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Ordering of hexagonal layers in Mg_2Al_3 - β and β' phases

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Abstract

Two phases, β and β', around the Mg_2Al_3 composition have been compared. Structural rod-like domains composed of sets of hexagonal layers have been described. The main set containing 11 layers does not change during the β'- β transformation. The short sequences of layers presented on the β' phase transforms into clusters emerging in the β-phase. The centres of the domains form a superstructure with the modulation vector equal to 3/22.

1. Introduction

The Mg_2Al_3 compound has been intensively investigated by Samson [1] and many other authors (for the review see [2]). The β-Mg_2Al_3 Samson structure is an example of the complex intermetallic structures. Its crystal lattice is faced centred cubic - FCC (*Fd*-3m, no. 227 space group, a_c=2.8242(1) nm) and an elementary cell contains 1168 atoms distributed over 1832 atomic positions. The β-phase skeleton consists of 528 aluminium atoms and 351 magnesium atoms, for which the site occupation factor (SOF) is equal to one. As it has already been pointed out [3] the skeleton Al atoms form a sequence of hexagonal layers. The remaining 289 (25%) atoms partially occupy 953 positions with the average SOF equal to 0.3. Many of them belong to clusters which form a tetrahedral lattice. Their structure has been described in detail by Feuerbacher *et al*. [2] and the following references, and by Sikora *et al*. [5]. The Samson phase is stable at a temperature above 214°C.

At lower temperatures the structure of Mg_2Al_3 compound undergoes a phase transformation to the rhombohedral β'-phase (space group *R3m*, no. 160, which is a subgroup of the *Fd*-3*m* group - index 4) with a_r=1.9968(1) nm, c_r=4.89114(8) nm. Using rhombohedral unit cell and hexagonal coordinates for describing the FCC structure, one obtains the following values: $c_r/a_c=\sqrt{3}$ and $a_c/a_r=\sqrt{2}$ which are in very good agreement with the experimentally obtained ratio of β' and β phases lattice parameters. This also leads to the theoretical ratio of volumes of that unit cell equal to ¾, which perfectly fits to the same ratio obtained from the refinement of the diffraction patterns, equal to 0.74999. This means that there are only some local atomic position changes during the β-β' transition.

The crystal structures are close packed of hexagonal layers for both components of the Al-Mg intermetallic compound. The pure aluminium crystal lattice is FCC with the distance between the nearest neighbours equals 0.286 nm. In the case of Mg atoms, they crystallize in hexagonal closed packed structure (HCP) and the inter-atomic distance of the nearest neighbouring atoms is 0.319 nm. This value is about 12% larger than the corresponding one for the Al atoms. Both structures are close-packed, although they consist of differently arranged hexagonal layers: A, B or C. The sequence between these layers for the cubic structure is ABC, whereas it is AB for HCP. The local symmetry of the first neighbour's positions in the FCC and HCP structures is different, mainly due to the inversion. The

inversion symmetry of the nearest atoms presented for the FCC structure is not observed in the case of the HCP structure.

The hexagonal layer sequence in the β-Mg_2Al_3 structure has been published recently [3,4]. The 22 layers (only half of them, namely 11, are occupied by the skeleton atoms) form an object which is called a structural domain. The single rod-like domain consists of about five hundred atomic positions (many of them are only partially occupied). In that paper it was emphasized that there were three structural domains (called as: I, II and III) forming hexagonal superlattice in the basal (111) plane. The domains form a periodic sequence of the FCC type: I, II, III along the main diagonal ([111] direction) of the cubic unit cell. The relative distance between the centres of these domains is shifted by 1/3 of the length of the diagonal. All the length values were given in relation to the *z*-axis unit of the hexagonal reference frame which is equal to the length of the main cubic diagonal - for the β cubic phase, or its equivalent, lattice constant c_r - for the β' rhombohedral phase.

The present paper compares two phases, β and β', around the Mg_2Al_3 composition. The similarities and differences of the structures of those two phases are discussed. Detailed analysis is mostly concentrated on β' rhombohedral phase.

The paper presents the crystal structure analysis outcome performed on the elementary unit cell obtained from the study of the Mg_2Al_3 diffraction pattern. The study of Mg_2Al_3 diffraction pattern were performed by Feuerbacher *et al*. [2] and the atomic positions obtained by them were used. Different local atomic configurations consistent with the elementary unit have been discussed as well. Only the geometrical properties resulting directly from the atomic positions for β and β' phases have been discussed. The goal of this paper was to find some simple rules presented in such complex structures.

