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Project Research Activities

(A) Diamagnetic Scattering of Neutrons by Bismuth, C. G. Shull

During the present period we have completed the study of polarized neutron scattering by diamagnetic bismuth in Bragg reflections around the $[1\bar{1}0]$ axis. In these experiments a single crystal of pure bismuth held at room temperature is subjected to a large magnetic field (60 KG in our case) and the induced diamagnetization is sensed and measured by polarized neutron intensity measurement in a Bragg reflection. The coherence between the diamagnetic scattering amplitude and the nuclear scattering amplitude produces an intensity change upon neutron polarization reversal. Although the measured diamagnetic susceptibility of bismuth is some five times larger than that calculated, it is still very small on an absolute scale and the intensity changes that must be measured are very small, the largest being about 100 parts per 100,000. This can be measured with suitable polarized neutron technique and we customarily carry measurements to a significance level of 5 parts per 100,000 with long period counting.

We have collected data on seven reflections out to a maximum value of $\sin \theta = 0.310 \text{ \AA}^{-1}$ and these reflections, plus two very weak reflections not available to experiment, constitute all possible one-zone reflections to this limit. The measured diamagnetic scattering amplitudes for these reflections show pronounced directional effects being both larger and smaller than that calculated from basic diamagnetic theory using electron wave functions that are available for isolated atoms. These directional effects are thought to arise from the overlap of the outermost electron wave functions (bismuth has a compact core of 78 electrons plus two 6s and three 6p electrons which are much more extended than the core group). In overlapping regions the effective mass of the electrons is greatly reduced and consequently the diamagnetization there is enhanced. Such a picture arises directly by Fourier transforming the diamagnetic scattering amplitudes so as to yield a projection of the diamagnetization density upon a plane normal to the zone axis which has been studied in the experiments.

These diamagnetization density maps are most easily interpreted when the core electron contribution is subtracted from the measured amplitudes thereby showing up only the outer 6s-6p electron effects. Since the core electrons are so compact relative to atom separation in the crystal, their diamagnetization can be calculated with confidence. The density maps representative of the 6s-6p electron groups show pronounced positive and negative regions (relative to the mean diamagnetization level) at positions considerably removed (1 to 1.5 $\text{\AA}$) from the nuclear positions and unsymmetrically arranged relative to the nuclei. The two unique atoms in the bismuth unit cell show magnetic displacements in opposite direction. This illustrates that these magnetic atoms are very lop-sided on a scale much more pronounced than has been seen in the spin density distributions within paramagnetic, antiferromagnetic or ferromagnetic systems.

It is to be emphasized that these diamagnetization maps are unique in that they portray the electron current distribution in and between atoms in contrast to the electron spin distribution that characterizes the usual neutron scattering results. It should be pointed out also that these directional

effects represent a very different phenomena than the long established directional effect on the diamagnetic susceptibility. In the present experiments, the external field has been applied in only one direction and we are sensing the diamagnetization density as it is distributed around this polar axis. It will be very interesting to correlate these diamagnetization findings with the effective mass ellipsoid constructions that are available from cyclotron resonance and DeHaas-von Alphen studies. These experimental results will shortly be presented for publication.

(B) Nuclear Polarization of Li^7 , D. Frank and C. G. Shull

We have planned on studying nuclear polarization as induced in some nuclear systems by application of a high magnetic field to crystals held at low temperature. By determining the change of nuclear coherent scattering with polarized neutrons fundamental information on the nuclear spin state scattering amplitudes is obtained. There is interest among nuclear theorists in having such information for the Li^7 nucleus and we have concentrated in this direction.

In the interpretation of the Bragg reflection intensity with nuclear polarization it is necessary to establish quantitatively the degree of extinction occurring in the Bragg reflection. Experimental studies are usually performed with crystals where the effects of extinction are purposely made small, usually by increasing the mosaic spread of the crystal, so that it can be corrected for in a quantitative sense. For practical reasons of crystal availability we have decided to use LiF crystals. Our present crystals of both normal and isotopic form have been found to exhibit considerable extinction in some of the reflections and we have spent a great deal of effort in attempting to lessen the effects of extinction by increasing their mosaic spread. The efforts have been mostly in attempts at plastic deformation at high temperature. Several forms of furnace, atmospheric and pressure-application equipment have been tried. Even with heating to 800°C , about 30° below melting, it has been found that pressing, to the limit yielding cracking along (100) planes, has been ineffective in increasing the mosaic width of the crystals. This behavior with this material is very unexpected since equivalent treatment with other crystals (such as Si and Ge) is known to be very effective.

