08.5-1 CRYSTAL STRUCTURE OF TWO MODIFICATIONS OF ζ-Mn_5Ge_2. By T. Ohba, K. Kifune and Y. Komura, Department of Materials Science, Faculty of Science, Hiroshima University, Hiroshima, Japan.

It has been found by the electron microscope observation that the high-temperature phase (ζ) of Mn_5Ge_2 has two modifications making parallel intergrowth with common a- and c-axes. (Kifune & Komura, Cryst. Res. Technol. 21 (1986) 1229-1234) Selected area electron diffraction patterns showed that they have different lattice constants along the c-axis ; i.e. one is 39 Å and the other 13 Å in the hexagonal cell. We call the former ζ_1 and the latter ζ_2. A mixed crystal of ζ_1 and ζ_2 shows double peaks in the temperature dependence of magnetization. The crystal structure of ζ_1 was determined using the specimen which showed no such double peaks in the magnetization (Komura et al., Acta Cryst. C43 (1987) 7-10).

The crystal structure of ζ_2 is determined using diffraction data derived from a mixed crystal of ζ_1 and ζ_2 since it is found to be difficult to isolate a pure single crystal of ζ_2. The analysis is performed on the assumption that the scattering from both crystallites is incoherent. The assumption has been proved to be valid by plotting the diffraction data obtained from a mixed crystal against the ones from pure ζ_1.

Crystal data of two modifications are as follows :

		a (Å)	c (Å)	Z
ζ_1-$Mn_{5.11}Ge_2$	(P3c1)	7.198(1)	39.227(4)	18
ζ_2-Mn_5Ge_2	(P3c1)	7.198(1)	13.076(1)	6

The crystal structures of ζ_1 and ζ_2 have been refined with final R=0.0557 and 0.0885 respectively, by full-matrix least-squares refinement. Both structures are characterized by two kinds of fundamental layers having three atoms stacked alternately along their c-axes. Additional atoms are placed on three threefold axes. The atoms in ζ_2-Mn_5Ge_2 are located in averaged positions for three parts of ζ_1 which are obtained by deviding the structure into one-third. Bottom figures show a comparison of the structure of ζ_1 and ζ_2 projected along [010]. Fundamental layers and three threefold axes are represented by horizontal and vertical lines, respectively. Mn and Ge atoms on threefold axes are represented by open and filled circles respectively. Kinds of atoms in the fundamental layers are shown beside the horizontal lines.