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" Low Temperature and Neutron Physics Studies "

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"Low Temperature and Neutron Physics Studies"

Abstract

Progress on and completion of various studies in solid state and neutron physics through use of neutron spectrometers is outlined in the present progress report. Topics which are discussed include: (a) characterization of the low temperature magnetization in the Cu(Fe) Kondo alloy, (b) study of the charge-density-wave phase transition in the superconductors NbSe₂ and TaSe₂, (c) neutron scattering by nuclearly-polarized Li⁷, (d) extraneous scattering effects in the passage of polarized neutrons through high field magnets, (e) preparation of neutron interferometer systems and (f) revision of spectrometer facilities.

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Introduction

Our program on low temperature and neutron physics studies is normally centered around our use of neutron spectrometers operating at the 5 megawatt MIT Research Reactor. Since this neutron source has been shut down (from May 1974) for rebuilding during all of the past annual period, we have continued research activity at both Brookhaven and Oak Ridge National Laboratory. As well, our local activities have involved earlier data analysis, revising and up-dating of our spectrometer facilities and preparing for new experiments upon reactor start-up. At the time of this progress report, our reconstructed reactor, now known as MITR-II, has been loaded with new fuel elements and has become critical. This will be followed by some 6 or 8 weeks of reactor testing during which we shall be reinstalling our spectrometer equipment.

Project Research Activities

(A) Study of Charge Density Wave Transitions in 2H-TaSe_2 and 2H-NbSe_2 . D.E. Moncton and J.D. Axe (BNL)

Neutron scattering studies performed at Brookhaven National Laboratory on the isomorphic compounds 2H-TaSe_2 and 2H-NbSe_2 have revealed the presence of strong "Kohn-like" anomalies in the $\text{LA}(\Sigma_1)$ phonon spectra and also an incommensurate superlattice structure characteristic of a charge density wave (CDW) instability occurring at low temperature. These dynamic structure effects are of interest because of their correlation with the eventual superconductivity of these materials which sets in at still lower temperature. The static atomic displacements associated with the CDW superlattice are found to be of the same symmetry as the Σ_1 phonon eigenvector, but only a slight softening of the relevant phonon is observed as the transition is approached from higher temperature. The transitions in both compounds appear to be second-order with precursor critical scattering which is not measurably inelastic. Whereas the NbSe_2 superlattice which forms at $T_0 = 33.5$ K remains incommensurate reduced wave vector $\vec{q} = (1 - \delta) \vec{a}^* / 3$ to at least 5 K, the TaSe_2 superlattice ($T_0 = 122.3$ K) becomes commensurate, $\delta \rightarrow 0$, in a first-order lock-in transition at 90 K. The vector $\vec{a}^*$ is equivalent to the reciprocal lattice vector $\vec{b}_1$ of the hexagonal structure and values of δ decrease with decreasing temperature, ranging from 0.025 to 0.011 for NbSe_2 and 0.020 to 0 for TaSe_2 .

Interesting pressure dependent effects on the NbSe_2 transition have been found and it was established that pressures up to 6 k bar drive the NbSe_2 superlattice towards commensurability with only slight (less than 1 K) lowering of T_0 . The temperature dependence of the superlattice wave vector $\vec{q}$ in the incommensurate phase and the lock-in transition in TaSe_2 have been interpreted theoretically from free-energy arguments involving third-order "umklapp" terms and a secondary order parameter. The secondary lattice distortion which is predicted in this model agrees with the experimental observations.

This research problem has served as the doctoral thesis research for D.E. Moncton.

(B) Polarized Neutron Diffraction by Li^7F
D.P. Frank and C.G. Shull

The analysis of the polarized neutron diffraction data obtained earlier on nuclearly-polarized crystals of Li^7F was completed during the past period. Since the extinction correction effects turned out to be rather large for our crystals, considerable attention was given to the development of a modified Zachariasen extinction theory which would be best representative of our symmetric Laue transmission case. Following this, the data were analyzed leading to the Li^7 spin state scattering amplitude difference, $b_+ - b_- = -0.530(0.032) \cdot 10^{-12}$ cm. This value differs somewhat from that obtained by Roubeau, et al (Phys. Rev. Lett. 33 102 (1974) of $-0.460(0.014) \cdot 10^{-12}$ cm by polarized neutron precession in transmission through polarized samples. The latter experimental technique does not encounter the single crystal problems and nuclear spin relaxation effects that have bothered our Bragg reflection technique and so it is inherently simpler and capable of better precision. Our study was interesting in that it showed an anomalously large spin relaxation time of about 35 hours, i.e. it took this long for the nuclear spin temperature to adjust to that of the Li F lattice.

