High pressure transport and structural studies on Nb₃Ga superconductor

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Abstract

The crystal structure of A-15 superconductor Nb₃Ga with a critical temperature $T_c = 16.5$ K has been investigated by high pressure x-ray diffraction (HPXRD) using synchrotron x-rays and a diamond anvil cell under Ne pressure medium. The high pressure structural results indicate that Nb₃Ga is stable up to 41 GPa. The P-V plot shows an anomaly around 15 GPa even though there are no pressure induced structural transitions are observed. High pressure resistance measurements were performed up to 0.5 GPa to understand the variation of T_c under pressure. Our results show a positive pressure effect on T_c .

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1. Introduction

Nb_3Ga belongs to the A-15 family of superconductors, which has gained importance in recent years, due to their rising technological value from combination of the excellent performance with the good mechanical properties [1]. A-15 superconductors have relatively high transition temperature type I materials, also exhibit high critical current density and critical magnetic field values, which make these compounds for some viable applications [2]. Some of A-15 compounds with high critical temperatures are V_3Si ($T_c = 17$ K) [3], Nb_3Al ($T_c = 19$ K) [4], and Nb_3Sn ($T_c = 18$ K) [5]. Nb_3Ga has a transition temperature as high as 20.7 K [6] and used for commercial applications as superconducting wires. The T_c in this system is highly dependent on the stoichiometric ratio of the niobium and gallium. The phase diagram of Nb_3Ga suggests that the A-15 structure with the highest critical temperature and the highest critical magnetic field can be achieved by synthesizing the sample at 1750°C [7].

Nb_3Ga has a cubic β -W type crystal structure with space group $Pm-3n$ (space group no. 223) shown in Fig.1. It forms a body-centered cubic (BCC) lattice with gallium atoms in the center of the cube. In β -W phase, the Nb atoms form three mutually orthogonal chains that lie parallel to the edges of the unit cell [8]. Very short A-A nearest-neighbor distances consequently result in anisotropy along the chains in these materials. For compounds with electronically different A and X atoms, long-range order becomes an important factor governing many physical properties [9]. It is believed that the squeezing of the A atom chains improves the electron-phonon interactions from anisotropic density of states, which is obtained from the re-arrangement of the atoms in the crystal symmetry [10].

It has been further suggested that for niobium based A-15 compounds the microscopic parameters that imply to the superconducting properties of the material follow a tendency expressed by the electronic parameter, which is proportional to the density of states $N(E_f)$ [11]. Application pressure could change the $N(E_f)$ and thereby the electrical properties. Additionally, some of the vanadium and niobium based materials manifest anomalies in their electrical, magnetic, and structural properties. Those anomalies were observed to have strong temperature dependence. Cubic to

tetragonal transformation were observed in V_3Si and Nb_3Sn and however other compositions such as V_3Ge and Nb_3Al did not show such transformations indicating no general sequence [12]. Even though there are high pressure transport measurements available for these compounds crystal structure investigations are still elusive. Recently Yu *et al.* [13] have reported their high pressure results on Nb_3Al . This material shows an anomaly at high pressures around 15 GPa. The motivation for our research emerged from the interest in studying the pressure-induced anomalies of these Nb based A15 superconductors. We have investigated the structural behavior and phase stability of Nb_3Ga , as well as studied the electrical properties under high pressure in a piston type cell in order to shed more light on the high pressure behavior.

2. Experiment

High purity powders of niobium and gallium were mixed with a 3:1 atomic weight percentage and compacted into a pellet. The pellet was then arc melted in an Ar atmosphere. The synthesized samples were characterized using a Bruker Discover x-ray diffractometer operating with Cu k-alpha1 radiation ($1.5418 \text{ \AA}$) with Ni filter. The T_c measurements were performed using a Cryomech closed cycle refrigerator capable of reaching temperatures as low as 6 K. For high pressure low temperature resistivity measurements a piston-cylinder type Cu-Be type cell was mounted to the closed cycle refrigerator. The sample was loaded in the four probe configuration [14] into a teflon chamber of the cell with Daphne oil pressure medium and a ruby chip. The pressures were measured by the ruby fluorescence technique. The resistivity data was collected up to 0.5 GPa.

High pressure x-ray diffraction experiments were performed at Sector 16-IDB of the HPCAT - Advanced Photon Source (APS) - using a symmetric type diamond-anvil cell (DAC) with an incident monochromatic wavelength of $0.40662 \text{ \AA}$. Samples were loaded in a $100 \text{ }\mu\text{m}$ diameter hole of a $40 \text{ }\mu\text{m}$ -thick rhenium gasket in the DAC with diamond-culet sizes of $300 \text{ }\mu\text{m}$. Pressure was determined using the ruby fluorescence technique and Ne was used as pressure-transmitting medium. The monochromatic x-ray beam was focused down to $20 \times 20 \text{ }\mu\text{m}^2$ using Kickpatrick-Baez mirrors. The images

were collected using a MAR345 image plate. They were integrated and corrected for distortions using FIT2D software. The typical exposure time for each spectrum was 20s. The structural analysis was performed using JADE and RIETICA (LHPM) Rietveld packages.

