13.1-02 SINGLE CRYSTAL DIFFRACTOMETER AT THE LOS ALAMOS PULSED NEUTRON SOURCE. By Allen C. Larson and Phillip J. Vergamini, Los Alamos National Laboratory, MS-805, Los Alamos, New Mexico 87545.

A single crystal neutron diffractometer has been implemented for use at the Los Alamos Spallation Neutron Source. The instrument is conceptually similar to that developed at Argonne National Laboratory[1]. At the heart of the instrument is a 25cm x 25cm ^3He position sensitive proportional counter of the Borkowski-Kopp design. Positional information is combined with wavelength information generated by measurement of the neutron time-of-flight and is stored directly into a megaword sized front-end memory[2] in individual X-Y-time resolution elements.

Software used to acquire and analyse data, as well as to define and control this instrument, is being developed jointly with Argonne National Laboratory staff.

A complete data set has been obtained for K_2SO_4. All observed reflections have been indexed. Instrument parameters and cell constants have been refined to good accuracy. Refinement of positional and thermal atom parameters is in progress and will be reported.

1) S.W. Peterson, A.H. Reis, Jr., A.J. Schultz, and P. Day, (1978) Advances in Chemistry Series No. 186 p. 75-91, American Chemical Society (1980).

2) R.W. Hendricks, P.A. Seeger, J.W. Scheer and S. Suehiro, Oak Ridge National Laboratory Report ORNL/TM-7325.

13.1-03 APPLICATION OF THE FIXED SCATTERING-ANGLE SPECTROMETER FOR NEUTRON DIFFRACTION STUDIES OF POWDERED SAMPLES. By M. Adib, R.M.A. Maayouf, S.E. Gwaily and I. Hamouda, Reactor and Neutron Physics Department, A.E.E., Cairo, Egypt.

A fixed scattering-angle spectrometer, installed in front of one of the horizontal channels of the ET-RR-1 reactor, for neutron-diffraction studies of powdered samples is described.

The spectrometer consists of a rotor, suspended in a magnetic field, spinning at a maximum speed of 16000 rpm producing bursts of polyenergetic neutrons. The rotor, 32 cm in diameter, has two slits for producing two bursts of neutrons per revolution. The slits have curvature of radius 65.65 cm and a cross-sectional area of 7 x 10 mm^2.

The flight path from the chopper's centre to the centre of the sample is 400 mm while the flight path from the sample centre to the counter centre is 2000 mm. Two ^3He gas-filled detector batteries are used while fixed, both at 90 and zero degrees w.r.t. the neutron-beam direction. The diffraction data are collected by means of two 1024 multichannel time analyzers.

The wavelength resolution $\Delta\lambda/\lambda$ of the spectrometer at rotation rates 7300 rpm (corresponding to maximum transmission of neutrons of wavelength $\lambda \approx 4$ Å) and 16000 rpm ($\lambda \approx 1.8$ Å), with total flight path 2400 mm, is 1.5% and 1.7% respectively.

13.2-01 ELASTIC AND INELASTIC NEUTRON SCATTERING ON Cr_3Si. By J.-E. Jørgensen,+ J.D. Axe, L.M. Corliss, J.M. Hastings, Brookhaven National Laboratory,* Upton, New York 11973, and S.E. Rasmussen,+ +: Chemistry Department, Aarhus University, DK-8000 Aarhus C, Denmark.

Cr_3Si has the A15 structure. The material does neither become superconducting nor does it exhibit a structural phase transition at low temperature. It is therefore of interest to compare the properties of Cr_3Si with those of superconducting A15 compounds. Cr_3Si has been studied by elastic neutron diffraction to determine Debye-Waller factors and for estimating the crystal perfection of the crystals prepared by zone melting (J.-E. Jørgensen and S.E. Rasmussen (1979) Jr. of Crystal Growth 47, 124). TDS corrected neutron data were refined to R = 1.7% for 21 reflexions (F>2sig(F)) and 4 parameters. The Debye-Waller factors were determined to

$$U^{Cr}_{iso} = .0036(4)\ \text{Å}^2 \quad \text{and} \quad U^{Si}_{iso} = .0050(6)\ \text{Å}^2.$$

The diffraction experiment shows that the grown crystals are ordered and stoichiometric. Phonon dispersion curves for Cr_3Si have been studied by inelastic neutron scattering. Measurements of acoustic phonons in the principal symmetry directions and of low lying optic modes in the Γ-point have been performed. Mode assignments at the Γ-point were made by comparing scattering intensities at different reciprocal lattice points with predictions based upon symmetry and simple dynamical models. It was possible to make reliable assignments for 12 of the 24 normal modes which show much accidental near degeneracy.

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13.2-02 THE MODULATED STRUCTURES OF URANIUM. H. G. Smith, N. Wakabayashi, R. M. Nicklow, Oak Ridge National Laboratory,* G. H. Lander and E. S. Fisher, Argonne National Laboratory, and W. B. Daniels, University of Delaware.

The room temperature phase of uranium is the α form, which is orthorhombic (Cmcm) with four atoms in the set (0,y,1/4). Numerous experiments involving elastic constants, lattice constants, dilation, and specific heat measurements, etc. indicated anomalous behavior in these properties near 43 K, 37 K, and 22 K and suggested possible structural transitions at these low temperatures. Early crystallographic studies by X-ray and neutron diffraction techniques did not reveal superlattice formation or significant crystallographic distortion. However, lattice dynamics studies by inelastic neutron scattering did reveal a low frequency optic mode which softened considerably at low temperatures. Subsequent elastic neutron diffraction measurements showed the existence of a periodic lattice distortion (PLD) at low temperatures in the x-direction nearly commensurate with the α-lattice and was interpreted as evidence of a charge density wave formation. Intensity meaurements showed that the lattice distortion is suppressed under application of modest (<4 kbar) hydrostatic pressures. Recent neutron diffraction studies by Marmeggi et al. discovered an additional CDW with y,z components incommensurate with the b,c lattice constants. The relation, if any, between these two PLD's is not presently known; however, neutron scattering studies as a function of temperature and pressure are continuing and the results will be discussed.

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