Structural study under high pressure and low temperature of HTSC compound $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.10}$

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Introduction

For HTSC copper oxides, and particularly for $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8+x}$ (Hg,Tl-1223) [1], three structural anomalies have been observed previously: T_0~T_c+15 K, T_1~150-160 K and T_2~240-250 K (Fig. 1). External pressure leads to increase of temperature of superconductivity T_c of HTSC compounds, underdoped or nearly optimally doped by charge carriers, because of both intrinsic pressure induced structural change and increase of charge carriers concentration in superconducting CuO_2-planes due to charge transfer [2]. To investigate an influence of these factors on structural anomalies and to obtain more information about their origin the structural study of Hg,Tl-1223 at high pressure and low temperature has been undertaken.

Experiments and Results

The diamond anvil cell was used as a high-pressure cell, low temperature measurements were performed using helium cryostat. The imaging plate (R-AXIS IV, 0.10 mm resolution, 300×300mm area size) was used as the x-ray diffraction detector, λ=0.4959 . The exposure time of each measurement was 1-2 min. The measurements at room temperature have been performed at P= 1, 3, 12, 15, 20, 35 GPa. At P= 1, 20 and 35 GPa the measurements have been performed in the range 100-300 K with 5K step at cooling. GSAS program [3] was used for calculation of structural parameters, obtained discrepancy indexes were following: wR_p~3÷5%, R_p~3÷4%, χ^2~3-5.

a-parameter as function of temperature at P=1 and 20 GPa is shown in Fig 1 (the behavior of ***c***-parameter and lattice volume is the same), ***a*** and ***c*** as function of pressure at room temperature in whole are similar with literature data [4,5]. The atomic coordinates for P= 1 and 20 GPa almost does not change at temperature decrease.

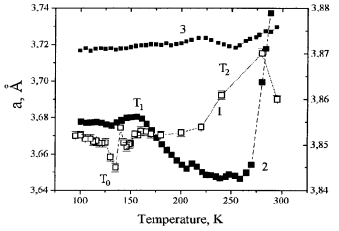

Figure 1. Temperature dependence of the unit cell parameter of Hg,Tl-1223 (x=0.1) at ambient pressure (1, right axe) [1], 1 GPa (2) and 20 GPa (3).

The BaO-layer is situated between Hg,Tl-O and CuO_2-planes and its splitting is controlled by difference of electric charge in surrounding plans. We calculated this splitting as $\Delta=c^*(z_{Ba}-z_{O3})$. This parameter almost has not a change by temperature, so we can conclude that the charge transfer does not occur at temperature decrease.

All structural anomalies are suppressed for P=20 GPa, while for P=1GPa the T_0 anomaly is very weak but still noticeable and its temperature is the same as for ambient pressure. The increase of ***a***-parameter between T_1 and T_2 is more surprised fact we observe. Together with very small splitting of CuO_2-planes for P=1 GPa it means that external pressure suppress the formation of stripes and leads to change of polarizability of the material, which cause a negative thermal expansion.

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X-Ray Diffraction Measurement of Pressure-Induced Transformations of Boron Hydride

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Boron hydrides (boranes) have molecular structures where hydrogen atoms terminate or bridge boron frameworks with B-H and B-H-B bonds. In our previous work for decaborane ($B_{10}H_{14}$), which is a molecular crystal at ambient condition, high-pressure Raman scattering and infrared absorption spectroscopy indicated that $B_{10}H_{14}$ molecule changed into another molecular structure at 50 GPa and then into a non-molecular phase at 100 GPa [1]. However, no information has been obtained about the structural changes of the crystal unit, which might be accompanied by a change of the molecular structure. In the present study, we performed *in situ* XRD measurement to explore the crystal structure.

Decaborane crystals (Wako Pure Chemicals Industries, Ltd.) were loaded into a diamond-anvil cell (DAC) without a pressure medium. *In situ* XRD experiments were carried out at the BL10XU beamline. In order to collect all of the weak diffracted x-rays, a plate of diamond single crystal was used as a sheet for the diamond-anvil instead of a tungsten carbide hemisphere with a slit.

The XRD peaks observed at 1.2 GPa were indexed with a monoclinic structure, which is same with decaborane at ambient condition [2]. With increasing pressure, the x-ray peaks were continuously weakened and shifted without a drastic change (Fig.1). It suggests that the unit cell gradually collapses under compression independent of the structural change of the molecule inferred from the Raman measurement at 50 GPa, and that decaborane finally transforms into an amorphous-like phase.

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[2] A. Tippe et al., Inorg. Chem., 8, 464 (1969).

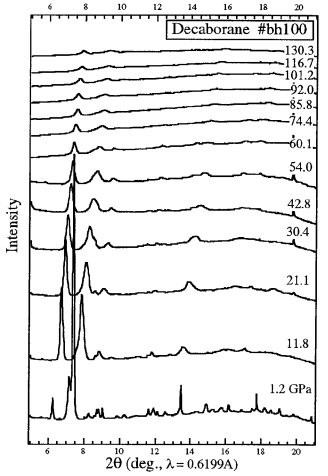

Fig.1. XRD patterns of decaborane obtained under compression.