a prominent increase in T_c at low pressures.

1 Introduction

In the periodic table, twenty-nine elements exhibit superconductivity at ambient pressure. Among them, eleven elements show the increase in the superconducting transition temperature T_c at high pressures [1]. The study on superconductivity of pure single elements has no more room for meaningful progress. For instance, the highest T_c of single element superconductors at ambient pressure is 9.20 K for Nb, and it exhibits the maximum value of 9.90 K at around P = 10 GPa [2].

Recently, it has been observed that enormous residual strain sometimes plays a positive role in stabilizing superconductivity, as observed in Nb [3], NbTi [4], and Re [5]. We expect any positive influence of residual strain stored in materials from the perspective of desiring high T_c under pressures. Indeed, in the severely strained Nb, we observed T_c of more than 9.90 K at around 2 GPa as seen in Fig.1. Now, the investigation on the crystal structure as a function of pressure is desirable in order to understand quite sensitive pressure response.

2 Experiment

High-purity (99.9\%) Nb discs were subjected to HPT processing at room temperature under a pressure of P = 6 GPa and revolutions of N = 0, 1, 2, 5, 10, and 20 [6, 7]. For N < 2, dislocations are stored, and the grain size largely changes [8]. The small-angle grain boundaries formed in these cases gradually transform to large-angle grain boundaries with increasing N. On the other hand, for $N \geq 2$, only the large-angle grain-boundaries are present, and the grain size hardly changes with further increase in N.

Further, at ambient pressure, T_c for AR is approximately 9.25 K, and T_c exhibits a maximum of approximately 9.37 K at N = 2. In addition, T_c remains unchanged at 9.35 K for N > 10 [3].

We performed X-ray diffraction (XRD) analyses under high pressure of up to P = 5.1 GPa at room temperature using a synchrotron radiation XRD system with a cylindrical imaging plate at the Photon Factory at the Institute of Materials Structure Science, High Energy Accelerator Research Organization [9].

The energy of the incident X-rays was 16 keV. Pressure was applied using a DAC that consisted of two diamond anvils with flat tips having a diameter of 0.8 mm and a 0.3-mm-thick CuBe gasket. The small pieces of HPT-Nb were placed in a randomly oriented manner in a sample cavity with a diameter of 0.4 mm along with a ruby of manometer and transparent pressure-transmitting-mediums (PTMs) such as fluorinated oil (FC77, Sumitomo 3M Ltd.) or MEW.

All the atomic positions in the unit cell are special positions, and therefore, the structural parameters were evaluated with the use of the diffraction peak angle and full-width at half-maximum (FWHM) values.

3 Results and Discussion

Prior to the experiments on hydrostatic pressure, we mention the crystal structure in the unit cell level for the targeted samples. The position of the diffraction peak of the (110) plane slightly shifts toward high angle sides with increasing the revolution number N in the turn as-received (AR) → N = 1 →2 → 5. However, between N = 5 and 10, there occurs the sudden shift toward low angle side. We assumed the reduction of structural symmetry such as the change from cubic to orthorhombic between N = 5 and 10.

Indeed, as seen in Fig. 2, each lattice parameter in orthorhombic system exhibits independent pressure dependence each other. At around P = 2 GPa, the elongation along *b*- and *c*-axes suggesting prominent structural deformation occurs. According to our first-principle calculations, the reduction in structural symmetry affords an increase in the density of states at the Fermi energy, thereby yielding a prominent increase in T_c at low pressures.

Thus, we can control T_c positively by realizing any quasi-stable structure, which would be realized by both large shear strain and hydrostatic pressure. The first-principle calculations suggest that the reduction in structural symmetry affords an increase in the density of states at the Fermi energy.

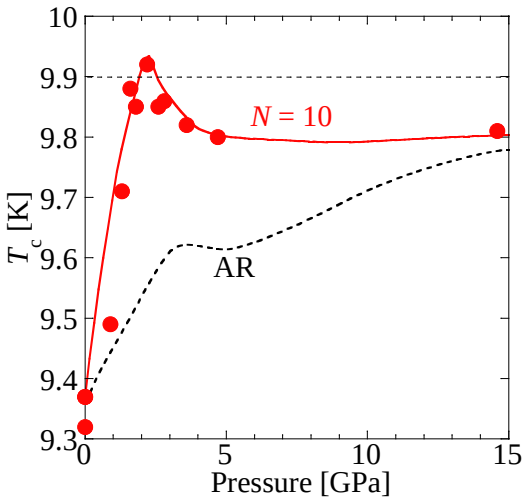

Fig. 1: Pressure dependence of superconducting transition temperature T_c for HPT-Nb with N = 10. Here, the Apiezon-J oil was used as the PTM. For reference, the guide curve corresponding to $T_c(P)$ of the sample AR using the Apiezon-J oil as PTM is also presented.

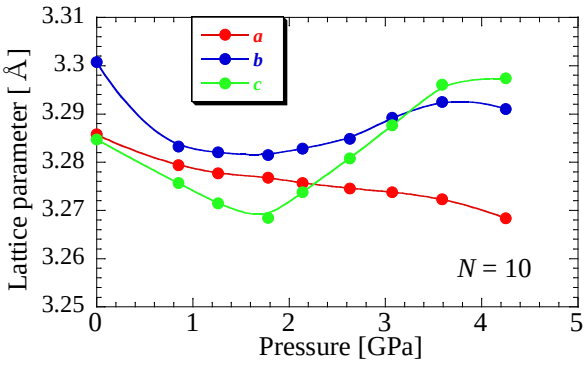

Fig. 2: Pressure dependence of lattice constants in orthorhombic system for HPT-Nb with N = 10.

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*mitoh@mns.kyutech.ac.jp