13.X-05 ON THE MODULATED MAGNETIC STRUCTURE OF $CeAl_2$ By B. Barbara, IBM T. J. Watson Research Center, Yorktown Heights, New York and Laboratoire Louis Néel C.N.R.S. 166X 38042, Grenoble; J. L. Buevos, I.L.L. 156X, 38042, Grenoble; M. F. Rossignol, Laboratoire Louis Néel C.N.R.S., 166X 38042, Grenoble; J. X. Boucherle and J. Schweizer, D.R.F./D.N. – C.E.N.G. 85X 38041 Grenoble and I.L.L. 156X 38042, Grenoble, and C. Vettier, I.L.L 156X, 38042 Grenoble.

The intermetallic Laves-phase compound $CeAl_2$ exhibits sinusoidally modulated magnetic structure with the propagation vector $\vec{q}_i = 1/2+\tau, 1/2-\tau, 1/2)$ (B. Barbara, J. X. Boucherle, J. L. Buevos, M. F. Rossignol, J. Schweizer, Sol. State Comm. 24, 481, 1977). There are twenty-four nonequivalent $\vec{q}_i$ vectors in the Brillouin zone which lead to a twenty-four-component order parameter. The existence of small magnetic peaks with $\vec{q}_c = (1/2,1/2,1/2)$ and the continuous character of the magnetic ordering transition suggest a coupling between different $\vec{q}_i$ vectors (S. M. Shapiro, E. Guerwitz, R. D. Parks, L. C. Kupferberg, Phys. Rev. Lett. 43, 1748 (1979). On the other hand the increase of diffracted intensity at some points of the reciprocal lattice and the correlative decrease at other points (under small uniaxial stress at $T \simeq T_n/2$) suggest a single $\vec{q}$ magnetic structure with an overall cubic symmetry restored by the coexistence of twenty-four magnetic domains (B. Barbara, J. X. Boucherle, M. F. Rossiguol, C. Vettier, Phys. Rev. Lett. 45, 11, 1980).

These two points as well as the evolution of the incommensurate magnetic structure of $CeAl_2$ under hydrostatic pressure will be discussed. Furthermore the fact that such modulated structures involving moment reductions characterize the ground state of a Kramers ion will be related to the ordered Kondo lattice model.

13.X-06 MAGNETIC PHASE TRANSITIONS IN SUPERCONDUCTORS By J. W. Lynn, Department of Physics and Institute for Physical Science and Technology, University of Maryland*, College Park, Maryland 20742, and National Measurement Laboratory, National Bureau of Standards, Washington, D.C. 20234.

The rare-earth (RE) ternary superconductors belonging to the $REMo_6X_8$ (X=S, Se) and $RERh_4B_4$ classes of materials have provided the first unambiguous examples of the coexistence of superconductivity and long range magnetic order. For systems in which the interactions between rare-earth moments are antiferromagnetic in nature, the magnetic order only weakly perturbs the superconductivity since there is no macroscopic magnetization associated with the magnetic state. There are now a rather large number of ternary materials which exhibit long-range antiferromagnetic order coexisting with superconductivity over a wide range of temperatures. The competitive nature of these two cooperative phenomena is illustrated for systems which display ferromagnetic interactions, such as $HoMo_6S_8$ and $(Er_{1-x}Ho_x)Rh_4B_4$, which first become superconducting at a temperature T_{C1} and then order magnetically at lower temperatures. At first the superconductivity is able to prevent ferromagnetic alignment, and a compromise long-wavelength oscillatory magnetization is established at intermediate temperatures. At sufficiently low temperatures, however, the superconductivity is destroyed (at T_{C2}) as ferromagnetism sets in. A similar reentrant superconducting transition has recently been found in $ErRh_{1.1}Sn_{3.6}$, although in this case the ferromagnetic order appears not to be truly long range in nature. The behavior of these reentrant ferromagnets contrasts with the pseudo-binary substitutional alloy systems such as $(Ce_{1-c}RE_c)Ru_2$, where rather long-range ferromagnetic correlations develop in the superconducting state, but true long range magnetic order only appears above the percolation threshold where the superconducting state is fully suppressed.

Inelastic neutron scattering studies have shown that the crystal field splittings of the rare-earth ions in these materials are large in comparison with the magnetic energies, as might be expected since the magnetic ordering temperatures are typically below 1 K. Consequently the nature of the magnetic state at low temperatures and its influence on the superconducting properties is dictated in each case by the crystal field ground state of the 4f electrons rather than the free-ion properties. The crystal field results obtained to date on these materials will also be reviewed.

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13.X-07 ANISOTROPIC AND ANHARMONIC INTERACTIONS IN CUBIC AB_3 INTERMETALLIC COMPOUNDS. By J. Faber, Jr. and G. H. Lander, Argonne National Laboratory, Argonne, Illinois, P. J. Brown, Institute Laue Langevin, Grenoble, France, A. Delapalme, Laboratori Leon Brillouin, Gif-sur-Yvette, France, C.-K. Loong and C. Stassis, Iowa State University, Ames, Iowa.

