Direct Observation of Enhanced Lattice Stability in V_3Si under Hydrostatic Pressure

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The lattice transformation temperature T_L of single-crystal V_3Si was directly observed to decrease linearly with hydrostatic pressure at a rate of $-(1.5\pm0.1)\times10^{-4}$ °K bar^{-1}. To explain the pressure dependence of T_L and the elastic behavior, the Labbé-Friedel model must be extended to include interband charge-transfer effects as a new variable, in agreement with a recent calculation of Ting and Ganguly. We give a discussion of these results related to structural instability and superconductivity.

Soft phonon modes have been observed upon cooling in almost all *A*15 compounds with high superconducting transition temperature T_c.[1] For some extreme cases, the phonon mode becomes so soft that a lattice distortion corresponding to a cubic-to-tetragonal lattice transformation results. V_3Si is one such example. Its lattice distorts when the shear mode $C_s=\frac{1}{2}(C_{11}-C_{12})$ decreases to a very small value at a temperature T_L slightly above T_c. T_L is defined as the lattice transformation temperature. By analyzing the elastic properties and the specific heat, Testardi *et al.*[2] predicted a strong, quadratically strain-dependent T_c in cubic V_3Si in agreement with the later thermal-expansion study by Fawcett.[3] It was further suggested that T_c of V_3Si was promoted by the soft phonon mode.[4] However, T_c was found to be enhanced by the application of hydrostatic pressure[5] in contradiction with the above prediction of a quadratically strain-dependent T_c. It was later proposed[1,6] that the effect of hydrostatic pressure on T_c could be related to the hydrostatic effect on T_L. The purpose of this experiment is to examine directly the hydrostatic-pressure effect on lattice instability in transforming V_3Si and the role of soft phonon modes in its high T_c.

Our study of the hydrostatic-pressure effect on T_L of V_3Si was carried out using the newly developed temperature-modulation technique.[7] It is a combination of the high-pressure clamp technique and an ac calorimetric method. This makes possible the determination of the relative specific heat C_p and the temperature slope of resistance $R'=dR/dT$ of a metallic sample under hydrostatic compression. A sample of size 1.2 mm$\times$0.8 mm$\times$5 mm was spark cut from a V_3Si single crystal. The resistance ratio between room temperature and 18 K of the sample investigated was 26. At zero pressure, $T_c=16.7$°K and $T_L=21.6$°K, typical for a transforming V_3Si crystal. Four electrical leads and a Chromel-(Au+0.07% Fe) thermocouple were soldered onto the sample. The temperature of the sample was modulated by an ac voltage fed through a wire heater closely coupled to the sample. By properly adjusting the thermal links between the sample and the heat reservoir (the high-pressure cell for our experiment) and the frequency of the ac heat source, the amplitude of the ac temperature modulation of the sample, ΔT_{ac}, was approximately inversely proportional to the specific heat C_p. ΔT_{ac} was measured by a thermocouple attached to the sample. The ac component of the voltage across the potential leads gave $IR'\Delta T_{ac}$, where I represents the dc current passing through the sample. The self-clamp technique provided the hydrostatic environment in a 1:1 mixture of n-pentane and isoamyl alcohol. The pressure was generated by a press and locked by the clamp at room temperature. The high-pressure clamp was then removed from the press and cooled slowly inside a cryostat. A superconducting-Pb manometer situated next to the sample was used to determine the pressure at low temperature. All electrical leads were brought out from the high-pressure cell with Stycast 2850 FT epoxy seals. The ambient temperature of the sample was measured by a Ge thermometer and/or a Chromel-(Au+0.07% Fe) thermocouple, depending on the temperature range.

In Fig. 1, we show the temperature dependence

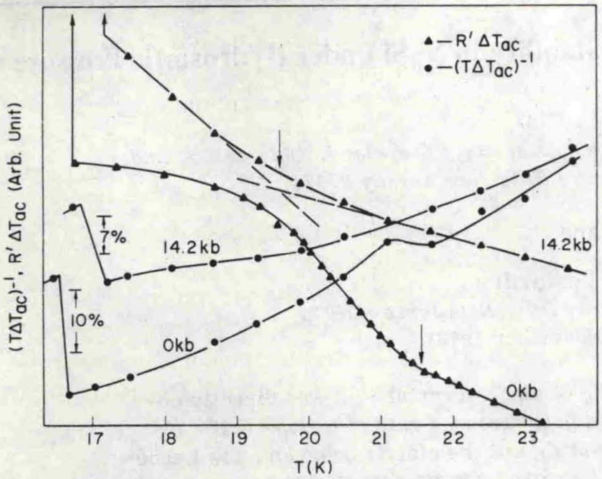

FIG. 1. Temperature dependence of the relative specific heat and the temperature slope of resistance of a V_3Si single crystal at different hydrostatic pressure.