3. Results and discussions

The pressure dependence of T_c was measured at three pressures up to 0.5 GPa and is shown in Fig. 2. The T_c at ambient pressure for the sample was measured to be 16.5 K. On application of pressure the T_c increases as a function of pressure as shown in the inset. The increase in T_c observed in Nb_3Ga is similar to other A15 type compounds. Recently Tanaka *et al.*, [15] have reported the effect of pressure on Nb_3Sn and V_3Si and as a function of pressure up to 4 GPa. The T_c is found to increase up to 4 GPa and becomes insensitive to application of pressure under further compression.

The T_c was suppressed above 9 GPa for Nb_3Al with an increase in transition width. They have speculated that the suppression of superconducting transition in Nb_3Sn is due to a martensitic transition. A similar isostructural material Zr_3Al [16] also exhibits such a martensitic transition on application of pressure. However our high pressure structural studies performed followed by the T_c measurements for Nb_3Ga did not show any evidence for structural transitions below 10 GPa. The HPXRD patterns are shown in Fig.3 for representative pressures.

The absence of any major changes and splitting of the peaks in the XRD patterns obtained indicate that there is no structural phase transition up to the highest pressure studied. The indexing was done by JADE7 program, with space group $Pm-3n$ for the whole pressure range, since phase changes were not observed. After refining, the lattice constant was found to be 5.1673 (4) (1) Å at ambient pressure. The lattice constant, along with the Wyckoff positions for β -W phase were used to model the crystal structure of Nb_3Ga . The Rietveld refinement for the XRD pattern at 1.1 and 41 GPa is shown in Fig. 3. The atomic positions remain unchanged for both Ga and Nb under pressure. The lattice constants are provided at 1.1 GPa and 41 GPa in Table 1. The P-V data was plotted and shown in Fig.4.

As seen in the P-V data we have observed an anomaly around 15 GPa very similar to Nb₃Al [13]. In the pressure range between 15 and 19 GPa, where the volume anomaly takes place, the volume is observed to change by only 0.5%. This suggests that the transition is second order and is not accompanied by significant volume collapse. The B_0 and B_0' were derived by fitting the P-V data to a Birch-Murnaghan 2nd order equation of state (EOS) [17]. The bulk modulus was determined by separately fitting the data points at low pressure and high pressure regions. The fitting for the low pressure region yielded the bulk modulus and the derivative $B_0 = 198$ (7) GPa, $B_0' = 5$ while the results for high pressure region gave $V_0 = 139.0$ (0.4) Å³, $B_0 = 217$ (3) GPa, $B_0' = 5$. The chi-square values obtained were 0.12 and 0.95 for LP and HP phases respectively. The values obtained are consistent with Nb₃Al [13]. Recently Rajagopalan, studied the electronic properties of Nb₃Al by all electron full potential linear augmented plane wave method (FP-LAPW) [18] to understand the compressibility anomaly. The discontinuity in compressibility of this intermetallic compound was explained by the movement of the 'd' like band of niobium. They reported a rise in the band from 12 GPa, up to the Fermi level at 17 GPa, then a downward trend under pressures higher than 17 GPa. Isostructural transitions were, also, observed in a similar binary alloy Pd₃Fe [19]. For Pd₃Fe, the change in bulk modulus is accompanied by a collapse in the magnetic moment of iron. Garg et al. have investigated the compressibility behavior of similar A15 type Co₂FeSi and Ni₂MnGa [20]. They have observed a normal P-V variation for Ni₂MnGa, whereas for Co₂FeSi the pressure dependence of volume becomes linear past 5 GPa. It was concluded that negative electronic or lattice Gruneisen parameter may attribute to the results, since in strongly correlated electron systems the negative γ can have an effect on enhancing the compressibility anomalies. In order to shed more light further high pressure structural studies are required for A15 type materials. In conclusion, we have investigated the T_c of Nb₃Ga as a function of hydrostatic pressures up to 0.5 GPa using the four probe resistivity technique in a piston cylinder cell. Application of pressure enhances the onset transition from 16.5 K to 17.2 K. High pressure XRD measurements were performed to study the structural stability up to 41 GPa. The results revealed a pressure-induced isostructural transition.

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Fig.1. A15 crystal structure of Nb₃Ga. Green spheres represent Ga atoms, purple spheres are Nb atoms. The Nb atoms are located at 6c (0.25, 0, 0.5) and Ga at 2a (0, 0, 0) positions.

Fig.2. High pressure resistivity measurements for Nb₃Ga. The inset shows the pressure dependence of T_c .

Fig.3. X-ray diffraction patterns collected at various pressures for Nb₃Ga. The Rietveld refinement plots are shown at 1.1 GPa and 41 GPa. The markers, simulated pattern and the difference and phase markers are shown.

Fig.4. P-V plot for Nb₃Ga. The shaded region shows the pressure range where the compressibility anomaly is observed. The error bars are smaller than the symbols.

Pressure (GPa)	a (Å)	Volume (Å³)	R_p	R_{wp}	χ^2
1.1	5.1673 (4)	137.97(1)	1.4	2.8	3.9
41	4.9284 (7)	119.86(4)	1.5	3.1	4.4

Table 1. Structural parameters obtained at two different pressures for Nb₃Ga from the refinement.