Pressure-Enhanced Lattice Transformation in Nb_3Sn Single Crystal*

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We report the first observation of pressure-enhanced lattice transformation in the high-temperature superconductor Nb_3Sn. The opposite pressure effects on the lattice transformation and the superconducting transition in A15 compounds can thus be understood on the basis of the Weger-Labbé-Friedel model by taking into account the pressure-induced interband charge transfer.

Many high-temperature superconductors exhibit a lattice transformation from cubic to tetragonal symmetry at temperature T_L above their superconducting transition temperature T_C. This concurrence of lattice transformation and high-temperature superconductivity has stimulated extensive investigations, both experimental and theoretical, on the two phenomena.[1] Hydrostatic pressure studies were recently made on T_L and T_C of near equiatomic V-Ru,[2] $(Hf_{1-x}Zr_x)V_2$,[3] and V_3Si[4] compounds. Without exception, T_L always decreases while T_C increases with pressure. In view of the negative pressure dependence of T_C in polycrystalline Nb_3Sn,[5] the determination of the pressure behavior of its T_L is particularly important in the understanding of lattice transformation and high-temperature superconductivity. We have determined calorimetrically the pressure dependence of T_L of an Nb_3Sn single crystal up to 18 kbar. For the first time, lattice transformation was observed to be enhanced by the application of hydrostatic pressure in a high-T_C superconductor. T_C was also measured inductively at different pressures. It is suppressed by pressure at the same rate as that previously observed for polycrystalline samples.[5]

An ac temperature-modulation technique[6] was employed to determine the temperature variation of the relative specific heat C_p and the temperature derivative R' of the resistance of the Nb_3Sn single crystal under hydrostatic pressure. It is a combination of the high-pressure clamp technique and an ac calorimetric method. The pressure medium was a fluid mixture of 1:1 n-pentane and isoamyl alcohol. A superconducting lead manometer situated next to the sample was used to measure the pressure at low temperature. The pressure change[7] due to cooling usually is small and was shown to occur mainly at the freezing of the pressure medium. The pressure medium used freezes at ~180 K at atmospheric pressure. Hence the quoted pressure is that determined at low temperature (7 K). The temperature of the sample was determined by a Au plus 0.07% Fe–Chromel thermocouple and/or a Ge thermometer depending on the temperature range.

The Nb_3Sn sample studied was part of the RCA single crystal which was observed[8] to transform at low temperature in the x-ray–diffraction and neutron-scattering experiments. The resistance ratio between 300 and 20 K was 7. The lattice transformation was clearly evidenced by anomalies in C_p, R', and resistance R. At atmospheric pressure, both in the absence and then in the presence of the pressure medium, T_L was found to be ~43 K which is ~2 degrees lower than that previously observed.[8] This may be due to the inhomogeneous nature[9] of the big crystal from which our small sample was cut. In Fig. 1, the temperature dependence of the relative C_p is shown at several pressures. The numbers underlined represent the sequential order of the experimental runs and the others stand for the pressure in kilobars. The arrow bars define the width of the lattice transformation, which varies from a few tenths of a degree at low pressure to about one degree at 18.3 kbar. Over the same temperature region, R exhibits a drop which gives rise to a large peak in R' corresponding to a change of over 100% at atmospheric pressure, as depicted in the inset of Fig. 1. However, at high pressure, e.g., >10 kbar, the R drop becomes sluggish and the R' peak degenerates into a broad jump. T_L defined above was plotted as a function of pressure in Fig. 2. It is enhanced by the application of hydrostatic pressure, linearly with $dT_L/dP = +(2.8 \pm 0.1) \times 10^{-4}$ kbar^{-1} for $P > 5$ kbar but nonlinearly at a higher rate for $P < 5$ kbar, in contrast to $dT_L/dP = -(1.5 \pm 0.1) \times 10^{-4}$ kbar^{-1} for V_3Si for pressures up to 18 kbar.[4] dT_L/dP is estimated to be $+(3.3 \pm 0.3) \times 10^{-4}$ kbar^{-1} as P approaches zero. In the same figure, the pressure dependence of T_c determined

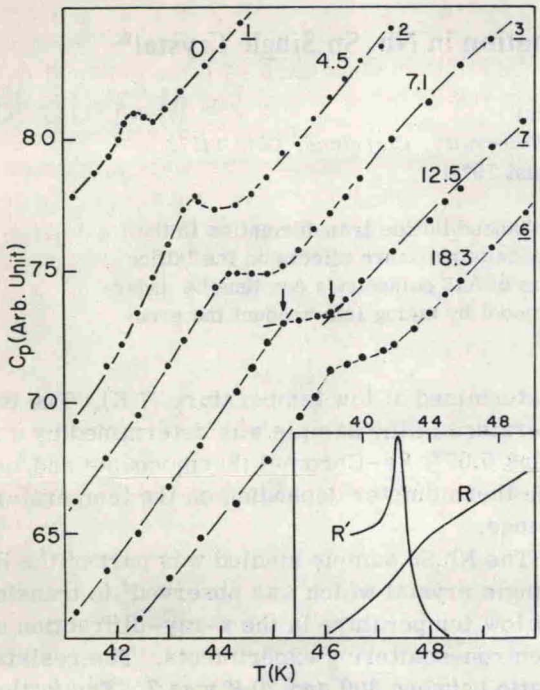

FIG. 1. Temperature dependence of the relative C_p at different pressures for Nb_3Sn single crystal. The inset shows the anomalies of resistance R and resistance slope R' at the T_L and atmospheric pressure.

