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STUDIES OF LOW TEMPERATURE PHASE TRANSFORMATIONS IN
HIGH FIELD SUPERCONDUCTORS AND THE PHONON SPECTRUM
AND MECHANICAL PROPERTIES OF VANADIUM

Final Report

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ABSTRACT

In the research on this contract we have made extensive studies of the structure and phase transformations of high field superconductors of the β -tungsten type. We discovered a phase transformation at 43°K in Nb_3Sn and have measured the structure of the low temperature phase. The details of the transformation in terms of the formation of the low temperature tetragonal phase from the high temperature cubic phase was investigated both by x-ray observations and optical microscopy below 40°K .

The complete phonon dispersion of vanadium was measured by x-ray diffuse scattering, thus complementing the neutron measurements on other body-centered cubic elements. Incidental to the work on phonons in vanadium we discovered a strong effect which we were able to relate to hydrogen precipitations in vanadium. In separate electron microscopy studies we determined the structure of the vanadium hydride phase directly and determined the relative positions of the hydrogen atoms. In a neutron diffraction study complementing our phonon work with x-rays we were able to show directly the existence of anharmonic vibrations in single crystals of silicon by determining, for the first time, a nuclear forbidden reflection. This reflection is due solely to anharmonic vibration of the nucleus of the atom and we were able to show that its intensity increases with increasing temperature roughly as the 4th power of temperature.

This final report describes the work performed under contract number AT(11-1)-3164 entitled "Studies of Low Temperature Phase Transformations in High Field Superconductors and the Phonon Spectrum and Mechanical Properties of Vanadium".

The initial phase of this work was concerned with the compounds Nb_3Sn and V_3Si which are high temperature superconductors. When this work was initiated it had been established previously in the literature that V_3Si underwent a structural phase transformation at a temperature of about 23°K compared to a superconducting transition temperature of 17.3°K . Attempts to show that Nb_3Sn whose superconducting transition temperature is 18.5° and also has the same transition as V_3Si had failed. When we started this work we were able to obtain from J. J. Hanak of the RCA Laboratories a single crystal of Nb_3Sn and were able to show after appropriate heat treatment of that crystal that Nb_3Sn also underwent a phase transformation in a way similar to V_3Si with interesting differences. The transition temperature of the structural transformation was 43°K and that the change from cubic to tetragonal in Nb_3Sn was such that the c axis became smaller than the two a's whereas the reverse was the case in V_3Si . We then undertook a detailed study using optical techniques at helium temperatures to get information on the mechanism of the low temperature transformations. We were able to do optical microscopy at helium temperatures and to record the progress of the transformation using ciné techniques. We could see the formation of the

tetragonal structure and its propagation and stress dependence while the transformation took place.

Detailed x-ray measurements on both V_3Si and Nb_3Sn were made to establish that there was no volume change to one part in 10^4 in the transformation from cubic to tetragonal. All our results indicated that the transformation was at least second order as far as the strain parameters were concerned.

It was known that acoustic modes became soft in both these materials as the transformation temperature was approached. We attempted to measure an expected increase in the thermal x-ray scattering as the transformation temperature was approached.

To develop our techniques for the measurement of thermal diffuse scattering we measured the thermal scattering from single crystals of vanadium to get the phonon dispersion curves. Vanadium is a material which is unsuitable for neutron diffraction determinations of the phonon spectrum because of its low coherent scattering cross-section. We made the first x-ray measurements on single crystals of vanadium to get the phonon dispersion curves. This work was published in 1970.

During these x-ray measurements of thermal scattering we incidentally discovered peculiar effects of hydrogen in the vanadium samples and this led to a study of the effects of hydrogen in vanadium. In collaboration with Professor S. L. Sass and graduate student John Wanagel we made a detailed study of the formation of vanadium hydride precipitating in a vanadium matrix. Electron microscopy studies showed the ordering of hydrogen atoms in the vanadium hydride and we were

able to get a structure, for the first time, of the tetragonal vanadium hydride phase. We were also able to obtain the relative positions of hydrogen atoms in the hydride and thus determined the superstructure of the hydrogen atoms.

Incidental to our study of phonon properties in solids we were interested in anharmonic vibrations which we would expect to take place in solids in which soft phonons appear. One unique method of directly seeing anharmonic vibrations is to look at the neutron diffraction intensities of certain forbidden reflections, e.g., the (222). This reflection would normally be forbidden, but if the nucleus vibrates in an anharmonic way, the symmetry of the lattice, would allow a weak (222) reflection. Furthermore, contrary to the usual dependence of Bragg reflections on temperature these reflections increase with temperature roughly as the power of T^4 . The reason for the increase is that the degree of anharmonicity will increase as the vibrational amplitude of the nucleus increases with increasing temperature. We were able to detect and measure this anharmonic reflection.

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