2. Hexagonal layers of a single domain

Normalized hexagonal reference frame to describe both β and β' structures are used. It follows that a new *z*-axis should be set for a cubic cell. It is presently directed along the main diagonal of a cube, i.e. [111] direction. The remaining two coordinates which describe a relative atomic position within the hexagonal plane (also called the base plane) are directed along the Cartesian coordinate system axes. The relations between the lattice constants are as follows:

$$x_1 = x_c\cos(\alpha_1) - z_c\sin(\alpha_1); \qquad y_1 = y_c; \qquad z_1 = x_c\sin(\alpha_1) + z_c\cos(\alpha_1); \qquad \alpha_1 = 45^\circ$$

$$x_2 = x_1; \quad y_2 = z_1\cos(\alpha_2) - y_1\sin(\alpha_2); \quad z_2 = y_1\cos(\alpha_2) + z_1\sin(\alpha_2); \quad \alpha_2 = \operatorname{arctg}\left(\sqrt{2}\right) \approx 54.74^\circ$$

$$x = x_2\frac{2.824}{1.997}; \qquad y = y_2\frac{2.824}{1.997}; \qquad z = \frac{z_2}{\sqrt{3}} \qquad (1)$$

where: x_c, y_c and z_c are atom coordinates written in the cubic reference frame. Atomic coordinates written for the β-phase in cubic and hexagonal reference frames can be found in Table 1. Atom coordinates occupying the rhombohedral β'-phase cell are normalized, as well, which allows the direct comparison of the positions for β and β' phases.

Domain	Samson positions	x_c	y_c	z_c	x	y	z	Description of layers
I	Al16	0.0348	0.0348	0.0348	0.0	0.0	0.0348	4
	Al22	0.1250	0.1250	0.1250			0.1250	6
	Al16	0.2152	0.2152	0.2152			0.2152	8
	Mg17	0.3162	0.3162	0.3162			0.3162	11
	Mg18	0.3808	0.3808	0.3808			0.3808	11
	Mg23	0.5000	0.5000	0.5000			0.5000	~14
	Mg23	0.7500	0.7500	0.7500			0.7500	~20
	Mg18	0.8692	0.8692	0.8692			0.8692	1
	Mg17	0.9338	0.9338	0.9338			0.9338	1
II	Mg23	0.2500	-0.2500	0.2500	0.0	0.5774	0.0833	~20
	Mg18	0.3692	-0.1308	0.3692			0.2025	1
	Mg17	0.4338	-0.0662	0.4338			0.2671	1
	Al16	0.5348	0.0348	0.5348			0.3681	4
	Al22	0.6250	0.1250	0.6250			0.4583	6
	Al16	0.7152	0.2152	0.7152			0.5485	8
	Mg17	0.8162	0.3162	0.8162			0.6495	11
	Mg18	0.8808	0.3808	0.8808			0.7141	11
	Mg23	1.0000	0.5000	1.0000			0.8333	~14
III	Mg18	0.3808	-0.1192	-0.1192	0.5000	0.2887	0.0475	11
	Mg23	0.5000	0.0000	0.0000			0.1667	~14
	Mg23	0.7500	0.2500	0.2500			0.4167	~20
	Mg18	0.8692	0.3692	0.3692			0.5359	1
	Mg17	0.9338	0.4338	0.4338			0.6005	1
	Al16	1.0348	0.5348	0.5348			0.7015	4
	Al22	1.1250	0.6250	0.6250			0.7917	6
	Al16	1.2152	0.7152	0.7152			0.8819	8
	Mg17	1.3162	0.8162	0.8162			0.9829	11

Table 1. Samson positions coordinates indicate the centres of the domains of the Mg_2Al_3 intermetallic compound. They are written in a cubic [2] and hexagonal reference frame. A number is assigned to each position (the last column). These are the numbers of particular layers – the same as in the other figures.

The single rod-like domains for Mg_2Al_3 compound β and β' phases are shown in Figure 1. It has already been proven for β phase [3,4] that the core of the domain consists of eleven parallel and evenly distant hexagonal layers occupied by skeleton atoms, for which SOF=1. A detailed analysis of the crystal structure of each layer is gathered in Table 2. There, one can find all domain I Al atom properties that belong to the β'-Mg_2Al_3 phase. The first column contains z coordinates of the layers. The next one stores the layers' identifiers: the number from 1 to 22, the position occupied: A, B or C and, when needed, a complex symbol (α, β, γ) that is formed by the given Al layer along with the neighbouring Mg layers. The

following columns contain numbers of atoms belonging to the layer within its inner part ($r \leq 0.22$) and within its outer part ($0.22 < r \leq 0.29$). These two parts are shown in Figure 2 and discussed bellow. Asterisk symbols indicate atoms which lie outside domain I and, therefore, which belong to neighbouring domains. Symbol *III-2B* describes domain III atoms of the 2B layer that grow into the area of domain I. The same description holds for other symbols written in italics.