inductively was shown to be $-(1.40\pm0.05)\times10^{-5}$ kbar^{-1}. This is identical to that recently measured calorimetrically.[10] Hence the T_C data so obtained are characteristic of the tetragonal phase of the sample. $|dT_C/dP|$ is 2–3 times smaller than that for V_3Si.[4]

It has been shown that many of the unusual physical properties at atmospheric pressure of high-T_C A15 compounds, such as Nb_3Sn and V_3Si, could be understood in the framework of the Weger-Labbé-Friedel (WLF) model.[11] According to this model, the band structure exhibits sharp and narrow density-of-states peaks at the d sub-band edges, characteristic of the linear-chain arrangement of the transition-metal atoms in the A15 compounds. The relative position of the Fermi level with respect to the band edge depends on the number of d electrons in the sub-band Q. The Q dependence of both T_L and T_C for cubic Nb_3Sn and V_3Si were calculated by Labbé, Barišić, and Friedel.[12] They found that T_L and T_C, instead of being monotonically varying functions of Q, peak at Q_{LM} and Q_{CM}, respectively, as shown in Fig. 3. T_L drops back to zero when $Q > Q_0$. Because of the larger Q and less localized atomic d orbital for Nb_3Sn, its Q_{LM}/Q_{CM} ratio was found to be >1 in contrast to the case of <1 for V_3Si. In addition, Labbé, Barišić, and Friedel[12] also estimated that $Q_{CM} \simeq Q < Q_{LM}$ for Nb_3Sn while $Q_{CM} > Q \simeq Q_{LM}$ for V_3Si. The application of hydrostatic pressure will undoubtedly bring the linear chains closer together and will thus lead to a redistribution of charges in different bands. Therefore the observed opposite pressure effects on T_L and T_C of Nb_3Sn and V_3Si can easily be understood qualitatively in terms of the WLF model, provided that pressure enhances Q of these compounds and that Q remains in between Q_{LM} and Q_{CM}. Any crossover between Q and Q_{LM} or Q_{CM} will result in a sign change of dT_L/dP or dT_C/dP. In addition, the observed smaller value of $|dT_L/dP|$ for V_3Si can be attributed to the close proximity of Q to Q_{LM}, and that of $|dT_C/dP|$ for Nb_3Sn to the close proximity of Q to Q_{CM}. It should be noted that the experimental T_C results of the transforming samples are for tetra-

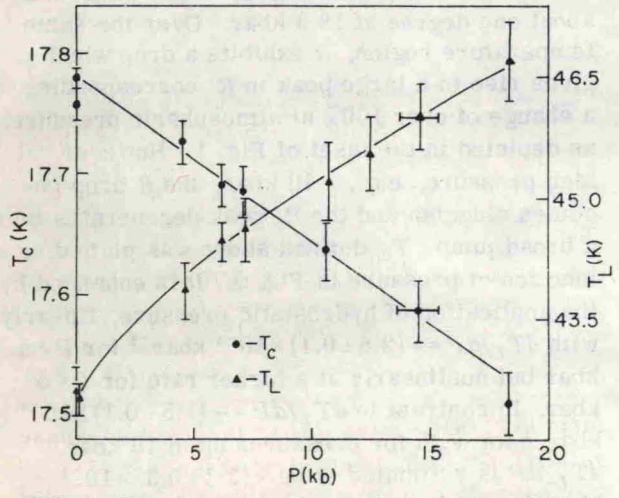

FIG. 2. Pressure dependence of T_L and T_C of Nb_3Sn single crystal.

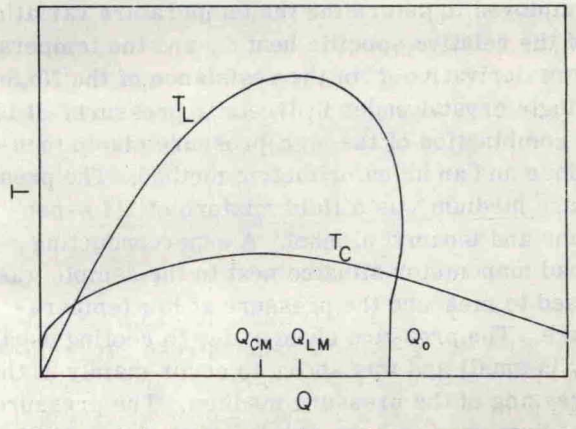

FIG. 3. Schematic variations of T_L and T_C with Q for Nb_3Sn (after Ref. 12).