Study of Transforming and Nontransforming V_3Si up to 29 kbar

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Well-characterized transforming (T) and nontransforming (NT) V_3Si single-crystal samples have been investigated under hydrostatic pressures up to 29 kbar. Above the critical pressure P_c, the superconducting transition temperature T_c of the T sample was found to increase continuously with pressure, with only a reduction in $\partial T_c/\partial P$. The value of $\partial T_c/\partial P$ for the T sample above P_c is similar as to that for the NT sample. A pressure-induced phase transition in the NT sample at 28.6 kbar was observed. The results are discussed and compared with some of the predictions of various models on $A15$ high-T_c superconductors.

$A15$ compounds with high superconducting transition temperature T_c, like V_3Si and Nb_3Sn, are known[1,2] to behave anomalously compared with the low-T_c superconductors or the "normal" metals, even in the nonsuperconducting state. Therefore, any models proposed to explain high-temperature superconductivity have to be able to account for the anomalies. Of particular interest among the anomalies is the appearance of lattice instabilities[3,4] above T_c, which, in some cases, leads to a lattice transformation at T_L.[5] Since hydrostatic pressure can reversibly vary and even arrest (above the critical pressure P_c) the lattice instabilities,[6] it provides some direct experimental tests on the different models. At the moment, hydrostatic-pressure effects on superconductivity and lattice instabilities of well-characterized high-T_c samples has been investigated only below[7] P_c and the results can be indiscriminatorily described in terms of all existing models. However, differentiation between the predictions of different models begin to emerge above P_c. Therefore the crucial test on the validity of the various models lies in the successful determination of the pressure effects on superconductivity and lattice instabilities of well-characterized samples above P_c.

The pressure dependence of T_c of a transforming (T) and a nontransforming (NT) sample of V_3Si single crystals was measured under hydrostatic condition up to 29 kbar by both the resistive and inductive methods operated at 10 Hz. The pressure dependence of T_L of the T sample was simultaneously measured, using the temperature modulation technique[6] by which the relative specific heat and the temperature derivative of the resistivity were determined. The T sample with dimensions ~5 mm×1.2 mm×0.8 mm has a T_c=16.6 K, a T_L=21.5 K, and a resistance ratio R(300 K)/R(20 K)=25 at atmospheric pressure. The NT sample with dimensions ~3 mm×0.9 mm ×0.3 mm has a T_c= 16.5 K, and a R(300 K)/R(20 K)=16 at atmospheric pressure. Both samples were spark cut but from different large single crystals[3,8] whose low-temperature structural states have previously been determined by measuring the shear modulus C_s as a function of temperature between 17 and 300 K. This is essential, in view of the sensitive dependence of T_L and the elastic properties of V_3Si on the sample condition. The pressure was generated in the 1:1 fluid mixture of n-pentane and isoamyl alcohol contained inside a 3.2-mm-diam Teflon cell, employing the self-clamp technique with a WC insert. The pressure was determined by a superconducting Pb manometer situated right next to the sample. The temperature was determined with a Ge thermometer below 23 K and a Chromel-Alumel thermocouple above 18 K. The relative uncertainty is estimated to be <1 kbar for pressure and <0.003 K for temperature within our experimental ranges.

The results[9] of the pressure dependences of T_c and T_L of the T single crystal of V_3Si are shown in Fig. 1. The rate of T_c enhancement $\partial T_c/\partial P$ drops from $(4.0\pm0.2)\times10^{-5}$ kbar^{-1} below 19 kbar (similar to previous experiments[6]) to $(2.8\pm0.2)\times10^{-5}$ kbar^{-1} above. T_L decreases with pressure increase, consistent with previous study[8] on the C_s below ~2.5 kbar on the same crystal from which the present T sample was cut. An extrapolation gives a P_c of 20 kbar for the stabilization of the high-temperature cubic phase in the superconducting state, suggesting that the sudden decrease of $\partial T_c/\partial P$ above 19 kbar is a direct consequence of the complete suppression of the structural transformation. A direct determination of the T_L-P curve near P_c is extremely difficult because of the diminishing anomalies associated with the structural transformation at high pressure. The pressure dependence of T_c for the NT sample is also shown in