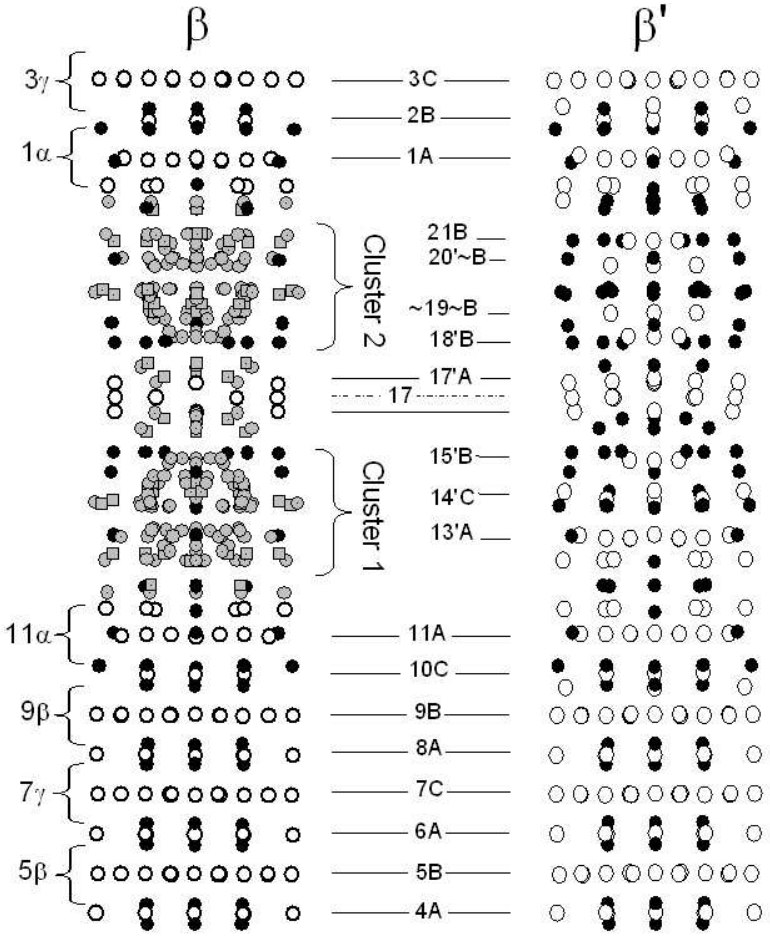

Figure 1. Single domain of Mg_2Al_3 intermetallic compound. The rod-like domain is oriented along the [111] direction for cubic β-phase and z-direction for the rhombohedral β'-phase. Open circles represent Al atoms, and full circles – Mg atoms. The black and white symbols describe atoms with SOF=1, grey symbols correspond to positions with SOF<1. There are 11 layers of Al atoms occupying A, B or C hexagonal positions for both phases. The Al layers with the neighbouring Mg layers form the α, β or γ slabs. Two cluster positions are marked for the β-phase. They correspond to short sequences of hexagonal layers in the β' phase, namely three 13'-15' layers and two 17'-18' layers.

z	symbol	$r \leq 0.22$ No. of atoms	$0.22<r\leq0.29$ No. of atoms
0.034	**4 A**		6
0.035		1	
0.078	**5 B (β)**		6
0.079		9	
0.124	**6 A**		6
0.125		1	
0.169	**7 C (γ)**	6	
0.170		3	6
0.214	**8 A**	1	
0.215			6 + 3*
0.259	**9 B (β)**	6	
0.260			6
0.261		3	
0.308	**10 C**	3	3*
0.353	**11 A (α)**	6	3
0.382	*III-M intergrowth*	*two identical layers*	6
0.438			6
0.463	**13' A (α)**	6	
0.508	**14' C**	3	
0.552	**15' B (β)**	3	
0.608	*III 2 B*		3
0.624	*17 M*		6
0.641	*II 10 C*		3
0.643	**17'~C**	3	
0.646	**17' A**	1	
0.694	**18' B (β)**	3	
0.721	*II-M intergrowth*	3	*two identical layers*
0,776		3	
0.804	**21 B**	3	
0.868	*II M*		6
0.898	**1 A (α)**	6	
0.902			3
0.942	**2 B**	3	0 + 3*
0.988	**3 C (γ)**	3	
0.989			6 + 3*

Table 2. A precise description of Al atoms positions within a volume of domain I for the β'-Mg_2Al_3 phase. In the table, there are: z-coordinates, a symbol of the hexagonal lattice and the numbers of atoms occupying positions within the inner area of the domain ($r \leq 0.22$) and within the outer area ($0.22 < r \leq 0.29$). An asterisk pertains to the number of atoms that come from domain I and lie outside its border.