(C) Neutron Diffraction Study of the Cu(Fe) Kondo System
M.H. Dickens, C.G. Shull, W.C. Koehler (ORNL) and R.M. Moon (ORNL)

Data obtained earlier on polarized neutron diffraction by a series of dilute alloys of Fe dissolved in Cu were given final analysis during the past period and prepared for publication. The last phase of the data collection were obtained after the MIT Reactor shutdown with experiments being continued at Oak Ridge National Laboratory in collaboration with the above staff. Careful extinction analysis was given to the data following the development of a new improved extinction theory based upon an earlier Zachariasen treatment, and this along with the incorporation of new Cu nuclear polarization data from Meriel et al at Saclay, was used in arriving at final conclusions. By studying the concentration dependence of the polarized neutron, magnetic scattering, it was possible to determine the magnetization of isolated Fe centers at different temperatures. This was found to be over three times larger than the bulk, or total magnetization at the lowest temperature of 1.2 K with the two quantities approaching each other in the vicinity of 10 K. This observation suggests the presence of a compensating magnetization component whose spatial extent $\sim 1 \text{ \AA}$ makes it unobservable in a diffraction experiment because of its compressed form factor. Such a conclusion lends strong support to the development of a Kondo spin-compensated singlet state at low temperature and it would argue against the validity of a localized-spin-fluctuation model in which a single-entity magnetization source is envisaged.

(D) Study of High-Magnetic Field Effects in Polarized Neutron
Diffraction
R.M. Moon (ORNL), W.C. Koehler (ORNL) and C.G. Shull

In attempting to explain some peculiarities in the diamagnetic scattering by Bi as described in our last Progress Report (MIT-3342-2), the influence of the high magnetic field and resulting magnetic force on the passing neutron beam was investigated. Such experiments involve the use of asymmetric, split, superconducting coils for field production with associated longitudinal and transverse field gradients. It has been established both theoretically and experimentally that these gradients can produce under certain conditions shifts in both the Bragg reflection position and the Bragg intensity. It follows that this can introduce spurious effects in addition to the real specimen contributions and this must be considered. It is not clear that this is the origin of the Bi scattering anomalies and further investigation must continue when the HFIR reactor at Oak Ridge again becomes operative.

(E) Revision of MIT Spectrometers
C.G. Shull, S. Collins, J. Callera, and A.D'Addario

Since the MIT reactor has been shut down for rebuilding during all of the past period, we have been revising most of our spectrometer equipment. One of our two-axis spectrometers has been changed effectively into a three-axis unit with incorporation of a double, parallel pyrolytic graphite crystal energy analyzing system before the final detector. This will permit inelastic scattering studies when desired and it can be conveniently returned to the original two-axis mode when wanted. A new computer has been procured and this will serve for controlling spectrometer operations and processing the scattering data. The computer is of such capacity that it will also be used for controlling operations on our other spectrometers most notably our high-field-magnet, polarized beam spectrometer. New monochromating crystals are being installed in our spectrometers, and entrance collimation changes and shielding modifications are being affected.

(F) Preparation of a Neutron Interferometer
J. Callera and C.G. Shull

We plan on pursuing an active program of neutron interferometry during the next period and to this end have been orienting and cutting a three slice Laue transmission interferometer from a silicon crystal ingot. The work has been done primarily in the laboratory of Dr. R. Deslattes at the National Bureau of Standards where there is expertise in preparing x-ray interferometer systems. We have prepared one system and this has been tested with x-radiation showing interference action. Further work is continuing with x-radiation before we attempt to use neutron radiation.

Laboratory Staff

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Theses Prepared

- "A Neutron Diffraction Study of the Magnetization in Dilute Cu(Fe) Alloys"
M.H. Dickens, Ph.D. Thesis, September, 1974
- "An Investigation of Slow Neutron Scattering from Polarized Li^7 Nuclei"
D.P. Frank, Ph.D. Thesis, January, 1975
- "A Neutron Scattering Study of the Charge Density Wave Transitions in 2H-TaSe_2 and 2H-NbSe_2 "
D.E. Moncton, Ph.D. Thesis, May, 1975

Laboratory Publications

- "A Study of Superlattice Formation in 2H-NbSe_2 and 2H-TaSe_2 by Neutron Scattering"
D.E. Moncton, J.D. Axe and F.J. DiSalvo
Phys. Rev. Lett. 34 734 (1975).
- "Neutron Diffraction Observations on the Cu(Fe) Kondo System",
M.H. Dickens, C.G. Shull, W.C. Koehler and R.M. Moon
Phys. Rev. Lett. August (1975).
- "Limitations on the Accuracy of Polarized Neutron Diffractometry"
R.M. Moon, W.C. Koehler and C.G. Shull
J. Nucl. Instr., in press (1975).