The usual assumptions for cubic solids are that the atoms vibrate isotropically and harmonically. However, the recognition that bonding effects play an important role in determining the properties of solids, and the observation that solids expand contradict these assumptions. It is precisely the higher-order corrections to these approximations that give us information about bonding and the restoring potentials associated with atom vibrations. Here we report the results of single crystal neutron Bragg scattering studies on the intermetallic compounds UGe_3, USn_3, URh_3, URu_3, $CeSn_3$ and $AuCu_3$. In the temperature range, $80 \lesssim T \lesssim 600$ K, these crystals exhibit the ordered cubic Pm3m structure (O_h^1). Both strong fundamental and weak superlattice reflections have been measured out to high $Q = 4\pi \sin\theta/\lambda$ ($Q \lesssim 15$ Å^{-1}) values. Large anisotropies in the superlattice intensities are observed that cannot be explained in the harmonic approximation. However, the point group symmetry for the B atoms in AB_3 is tetragonal (D_{4h}), and an anisotropic potential well is anticipated. The effects of anisotropic (but harmonic) thermal motion are enormous, e.g., in $CeSn_3$ the thermal vibration ellipsoid is 1.6 times as extended along the unique tetragonal axis as compared with perpendicular to it. We will show that the detailed shape of the thermal vibration ellipsoid is sensitively dependent upon the outer electron configuration at the B atom site, thus reflecting *p*-type bonding for Ge or Sn, but *d*-type bonding for Rh or Ru. Information about these hybridization effects has also come from polarized-beam experiments on UGe_3 (G. H. Lander et al., Phys. Rev. Letters 44, 603 (1980)) and $CeSn_3$ (C. Stassis et al., J. Appl. Phys. 50, 7567 (1979)). Our results will be discussed in light of these experiments as well as phonon and x-ray measurements on $CeSn_3$.

Finally, to achieve excellent agreement between theory and experiment, we must consider anharmonic effects, i.e., terms in the B atom potential to fourth-order in atomic displacements. For $CeSn_3$, the dominant fourth-order term is along the unique tetragonal axis, whereas for UGe_3, it produces a modulation of the potential in the x-y plane. This modulation yields a partially attractive interaction with respect to unlike nearest neighbors. The implication of these results for $AuCu_3$ near T_c will be discussed.

13.X-08 NEUTRON DIFFRACTION STUDIES OF CHEMICAL REACTIONS. By C. Riekel, Max-Planck-Institut für Festkörperforschung, 7000 Stuttgart-80, FRG.

Structural studies of heterogeneous (solid/gas; solid/liquid) reactions are usually performed on stable or metastable phases, with the aim of a high structural resolution. This approach may be quite time consuming for complicated phase sequences and it may not be possible to isolate all phases.

An alternative approach is real-time neutron diffraction which allows study of the dynamics of the structural development. Information on phase sequences and low resolution structural data are thus obtained (C. Riekel, Progr. in Solid State Chem. (1980) 13, 89). Neutrons are especially interesting for this approach as the high transmission of most materials facilitates the construction of reaction cells.

Most experiments were done on powders, and 1D-multiwire detectors were used to record the diffraction patterns. The time scale is in the range 0.5>t<15 min./spectrum. To cope with the multitude of spectra recorded, automatic peak fitting routines were developed.

The establishment of phase sequences will be shown for solid/gas reactions, i.e. the formation of KC_x, $KC_{24}(C_6D_6)_x$ and $|C_6D_4(AsF_5)_x|_n$. Examples for solid/liquid reactions are the electrochemical formation of $K_x(D_2O)_yTaS_2$ and $Li_xA\ell$.

Model calculations will be reported for $K_x(D_2O)_yTaS_2$ (stoichiometry and stabilisation of intercalate layer), D_xTaS_2 (deuteron sites).

13.X-09 NEUTRON DIFFRACTION AS A PROBE OF ADSORBED FILM STRUCTURES.* By L. Passell, Brookhaven National Laboratory, Upton, New York 11973 U. S. A.

There are cases where neutron diffraction is the technique of choice in the investigation of surface films. Applied, for example, to weakly-bound, light atom (or molecule) overlayers on substrates with large specific areas (and with single facet exposure), neutrons are often able to provide information unobtainable by more conventional methods. Thus neutrons have provided new insights into the properties of a number of overlayer phases which--by virtue of their weak interaction with the substrate--are predominantly two-dimensional in character. The general application of neutrons to surface film studies will be reviewed and illustrated by selected examples from the literature.

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13.X-10 COMMENSURATE AND INCOMMENSURATE STRUCTURES OF MONOLAYERS ON GRAPHITE. By P.M. Horn, IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA.

We have performed a series of X-ray diffuse scattering measurements on monolayers of krypton, xenon and oxygen on the surface of exfoliated zyx graphite using both synchrotron (see e.g. R.J. Birgeneau, G.S. Brown, P.M. Horn, D.E. Moncton and P.W. Stephens, J. Phys. C (1981) 14, L49) and conventional rotating anode (see e.g. R.J. Birgeneau, E.M. Harmmonds, P. Heiney, P.W. Stephens and P.M. Horn in "Ordering in Two Dimensions" dited by S.K. Sinha (North Holland, 1980; p29)) sources. In the submonolayer regime krypton is commensurate with $\sqrt{3}x\sqrt{3}R30$ structure. As the coverage is increased krypton undergoes a hexagonal commensurate to hexagonal incommensurate transition which is at least nearly second order. At this transition the substrate-limited coherence of the commensurate monolayer (2300Å) deteriorates to less than 100Å demonstrating that liquid-like disorder is the dominant feature of the weakly incommensurate system.

In contrast to krypton, both xenon above ∿70K, and oxygen above 10K, are incommensurate at all coverages. The xenon system exhibits a 2D triple point with first and possibly continuous melting.