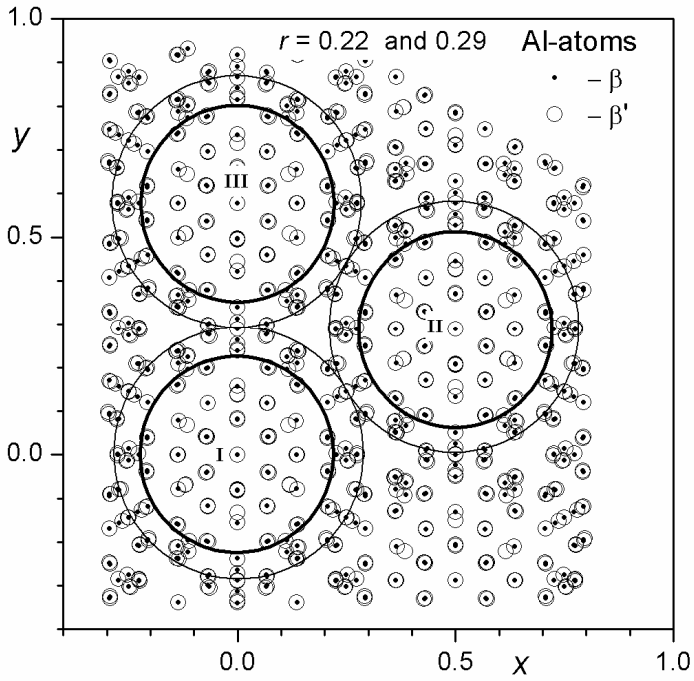

Figure 2. The skeleton Al atoms projected onto the (111) plane for the cubic structure β-Mg_2Al_3 (black dots) and compared to the projection of all Al atoms onto the base plane of the rhombohedral β'-phase (open circles). In the figure, three neighbouring domains I, II and III are marked. All values presented in the figures are in the units of rhombohedral lattice constant a_r. Circles with the radius $r = 0.22$ indicate the inner areas of the domains (the core of domains). The circles with radius $r = 0.29$ are tangential to each other. All points of the β-phase can also be found within the β'-phase. There are six β'-phase points within the inner area of each domain (open circles without dots in their centres – for details see also Figure 3) which do not belong to the hexagonal structure. These points cause clusters to form.

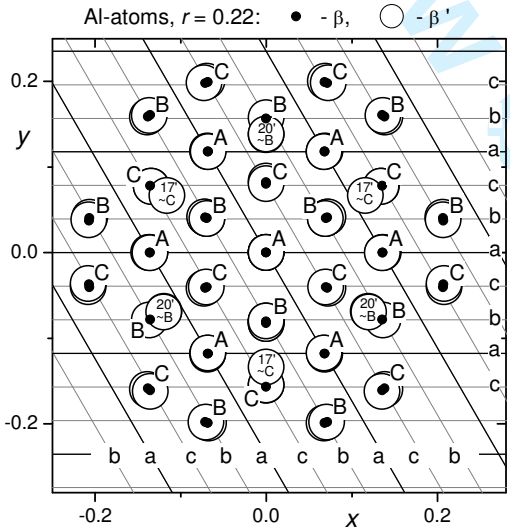

Figure 3. Similar as in Figure 2 but for single domain only. Lines a, b, c of hexagonal grid are also shown. Al atoms occupy A, B or C positions of the hexagonal lattice. Three atoms of layer 17' and three of layers 20' are shifted from the perfect hexagonal positions for the β' phase only.

Figures 2&3 show the skeleton Al atoms positions projected onto the base plane. Three neighbouring domains along with circles with the radii of 0.22 and 0.29 are marked respectively. The lengths of the radii are given as a relative number – a multiple of lattice constant a_r. The small circle with the 0.22 radius encloses an approximate inner area of the domain (a core of domain). The big circle with the 0.29 radius (the exact value: $\sqrt{3}/6 \approx 0.2887$) determines the maximum radius value of the circles which are associated with domains and tangent to each other. The region between 0.22 and 0.29 is an outer part of the domain. The core of the domain is occupied by Al and Mg atoms. Excluding six β'-phase Al-atoms, all other atoms occupy commensurate positions of the A, B, or C of hexagonal layer within each domain. The same positions are occupied in both the β and β' phases. Six positions are marked in Figure 3 as 17' and 20' (see also Table 2) are incommensurate with the other ones, which lead to a clusters' creation for β-phase (Figure 1).

The α, β and γ complexes (Figures 1, 4 and 5) consist of a slab of three hexagonal layers occupied in the Mg/Al/Mg sequence. There are gaps occupied by Mg atoms within the middle layer, among Al atoms (Figures 4 and 5). The Mg layers are shifted by 0.06 along the *z*-direction with respect to the Al layers. This is so because the Mg atoms atomic radius is nearly 12% larger than the Al ones. Consequently, Al gaps are too small for Mg atoms. There is not enough space for them within a common hexagonal layer. Mg atoms situate themselves either above or below the hexagonal Al layer forming the complex. The α complex contains only A-type atomic positions. The β and γ complexes closely resemble the α complex, however, in their case, these are positions B (for β) or C (for γ) that are taken.