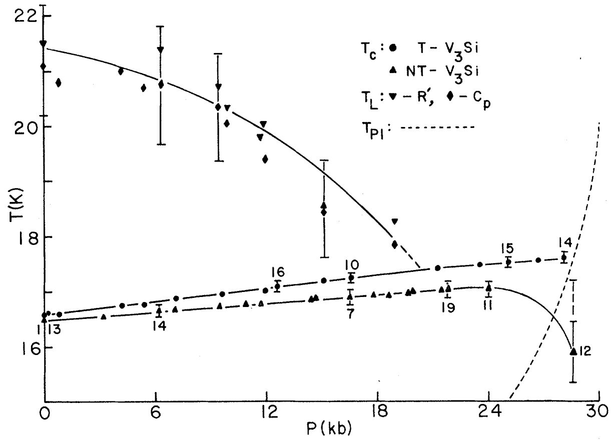

FIG. 1. The pressure dependences of T_c and T_L for T and NT samples of V_3Si single crystals. T_{PI} is the pressure-induced phase transition temperature, after Ref. 10. The number represents the sequential order of the experimental runs, and the bar the transition width. After the nineteenth run for the NT sample, unfortunately the WC insert of our high-pressure cell failed.

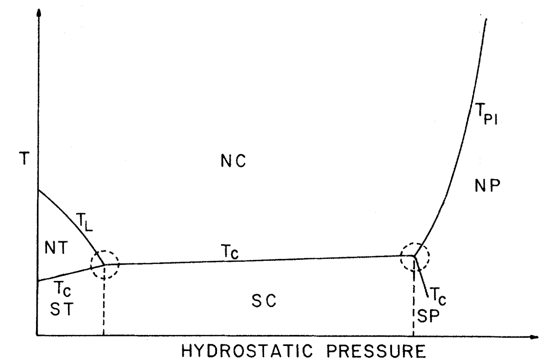

FIG. 2. The schematic phase diagram for transforming V_3Si single-crystal samples, suggested by the results of the present study and Ref. 10. Details near the critical point indicated by the circles and the boundaries separating the *ST* and *SC* (we are indebted to Professor I. Spain for pointing this out to us), and the *NP* and *SP* phases have yet to be determined. *N* stands for normal, *S* superconducting, *T* tetragonal phase, *C* cubic phase, and *P* the pressure-induced phase.

Fig. 1. T_c initially increases linearly with pressure at a rate of $(2.6 \pm 0.2)\times10^{-5}$ kbar^{-1}, similar to the value for the T sample above ~20 kbar. This is consistent with the above suggestion that P_c for the T sample is ~20 kbar. A large drop of T_c to 15.98 K occurs at 28.6 kbar, accompanying with a broad superconducting transition width of ~1.1 K, more than 4 times that at lower pressure. By comparing the results of the NT and the T samples at high pressure one can easily conclude that the drop of T_c of the NT sample at 28.6 kbar is not caused by pressure inhomogeneity due to the possible solidification of the pressure medium when the pressure is applied at room temperature. Furthermore, both the shift in T_c and the broadening of the transition are reversible with pressure cycling. The results therefore suggest the observation of a pressure-induced phase transition at 28.6 kbar in the NT V_3Si single-crystal sample. Such pressure-induced phase transition in a NT sample was inferred[11] from the negative pressure coefficient of C_s measured below ~2.5 kbar. The transition has a larger effect on T_c than the martensitic transition at 1 bar in the T sample. However, the nature of such a pressure-induced phase transition remains unknown. Included also in Fig. 1 is the dashed line representing the predicted pressure-induced phase boundary[11] for the NT sample.

The resemblance of $\partial T_c/\partial P$ for the T sample above P_c and for the NT sample below ~24 kbar (see Fig. 1) suggest a temperature–hydrostatic-pressure phase diagram as depicted in Fig. 2 for the V_3Si compound. It should be noted that details near the critical points indicated by the circles and the phase boundaries in dashed lines have yet to be determined. T_c of a T sample always increases with pressure but with a decrease of $\partial T_c/\partial P$ above P_c. Hydrostatic pressure above P_c stabilizes the lattice and the T samples thus behaves like a NT sample. Further increase of hydrostatic pressure (> 30 kbar) will result in a phase transition leading to a large drop in T_c as observed in the NT sample.

