20.4-01 SURSTRUCTURES ET INCOMMENSURABILITE DANS LA THIOUREE. By A. Moudden, F. Denoyer, M. Lambert, Université de Paris Sud, Laboratoire de Physique des Solides Bâtiment 510, 91405 Orsay, France.

Nous discuterons le diagramme de phase P.T de la thiourée $SC(ND_2)_2$, nous montrerons que la phase modulée se subdivise en plusieurs surstructures commensurables simples 3, 7, 9 ...

Nous présenterons qualitativement le mécanisme des accrochages de la période de surstructure aux multiples impairs de la période du réseau moyen. A partir des règles de sélection des reflexions satellites nous discuterons la valeur du déphasage entre sous-réseaux et déduire le super groupe d'espace possible lorsque la période de modulation est incommensurable et voir sa compatibilité avec le groupe d'espace tridimensionnel habituel lorsque la période est commensurable. Nous analyserons, ensuite, les variations de l'amplitude de l'onde de modulation et de ses harmoniques ; nous déduirons des facteurs Debye-Waller dits anormaux la contribution des défauts locaux de la période que nous comparerons à la théorie des fluctuations de phase des structures modulées.

20.4-02 $Er_{1.2}Mo_6S_8$--STRUCTURE WITH THREE INCOMMENSURATE SUPERSTRUCTURES AND DISORDER. H. Brigitte Krause, Physics Dept., Northern Ill. U., DeKalb, IL, 60115, USA, and John M. Cowley, Physics Dept., Arizona State U., Tempe, AZ, 85281, USA.

A series of $(Sn_xEr_{1-x})_{1.2}Mo_6S_8$ compounds was examined with selected area electron diffraction and high resolution electron microscopy. In addition to the expected rhombohedral (approximately cubic) Chevrel phase, several different superlattices and sublattices were observed. Furthermore, for $Er_{1.2}Mo_6S_8$ a new monoclinic, or nearly monoclinic, structure type was discovered. The b-direction of the monoclinic unit cell coincided with the b-direction of the pseudocubic Chevrel phase, and the lattice constant b_C=b_M 6.37Å is identical for both phases. The monoclinic a-axis is a_M=12.10Å, the c-axis is c_M=8.17Å, and the angle β_M=96.5°. The monoclinic axes are rotated with respect to the pseudocubic axes such that $[101]_M$ is in the direction of $[001]_C$ and $[10\bar{1}]_M$ approximatley in the direction of $[100]_C$.

In spite of the similarities between the cubic and monoclinic geometry, there are distinct differences: the volume ratio of $\frac{V_M}{V_C}$=2.4 does not allow a simple interpretation in terms of an Mo_6S_8 cube arrangement as in the Chevrel phase. In addition to regular monoclinic reflections, incommensurate reflections and diffuse scattering were observed. The diffuse scattering occurred in reciprocal lattice sheets perpendicular to the b-direction. One of the incommensurate doublets occurred at $[110]_M$ with a splitting parallel to the b-axis and corresponding to about 100Å in real space. Another doublet at [010] had splitting in the cubic [101] direction. A third series of incommensurate reflections occurred in the cubic [110] direction with splittings both in the direction of $[110]_C$ and $[010]_C$. The incommensurate reflections and lattice images indicate a modulation of the structure interpretable as antiphase domains. Structure models will be proposed.

20.4-03 THE MODULATED STRUCTURE OF CUBIC PHASE Cu_9BiS_6. By K. Tomeoka and M. Ohmasa*, Dept. of Geology, Arizona State University, Tempe, Arizona, U.S.A. *Inst. of Material Sci., University of Tsukuba, Ibaraki, Japan.

Quenched single crystals synthesized at about 550°C for compositions near Cu_9BiS_6 were found to reveal non-integral type satellite reflections in the X-ray diffraction patterns. The crystals reveal fundamental reflections corresponding to cubic α-chalcocite, which has a=5.54-5.57Å cell edge and a face-centered cubic cell. Around the fundamental reflections, many non-integral type extra reflections occur in clusters. These are described as follows: (I) The period of the satellite reflections corresponds to a non-integral multiple of the subcell and changes in the range of 6.0 to 6.75a. (II) The satellites appear three-dimensionally and make a body-centered cubic reciprocal lattice in the same manner as the main reflections. (III) Generally, intensities of the satellites are very strong, and some of them are much stronger than the main ones. (IV) Compared with the mains, the satellites are slightly diffuse. The degree of diffuseness differs in each sample. (V) Asymmetry of intensities between pairs of satellites is very remarkable. Generally, intensities of lower angle satellites are stronger than those of higher angle ones. This cubic phase has a solid solution range of some extent. The positions and the diffuseness of the satellites are correlated with the change of composition of the crystal.

The superstructure was investigated by using X-ray diffraction intensity data, measured on a crystal having a 6.5 multiple of the subcell, because the period can be made integral (13 multiple) simply by doubling 6.5. Since the satellites form a body-centered cubic lattice