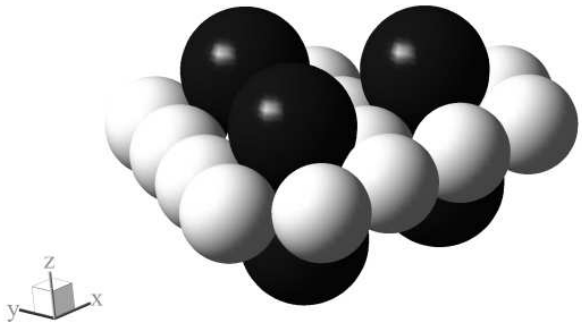

Figure 4. The central part of 3γ slab of the Mg_2Al_3 structure. Hexagonal rings of Al atoms with Mg atoms placed symmetrically in the centres of hexagons. All the atoms are placed in C positions of the hexagonal lattice. For α or β complexes the atoms occupy the A or B positions respectively.

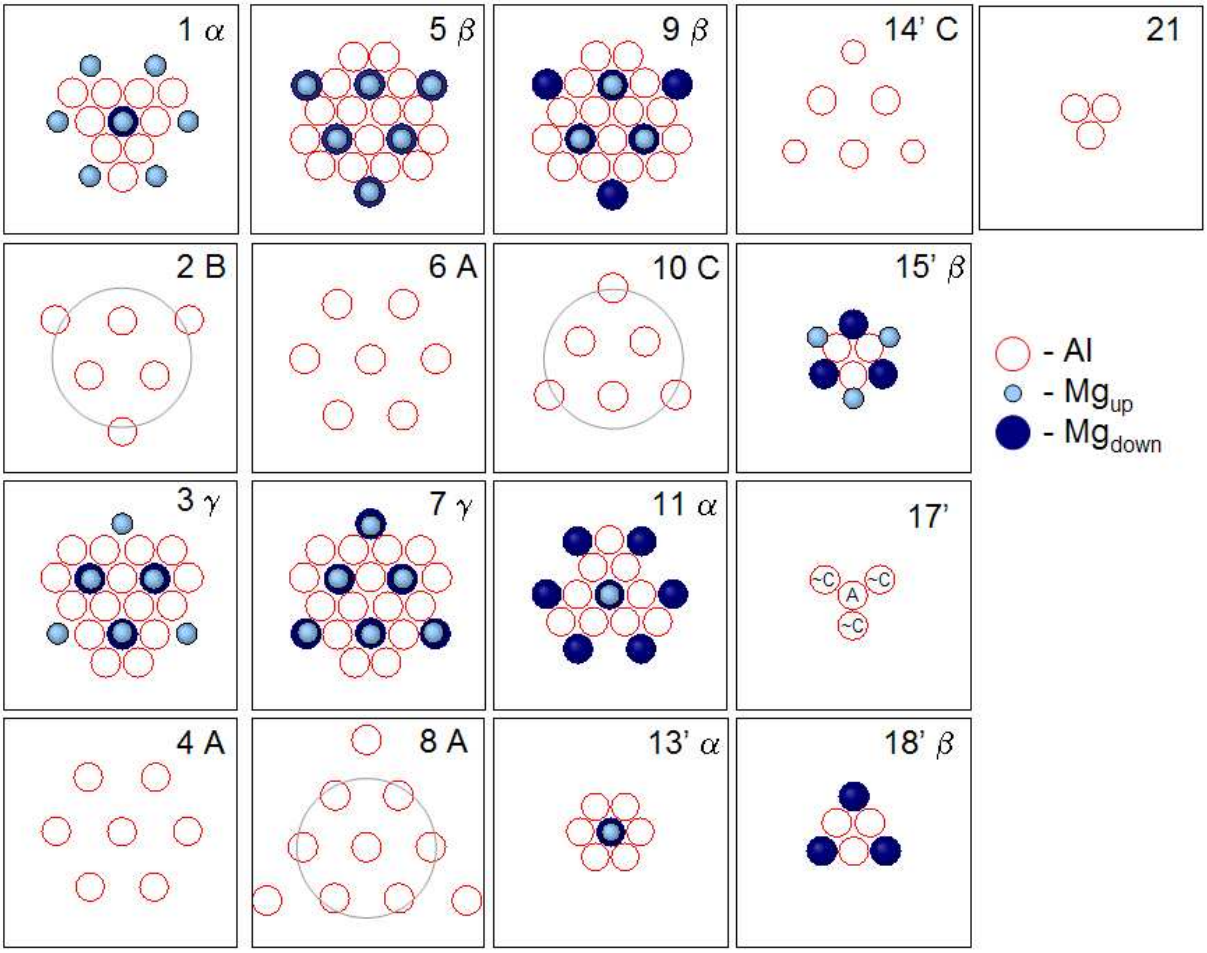

Figure 5. Cross-sections of individual hexagonal slabs presented in Figure 1. A cross-section is a hexagonal layer of Al atoms (open circles). There are gaps among these atoms. Each gap is occupied by a pair of Mg atoms (full circles). The first Mg atom of a pair is positioned above the cross-section and the other one below it. For layers: 2B, 8A and 10C, additionally, circles with radius $r = 0.22$ are marked. The central part of 3γ slab is presented in Figure 4.

