COMPLEX STRUCTURE OF Mg_2Al_3 β AND β' PHASES

J. Wolny [1*], M. Duda [1], and B. Kozakowski [1]

[1] *Faculty of Physics and Computer Science, AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland*

Keywords: Mg_2Al_3, Samson phase, hexagonal layers

**) e-mail: wolny@novell.ftj.agh.edu.pl*

The Samson phase structure is one of the most complex intermetallic structures. The first description of the β-Mg_2Al_3 structure was provided by Samson [1] in 60'. Because of its complexity and potential new technical applications, during the last few years the Samson structure aroused considerable interest among crystallographers. A good example of that interest is a review publication, written by 36 authors from 15 leading European laboratories [2].

Its cubic elementary cell (*Fd*-3*m*, no. 227 space group) contains 1168 atoms which are distributed over 1832 atomic positions. About 75% of atoms (879 to be exact) form the framework of the structure (skeleton atoms). The framework is made up of Samson's positions which are occupied by atoms with SOF equal to 1. The remaining 289 (25%) atoms partially occupy 953 positions with the average occupation probability of 30%. They form clusters arranged in an elementary cell in a tetrahedral lattice. Their structure has been described in detail in [2 and the following references] and in [3]. The lattice constant of the Samson structure is gigantic: $a = 2.8242(1)$ nm. At a temperature of 214°C, the structure undergoes a phase transformation to the rhombohedral β'-Mg_2Al_3 (space group *R*3*m*, no. 160, which is a subgroup of the *Fd*-3*m* group - index 4) with $a = 1.9968(1)$ nm, $c = 4.89114(8)$ nm. It should be pointed out that the constant *c* of a rhombohedral structure is practically equal to the length of the diagonal of the cubic structure $a_{\text{cubic}}\sqrt{3} = 4{,}89166\,\text{nm} \approx c_{\text{rhomb}}$. The near equivalence in length between the *c* axis of the rhombohedral β'-Mg_2Al_3 structure and the diagonal of the cubic β-Mg_2Al_3 is a consequence of lattice transformation connecting the hR cell of the β'-phase to the F cell of the β-phase.

Comparison of two different types of Mg_2Al_3 structure – cubic β and rhobohedral β' ones – leads to the conclusion that all skeleton atoms of a Samson structure don't change their position during the phase transformation. The skeleton atoms of a Samson phase lie within hexagonal layers [4]. These layers form three structural domains shifted with respect to each other by 1/3 of the length of the main diagonal of the cubic unit structure.

Besides within a hexagonal layer the length of every shift vector is a multiple of about 1/7 of the distances characteristic for hexagonal structures. Once the shift vectors were found, one could describe the structure as a modulated one.

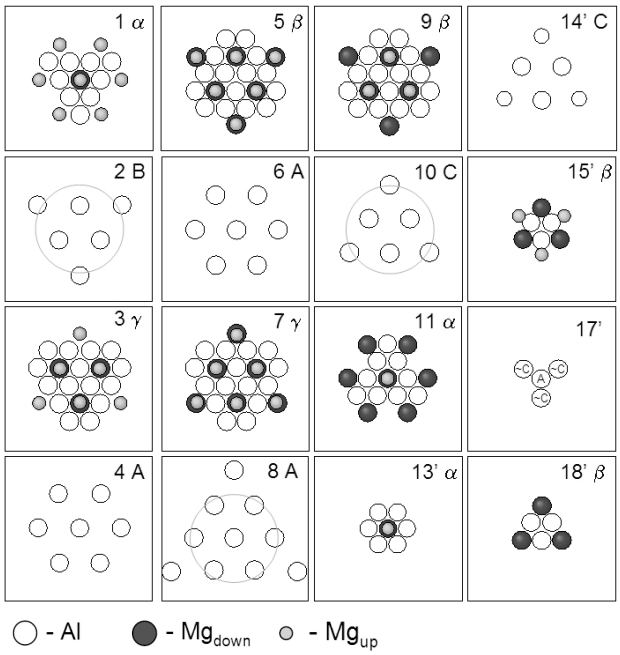

Figure 1. Eighteen layers forming a structural domain. Positions of Al and Mg atoms within the consecutive hexagonal layers for a structural domain of the Samson structure. Aluminium atoms take the hexagonal positions A, B, C. Magnesium atoms occupy positions which are shifted with respected to the Al layers.

References

[1] S. Samson, "The crystal structure of the phase ß-Mg_2Al_3", *Acta Crystallogr.* **19** (1965) 401–413.

[2] M. Feuerbacher *et al.*, "The Samson phase, ß-Mg_2Al_3 revisited", *Z. Kristallogr.* **222** (2007) 259–288.

[3] W. Sikora *et al.*, "Symmetry analysis in the investigation of clusters in complex metallic alloys", *J. Phys.: Conf. Ser.* **104** (2008) 012023.

[4] J. Wolny, B. Kozakowski, M. Duda, J. Kusz, "Stacking of hexagonal layers in the structure of β-Mg_2Al_3", *Philos. Mag. Lett.* **88** (2008) 501–507.