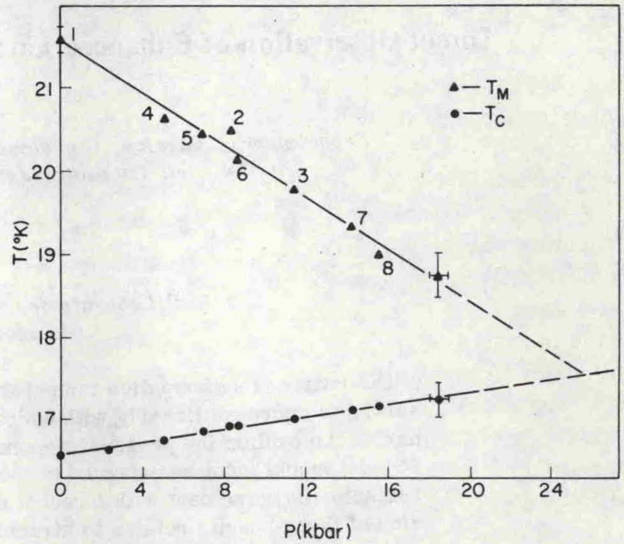

FIG. 2. Pressure dependence of the lattice-transformation temperature T_L and the superconducting transition temperature T_c of a V_3Si single crystal.

of $(T\Delta T_{ac})^{-1} \propto C_p/T$ and $R'\Delta T_{ac}$ of V_3Si at different pressures. The lattice transformation is evidenced by large changes in the slopes of the C_p and R' curves.[8] Under pressure, the lattice transition width increases and the anomaly weakens. We define T_L as the temperature at which the slopes increase drastically, as shown by the arrows in Fig. 1.

The results are summarized in Fig. 2. The number represents the sequential order of the experimental run and the bar denotes the experimental error. T_L decreases linearly with hydrostatic pressure with $dT_L/dP = -(1.5 \pm 0.1)\times 10^{-4}$ °K bar $^{-1}$ up to 18 kbar. We have also determined T_c inductively under hydrostatic compression and found $dT_c/dP = +(3.65 \pm 0.05)\times 10^{-5}$ °K bar^{-1} in excellent agreement with previous studies.[5] By extrapolation as shown in Fig. 2, a critical pressure of 24 kbar was obtained for a complete suppression of lattice transformation in V_3Si down to the superconducting state.

In view of the highly anisotropic nature of V_3Si,[1] it is not surprising at all to find that the hydrostatic-pressure effect on the lattice transformation differs greatly from the uniaxial-pressure effect. It was observed[2,9] that low uniaxial stress suppresses the lattice transformation but leaves T_L unchanged. Assuming an Ehrenfest second-order transition at T_L, Ehrenfest's equation gives

$$dT_L/dP = vT_L \Delta\alpha/\Delta C_p = \Delta\kappa/\Delta\alpha,$$

where α is the thermal volume-expansion coefficient, κ the compressibility, and v the molar volume of V_3Si. Since[2] $\Delta C_p = 0.054$ cal mole^{-1} °K^{-1}, $\Delta\alpha$ is thus expected to be -5×10^{-7} and $\Delta\kappa/\kappa = +1.33\times 10^{-4}$ as the lattice transforms from cubic to tetragonal symmetry. These values of $\Delta\alpha$ and $\Delta\kappa$ are too small to have been observed in the previous studies of thermal expansion[3] and elastic moduli.[1]

The lattice transformation occurs when $C_s(P,T)$ reduces to some small critical value in the cubic state. Assuming this critical value is pressure independent, and expanding $C_s(P,T_L)$ to its first-order terms, one has

$$\partial T_L/\partial P = -(\partial C_s/\partial P)_T(\partial C_s/\partial T)_P^{-1}.$$

With $\partial T_L/\partial P = -1.5\times 10^{-4}$ °K bar $^{-1}$ and $(\partial C_s/\partial T)_T = 20$ kbar °K^{-1}, we obtain

$$(\partial C_s/\partial P)_T = +3.$$

This shows that the application of hydrostatic pressure will stiffen the shear mode at low temperature, in agreement with the recent observation by Carcia and Barsch[10] for the transforming sample, but in disagreement with that by Larsen and Ruoff[11] for the nontransforming one. Carcia and Barsch[10] examined the temperature variation of $(\partial C_s/\partial P)_T$ between 37 and 298°K and found that $(\partial C_s/\partial P)_T$ becomes negative below ~100°K, exhibits a minimum at ~80°K, and finally changes sign back to positive below ~50°K.

The unusual behavior of $C_s(T)$ at atmospheric