There are hexagonal layers of type A, B or C filled partially by Al atoms in such a way that only every second position is occupied between the α, β and γ complexes (see even layers in Figure 5). If one considered three neighbouring layers of different atoms, e.g. layers 1-2-3, a sequence $A_{Mg}B_{Al}C_{Mg}$ is observed, where the Al atoms occupy every second position of the B-type positions, and Mg atoms – accordingly, every second A or C-type positions. The same holds also for other groups of layers: 3-4-5, 5-6-7, 7-8-9, and 9-10-11. Such a sequence (ABC) of half occupied hexagonal layers by the same type of atoms is typical for a body centred cubic structure (BCC).

For Mg_2Al_3 (both phases β and β') the resulting main sequence of 11 layers is as follows: 1α2B3γ4A5β6A7γ8A9β10C11α. The middle part of this chain consists of a regular sequence: 3γ4A5β6A7γ8A9β. Such a sequence of hexagonal layers resembles a double hexagonal closed packed structure (DHCP) with an ABAC sequence of hexagonal layers. The DHCP structure crystallizes some pure elements such as neodymium or praseodymium. The set of 11 layers corresponds directly to the Laves C36 and C14 phases. The central part of the set forms the C14 phase, while the two edges consist of two halves of C36.

In the case of Mg-Al intermetallic compound the main sequence of 11 hexagonal layers does not change during the transformation from β' to β phase. It is easy to show (Figure 6) that this part of the structure can be also constructed with the Friauf polihedra. The Friauf polyhedron describes very stable local configuration as it was discussed by Feuerbacher et al. [2]. The problem which arises is, however, the chemical composition of the compound. If the entire space is filled by Friauf polyhedra, the ratio of Mg atoms to Al atoms would assume a 1:2 value. Compared to the real ratio 2:3, the Mg atoms would be in deficiency. The chemical balance is restored by Mg atoms scattered within the outer parts of the structural domains. It should be emphasized here that the actual chemical composition of the studied sample was not fully stoichiometric – it was equal to $Mg_{38.5}Al_{61.5}$ [2].

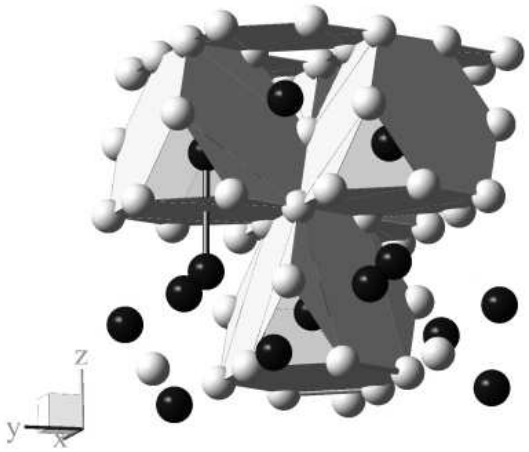

Figure 6. The Friauf polyhedra built on sequences of Al and Mg hexagonal layers of an Mg_2Al_3 single domain. Alumina atoms (light balls) form hexagonal layers 1A, 2B, 3C, 4A and 5B shown in Figures 1 and 5. Magnesium atoms (dark balls) belong to slabs 1α, 3γ and 5β.

Outside the region of the 11 ordered layers discussed above, there is an area where the structure of β and β' phases is significantly different.

The low-temperature β'-phase (Figure 1) is a more ordered structure. At the end of the main sequence (main chain) of 11 layers, one can observe transitional areas where Al and Mg atoms swap places. The narrow transitional area changes afterward into two short chains of hexagonal layers (Figure 1). They are: a three-layers chain (layers no. 13', 14' and 15') and a two-layers chain (layers no. 17' and 18') separated by an intermediate area. These two chains are short copies of the main chain. They keep the inter-layer distances; however, they are shifted, as a whole, with respect to the 22 reference layers. Layer 17 is filled with Al atoms occupying mixed positions marked by the letter M (Table 2). Such mixed positions are some commensurate positions described by intersections of different types of the hexagonal grid-lines a, b or c shown in Figure 3.