With this failure of mosaic structure alteration, we are now studying the extinction effects in some of the low reflectivity reflections from our Li^7F crystals. After assessing this quantitatively we shall proceed with the nuclear polarization measurements in our superconducting magnet. During the present period we have designed, tested and used a new specimen temperature control system as inserted into our superconducting magnet. This is working well and we can attain temperatures as low as 1.1°K . With 60 KG magnetic field and this temperature, the nuclear polarization should be 0.35% and this is sufficient for quantitative measurement.

(C) Low Temperature Transformation in ZrV_2 , D. Moncton

During the past year an initial set of X-ray and neutron diffraction experiments on the 120°K phase transition in the superconductor ZrV_2 have been concluded. The purpose of these studies was to determine whether

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this transformation involved either antiferromagnetic ordering or a lattice transformation resulting from a phonon instability. A cubic to rhombohedral lattice transformation was found to occur at 116.7°K with a large spontaneous lattice distortion of about 5%. No evidence was discovered for the existence of any local magnetic moments, either ordered or disordered in the temperature range investigated (5.4 K - 300 K).

The presence of such a lattice distortion has interesting implications for the superconductivity of ZrV_2 . It is felt that this transition is a result of an acoustic phonon instability similar to those found in the A15 superconductors V_3Si and Nb_3Sn . Group theoretical calculations have been carried out to enumerate the symmetries of the $q=0$ phonons. Using the Landau theory of second order phase transitions, the low temperature structures which would result from a phonon instability have been calculated for each optic and acoustic mode. Experiments are now underway to look for a sublattice distortion and determine which mode is involved in the transition.

Of further interest is the fact that the compound HfV_2 , which is isostructural with ZrV_2 , becomes orthorhombic below 120°K . This difference between the two components of the pseudobinary alloy $\text{Hf}_x\text{Zr}_{1-x}\text{V}_2$ is undoubtedly of importance in explaining the excellent superconducting qualities of the alloy at $x=0.5$. Therefore, further experiments may be carried out in search of sublattice distortions in HfV_2 to further understand the unique difference between these otherwise similar compounds.

(D) Dynamical Diffraction Experiments with Perfect Copper Crystals

C. G. Shull and H. Bradacsek

We have recently obtained two specimen crystals of copper prepared by Dr. F. Young at Oak Ridge National Laboratory which are perfect enough to exhibit an anomalous Borrmann effect. We are interested in studying these with neutron diffraction and if possible to measure their Pendellösung fringe structure as we have done in the past with perfect crystals of Si and Ge. This would permit a precision determination of the neutron scattering amplitude and as well a determination of residual curvature in the crystal specimen.

We have made preliminary measurements of the rocking width of these crystals as a study on their perfection and find their widths to be less than about 30 seconds arc. We are currently installing our high resolution torsion goniometer on one of our spectrometers that will permit a quantitative comparison with the perfect crystal Darwin width of a few seconds arc. If the perfection is found high enough we shall proceed to the Pendellösung fringe study.

(E) Neutron Flight-Time Transmission Measurements on Pyrolytic Graphite

R. A. Charpie

A small, cadmium disk chopper coupled with neutron flight-time analysis with a multi-channel analyzer has been used to measure the transmission spectrum of several pyrolytic graphite crystals. These crystals had been previously studied in Bragg reflection and it was desired to correlate these

results with those of the transmission spectrum. A collimated white beam of neutrons was chopped and passed through the pyrolytic graphite crystal oriented with its (002) base planes at known angle to the beam. Transmission dips were observed at the neutron energy calculated for Bragg reflection and the width of the dip and its magnitude agreed reasonably well with calculation using the mosaic width and reflectivity as measured earlier in Bragg reflection.

Laboratory Staff

Professor C. G. Shull, Department of Physics
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Theses Prepared

"Study of the Mosaic Structure in Graphite Crystals by Neutron Time of Flight Spectrometry", R. A. Charpie, B.S. Thesis, June 1973.

✓ "A Neutron Diffraction Study of the 120° K Phase Transition in ZrV_2 ", D. E. Moncton, M.S. Thesis, January 1973.

Laboratory Publications

"Refraction of Thermal Neutrons by Shaped Magnetic Fields", W. Just, C. S. Schneider, R. Ciszewski and C. G. Shull, Phys. Rev. B7, 4142-4145 (1973).

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