

**14.X-04** STUDY OF THE TWO-DIMENSIONAL ANTI-PHASE STRUCTURES IN THE ORDERED ALLOYS BY HIGH VOLTAGE - HIGH RESOLUTION ELECTRON MICROSCOPY. I. By D. Watanabe, O. Terasaki and K. Sato, Department of Physics, Tohoku University, Sendai, Japan.

Two types of two-dimensional long-period anti-phase domain structure (2d-APS) based on the  $L1_2$  structure have been found in several ordered alloys by X-ray and electron diffraction analyses; the  $Cu_3Pd$  type and the  $Au_3Mn$  type. Antiphase domain sizes  $M'$ s along the two directions estimated from the diffraction patterns are in general non-integral multiples of the fundamental  $L1_2$  cell, and it is not easy to understand the actual configuration of domains in real space from the diffraction study alone. Moreover, the weak superlattice reflections which cannot be explained by the idealized structure models have recently been observed on electron diffraction patterns; this means that the 2d-APS models proposed on the basis of diffraction patterns only need refinement or some modification. We have applied the structure imaging technique to the alloy systems concerned, using the 1 MV electron microscope with a theoretical resolution of 1.9 Å and solved these structural problems. In the present paper, results for the  $Au_3Mn$  type 2d-APS are given. The 2d-APS of this type is characterized by the antiphase vectors of the first kind along the two cubic axes and is observed in the Au-Mn and Cu-Zn-Au systems.

**Au-Mn:** Domain sizes,  $M_1$  and  $M_2$ , along the x- and y- directions are estimated to be 1.10-1.20 and 2.16-2.34, respectively, depending on composition and ordering temperature. It has been revealed in the course of the experiments that a new type of 2d-APS, which is based on the  $DO_{22}$  structure and gives diffraction pattern similar to that of the  $Au_3Mn$  type 2d-APS, exists in the composition range of 21-23 at.% Mn (Terasaki et al. J. Appl. Cryst. (1981) 14). It was confirmed by the observation of high resolution superstructure images, however, that the  $Au_3Mn$  type 2d-APS exists in the 23-24 at.% Mn alloys annealed at about 300°C, and the configuration of domains giving non-integral M values was clearly revealed.

**Cu-Zn-Au:** The 2d-APS exists in the  $Cu_{80-x}Zn_xAu_{20}$  ( $x=10-35$ ) and  $Cu_{55}Zn_{15}Au_{30}$  alloys annealed at temperatures below about 250°C. The characteristic of this system is that the M values along the two directions are always equal, i.e.,  $M_1=M_2$ , and they vary from 1.6 to 3.4, depending on the composition. From the high resolution superstructure images taken from the  $Cu_{55}Zn_{25}Au_{20}$  with  $M_1=M_2=2.0$ ,

we successfully derived a structure model which explains the intensities of all the superlattice reflections on the diffraction pattern, including the weak extra reflections. It is understood that the antiphase structure is basically of the  $Au_3Mn$  type. However, there is a strong tendency to avoid the formation of nearest neighbour pairs of Au atoms across the domain boundaries, and thus the two-dimensional density modulations are formed. This observation suggests a possibility of solving the structures of other compounds with non-integral M values.

**14.X-05** GAS ELECTRON DIFFRACTION: PRESENT STATUS AND FUTURE TRENDS. By Heinz Oberhammer, Universität Tübingen, West Germany.

For the past fifty years electron diffraction has been a powerful method for determination of molecular geometries. Apparatus and data analysis have been improved continuously and consequently accuracy and reliability of results have increased. The molecules studied by this method have increased in size and complexity. In recent years the combination of electron diffraction intensities and spectroscopic data (vibrational amplitudes and/or rotational constants) or theoretical results has been applied very successfully and will become even more important in the future. Very recent and future developments will include the study of molecules at very high temperatures, very low temperatures (molecular beam) and in excited states.

**14.X-06** ACCURATE MEASUREMENT OF DIFFRACTION INTENSITY AND ITS CONSEQUENCES. By M. Fink, The University of Texas, Center for Structural Studies, Austin, Texas, RLM 10.202, 78712, U.S.A.

During the last 5 years electron diffraction data from gaseous, molecular samples have been recorded with the special goal of achieving the highest accuracy which is obtainable with today's technologies. The results have been used successfully, addressing the following five questions of quantum chemistry. First: are experimental structure determinations still needed in spite of the great progress in quantum calculations (the case study, naphthalene)? Second: do diffraction data require additional corrections to include intramolecular multiple scattering when "harmonic" force fields are determined (the case study,  $Mo_2(O_2CCH_3)_4$ )? Third: can electron diffraction results contribute to the understanding of the multiphoton absorption process (the case study,  $SF_6$ )?

Fourth: are the anharmonic (cubic and quartic) force constants of the molecular potentials important in the description of the mean amplitudes of vibrations and the averaged mean atomic distances and their temperature dependence (the case study,  $CO_2$ )? Fifth: can electron diffraction data be used to derive molecular charge density distortion functions (the case study,  $O_2$ )? The answer

to all five questions is a conditional yes. This presentation will discuss the present situation and where further progress can be expected during the next five years, with special emphasis on even more precise data.