The clusters are formed in the β-phase outside the main chain of 11 hexagonal layers as it is shown in Figure 1. They are conglomerates of atoms which partially occupy their atomic positions in most cases (SOF<1). In Figure 7 more details of the cluster are shown. When selecting some Al atoms from the amorphous cloud a BCC-type surrounding of the Mg central atom can be found. One should remember that the BCC structure also consists of

hexagonal layers. The second-neighbour interaction favours the BCC-type arrangement of atoms instead of close-packed structures.

The space between the well ordered hexagonal layers and the clusters (Figure 1) are filled with Mg atoms which partially replace the outer Al atoms (this is the case of layers no. 11 and 1). Conversely, within the neighbouring Mg layers, Al atoms partially replace the outer Mg atoms. This replacing mechanism leads from 11 ordered hexagonal layers to some crystalline disorder and a formation of the atomic clusters for the β-phase.

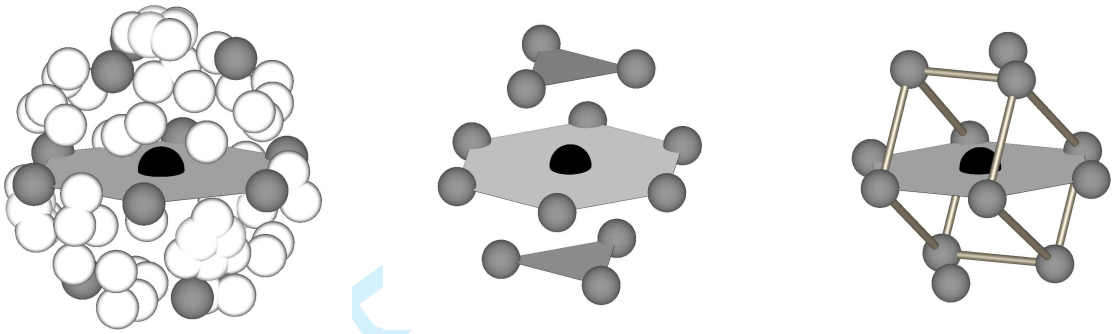

Figure 7. (left) The local arrangement of atoms for the Mg_2Al_3 β-phase clusters. A magnesium atom (dark ball with SOF=1) is placed in the centre of the cluster. The other atoms (Al and Mg with SOF<1) form an aperiodic cloud of atoms. Selected Al atoms (grey balls) with the central Mg atom form a local BCC-type atomic arrangement (right).

Having compared the β and β' phase's domains in Figure 1, a rather straight-forward conclusion follows: the Mg_2Al_3 compound structural stem is a set of stacked hexagonal layers filled interchangeably by Mg and Al atoms. In the case of the β'-phase (the lower-temperature phase) these layers are arranged into shorter and longer sequences of hexagonal layers and a transition from one sequence to another is realized by exchanging one type of atoms for another: Al for Mg and Mg for Al. There are so many possible combinations of the atomic layers arrangement that the exact periodicity along the z-axis may actually never occur. On the other hand, when an average structure is taken into account, one needs to include both shorter and longer atomic layer sequences into the structural model. This results in a very large elementary cell.

The structure becomes defected above room temperature. The defects destroy the initial layers periodic sequence. At higher temperatures Al atoms can easily swap positions between A and B (layer 2B instead 2A) or C (layer 10C instead of 10A). Position A should be rather expected for all even layers, as it is observed for 4A, 6A or 8A. Such a change of positions does not involve a considerable amount of energy. The change of energy would be equal to zero for a perfect set of close-packing spheres. Therefore, Al swaps can easily occur at the temperatures which are only slightly higher than room temperature. This kind of structural defect terminates the main chain of hexagonal layers and consequently layers 2B and 10C are the last even layers in this chain.

3. Super structure of domains

The basic hexagonal rings with the atomic distance a_0 are shown for a single domain in Figure 5. An average distance a_0 can be established by adjusting the hexagonal rings to the atoms' coordinates. Having done that for the 11 consecutive layers of the main chain, the value of this constant can be estimated as $a_0 \approx 0.1368$ (see also Table 3). This value is identical to the lattice length a of close-packed spheres arranged along the c_h into 22

hexagonal layers. The distance between two neighbouring layers can be expressed as $a\sqrt{2/3}$ for such a structure. This relation leads to the lattice constant value:

$$a = \frac{1}{a_r} \times \frac{c_r}{22}\sqrt{3/2} = 0.1364 \approx a_0 \qquad (2)$$

which is nearly equal to the one given above. The average value of near-neighbours distance (a_0) obtained for Al-atoms projected into hexagonal plane, equal to 0.273 nm, is only slightly smaller (about 4%) than the near-neighbours distance observed for the FCC aluminium structure (0.286 nm). The a_0 value is exactly 22/3 = 7.3(3) times smaller than the hexagonal lattice constant a_r, as illustrated in Figure 8. In this figure, the projected positions of 9B layer's atoms which belong to different domains are marked by symbols connected by thin lines. The 22/3 times larger superlattice (thick lines) connects the centres of the domains and stands for the in-plane hexagonal unit cell of Mg_2Al_3 compound.