To explain the different anomalies observed in V_3Si and Nb_3Sn, various models have been proposed. In spite of the many differences in details, they can be summarized into three, depending on the emphasis, i.e., the electron models,[2] the soft-mode model,[1,12] and the defect model.[9] The main feature of the electron models is the assumption of the existence of narrow peaks of density of states near the Fermi level.[2] The high-temperature superconductivity and lattice instabilities are considered to be two aspects of one phenomenon, namely the instabilities of the electron energy spectrum. According to these models, the application of hydrostatic pressure will increase both the interchain and intrachain couplings. This can induce[13] an interband charge transfer, broaden the density-of-states peak, and vary the electron-phonon interaction. T_c and T_L are then changed under pressure accordingly.[6,13,14] For instance, the pressure effects on T_c and T_L of V_3Si below P_c can be accounted for in terms of a positive pressure-induced charge transfer to the d sub-band of the compound. On the basis of the X-point model,[15] the pressure effects can be ascribed[16] to the suppression of the Peierls coupling constant by pressure. The change of $\partial T_c/\partial P$ above P_c can be attributed to the different pressure responses of the electron energy spectra of V_3Si in its cubic and the tetragonal states. At very high pressure, e.g., >24 kbar for the NT sample (or >30 kbar for the stabilized cubic phase of the T sample). the pressure-induced phase transition alters the band structure drastically and hence results in a T_c reduction which is larger than that caused by the ordinary martensitic phase transformation in a T V_3Si sample. Recently, the coupled-chain electron model with a density of states with logarithmic singularities was used to describe[17] the different low-temperature $\partial C_s/\partial P$ behavior[8,11] between the T and NT V_3Si samples by adjusting the Fermi levels of the samples. The large negative $\partial C_s/\partial P$ for the NT sample at low temperature was ascribed to the location of the Fermi level to the left of the density-of-states peak, whereas the small positive $\partial C_s/\partial P$ for the T sample to the location of the Fermi level to the right of the peak. Since pressure tends to increase the Fermi level,[13] a pressure-induced phase transition is expected to occur due to the increase in the density of states under pressure. In other words, a NT sample can be made into a T sample under hydrostatic pressure but a NT sample is unlikely to transform under any pressure above 20 kbar, in contrast to that suggested by Fig. 2.

In the soft-mode model, it is assumed[12,18] that high-T_c $A15$ structure is extremely unstable and large anharminicity exists near the bottom of the lattice potential well. High-temperature superconductivity is attributed mainly to the soft-phonon modes due to the large anharmonicity, using the strong-coupling theory of superconductivity. According to this model, hydrostatic pressure varies the lattice potential and thus the lattice instabilities. Since instability is maximum at T_L, T_c is therefore enhanced (suppressed) as T_L is driven by pressure towards (away from) T_c. A maximum in the T_c-P curve at P_c is predicted. Unfortunately, the results shown in Figs. 1 and 2 do not bear out such a prediction, although data below P_c seem to be consistent with the prediction. On the other hand, if T_L approaches T_c asymptotically above ~20 kbar for the T sample, instead of crossing T_c, the absence of the T_c maximum is not incompatible with the model. However, the existing data strongly suggest the crossing of the T_L with T_c above ~20 kbar, or the stabilization of the cubic lattice by pressure above P_c.

The defect model[9] focuses only on the relief mechanism for instabilities by assuming that all high-T_c $A15$ compounds are intrinsically unstable and thus extremely susceptible to defect formation. The lattice softness is preserved for the case of low defect concentration but removed for high defect concentration depending on the nature of the defects in the compounds and hence to vary T_c and T_L.[19] This model predicts the T_c-P and T_L-P relations, similar to those expected by the soft-mode model, which are in contrast to our observations. The defect model was also used to explain the drastic differences of $\partial C_s/\partial P$ between the T and the NT V_3Si samples.[20] According to this model, hydrostatic pressure would reduce the defects which were supposed to contribute positively to C_s, and hence would account for the large negative $\partial C_s/\partial P$ in a NT sample which had more defects than the T sample. Therefore, C_s of a NT sample is supposed to decrease towards that of a T sample under hydrostatic pressure asymptotically. Since pressure-induced phase transition was not detected in the T sample below 29 kbar, no transition below 29 kbar would be expected in the NT sample, in contradiction with our observation shown in Fig. 1.

In conclusion, we have found that hydrostatic pressure always enhances T_c of both the cubic and the tetragonal phases of V_3Si, and induces in the NT sample a phase transition leading to a large drop in T_c. The results tends to favor qualitatively the electron model, although inconsistency still exists, e.g., the existence of the pressure-induced phase transition in the NT sample. However, it is an experimental fact that soft phonon modes (including the ones with long wavelengths) exist in all high-T_c $A15$ material investigated, and that defects drastically suppress T_c. Since it is believed that the properties of matter must ultimately be predictable from the electron energy spectra of the matter, it becomes necessary that in any future attempt to formulate a more realistic electron model, the roles of anharmonicity and defects should also be taken into consideration. Further experiments on NT V_3Si under hydrostatic pressure both below and above 29 kbar are planned to determine the T_{pI}-P phase boundary shown in Figs. 1 and 2. By linearly extrapolating the C_s under low pressure, T_{pI} below T_c was predicted.[11] On the other hand, an electronic model[16,21] suggested that the existence of a superconducting gap should prohibit any structural transformation from taking place, i.e., T_{pI} could not be below T_c.

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