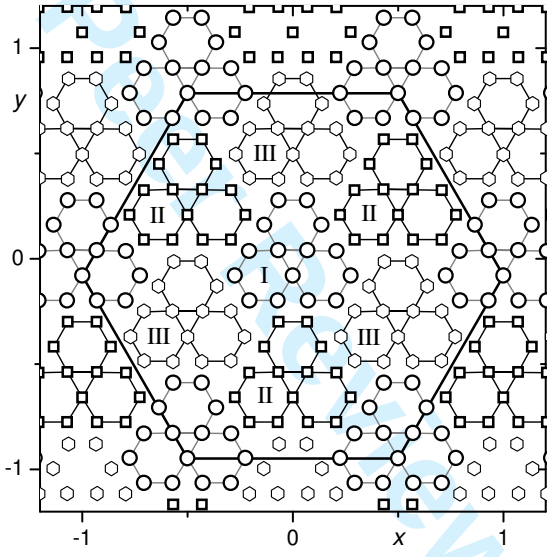

Figure 8. The centres of the domains form a hexagonal superstructure (a big hexagon marked by thick lines) which is 22/3 bigger than the size of the hexagonal rings (thin lines) of the individual domain. Atoms of layers 9B of the neighbouring domains are shown within a common plane. Small thick circles represent Al atoms of domain I, thick squares – atoms of domain II, and thin hexagons – atoms of domains III. All the experimentally determined atomic positions fit perfectly to the superstructure model.

Layer	a_0	a_0'
1 A	0.1369	0.1369
2 B	0.1356	0.1364
3 C	0.1375	0.1381
4 A	0.1373	0.1372
5 B	0.1368	0.1356
6 A	0.1367	0.1371
7 C	0.1368	0.1387
8 A	0.1374	0.1376
9 B	0.1375	0.1368
10 C	0.1356	0.1345
11 A	0.1369	0.1374
$\bar{a}_0$	**0.1368** (2)	**0.1369** (3)

Table 3. Hexagonal lattice constants adjusted to 11 layers of the main chain of the β-Mg_2Al_3 phase (a_0) and β' (a_0')

4. Conclusions

The Mg_2Al_3 intermetallic compound structure is built with rod-like domains. The core of each domain contains the main set of 11 hexagonal layers. The structure building element is a hexagonal ring of aluminium atoms completed with magnesium atoms, as shown in Figure 4. The structure forms a sequence of Al hexagonal layers (with holes) separated by appropriate Mg layers. An arrangement of such building blocks can be also described by the Friauf polyhedra which are very common for the Laves C14 and C36 phases. The main chain of 11 layers does not change during the β'-β transformation. The problem is, however, with the concentration of atoms in the core of the eleven layers. The concentration corresponds to $MgAl_2$ rather than Mg_2Al_3. The magnesium atoms are in deficiency and they are mostly located in outer part of the domains.

During the transition from β to β' the skeleton atoms do not change their positions. The origin may come from the bonding nature in Friauf polyhedra [7]. The dimensions of the corresponding hexagonal unit cells for both β and β' phases are identical which is in controversy to a statement about expansion and contraction of some fragments observed in $MgCu_2$ [2]. There is a change of the two clusters of the single domain into short sequences of hexagonal layers, different for each cluster. Such transformation of the clusters' structure leads to the symmetry reduction from cubic (β) to rombohedral (β')

One can distinguish an FCC-type superstructure for the Mg_2Al_3 compound. The superstructure lattice constant in the base plane is commensurate with the hexagonal lattice constant for Al atoms, with the ratio between them equal to 22/3. Along the *z*-direction the neighbouring domains are shifted by 22/3 of the distance between the hexagonal layers of Al atoms. Such a superstructure, together with the symmetry of individual domain, is responsible for very big unit cell with a cubic or rhombohedral symmetry. The appropriate modulation vector is equal to 3/22.

The structural features similar to the Samson structure's have already been observed in some other complex phases, e.g.: Cu_4Cd_3 [6] or $NaCd_2$ [8] where the regions corresponding to the hexagonal domains consisted of fragments of the Laves phase structures. The Laves

structures are frequently described in terms of the stacking of hexagonal layers. Additionally, it is probable that the skeleton atoms which form hexagonal layers play an important role for other Laves phases. For example, there should be a certain simple explanation of the commensurate modulated vectors for Mg_2Al_3 and $Mg_{17}Al_{12}$ described by Donnadieu *et al*. [9].

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