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Full Length Article

3d-visualization of magnesium strengthening mechanisms for a description of experimentally obtained data of alloying effect in Mg-Ga system

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Abstract

Based on laws of theory of materials strengthening were discribed the experimentally obtained alloying effect in Mg-Ga system and shown using program for 3d atomic structures.

As known from our experiments a homogeneous "wavy" microstructure of the diffusion zone forms as result of mass-transfer of molten gallium into the volume of magnesium alloys. SEM chemical composition shows Mg 65% wt. and Ga 35% wt. and X-ray spectra diffraction data - Mg_5Ga_2 intermetallic phase formation. Such intermetallic diffusion zone provides the significant strengthening effect of microstructure which was determined experimentally by the indentation method.

The 3-d visualization shows the reaction and changing of an original crystal structure of magnesium atomic lattice upon diffusion doping with foreign atoms of gallium and then is shown the coalescence of Mg_5Ga_2 intermetallic crystal with crystals surfaces of Mg-matrix. So, investigated Mg-alloy strengthening at alloying with Ga explained by two main factors. At first is the formation of intermetallic phases with the ordering and consolidation of the crystal structure of the matrix by the ligature atoms, which is the key factor of the strengthening mechanism fixed experimentally. Second, when hexagonal and orthorhombic atomic structures growth according to their spatial type, a significant disorientation of structural fragments occurs, an increase in the density of the amorphous transition layer, a twinning of the structure in the interphase boundaries, which leads to the formation of intrinsic mutual deformation and a high level of internal stresses.

Keywords: Magnesium; Gallium; Alloying; Strengthening; Atom; 3d.

1. Introduction

The aim of the study is to attempt to visualize the experimentally fixed effect of doping in the Mg–Ga system during the formation of intermetallic phases, which increase the hardness and elasticity. Classical theoretical descriptions of the mechanisms of intermetallic and intergranular hardening were used, as well as the capabilities of a three-dimensional atomic simulation program for constructing crystal structures of phases. It should be noted that gallium, from a fundamental point of view, is on the boundary between metals and semimetals, therefore it is a good model object for understanding the nature of the chemical bond in intermetallic compounds for research relationships between the structure and materials physical properties [1].

Such chemical interaction studied has applied values - gallium used as an activator in diffusion welding of Mg-alloys and other metals.

2. Experiments

Previous studies [2] have shown that when applying a thin layer of molten gallium and heating up to 300°C in a magnesium alloy of the Mg-Al-Zn system forms the diffusion zone with a width of up to 100 μm (Fig. 1) with a microhardness increasing of 1.5-2.0 GPa and Young's modulus 50-72 GPa, at values for the base magnesium alloy respectively: 1.2 GPa and 43 GPa. The SEM chemical composition of the diffusion

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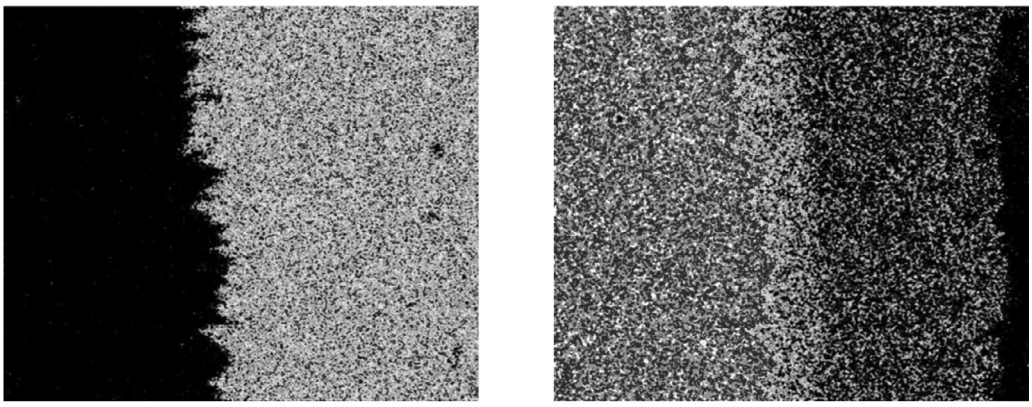


Fig. 1. SEM maps of the Ga (a) distribution in Mg alloy (b).

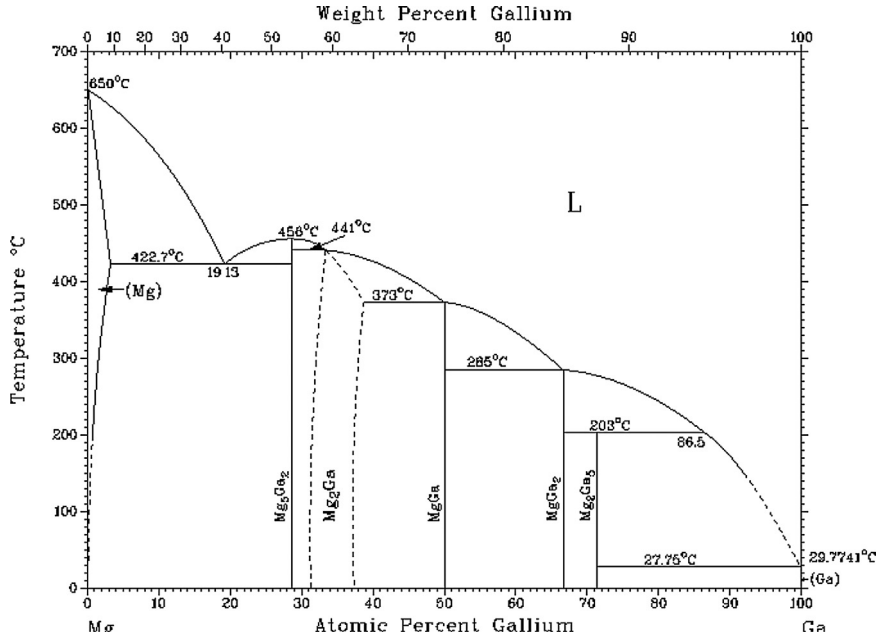


Fig. 2. Binary diagram Mg-Ga.

zone can be Mg_2Ga and Mg_5Ga_2 intermetallics according to binary diagram (Fig. 2).

According to Mendeleev's Periodic Table, gallium in alloys of the Mg-Al-Zn system forms chemical compositions only in pairing with magnesium, therefore the process of strengthening is considered only in the Mg-Ga system.

Physical and computer simulations of such interaction were carried out for the exact determination of the physicochemical mechanisms of strengthening at the interaction of gallium with magnesium alloy. Physical modeling was to study the phase composition of the alloy formed by the interaction of magnesium with gallium in the remelting [3]. Computer simulation will allow visualization at the atomic level of phase mechanisms of strengthening during the construction of crystalline lattice of phases, the type and crystallographic characteristics of which will be determined in the experimental part of this study by the X-ray method.

The presence of two types of structures is found on the cross-section of the ingot (Fig. 3): globular "dark" grains of the primary structure and an intergranular "light" eutectic of a secondary structure with irregular morphology. Indentation test fixed hardness 1.2-2 GPa and Young's modulus 43-73 GPa. The X-ray diffractograms (Fig. 4) showed the presence of the composition:

- 32.54 wt.% Mg_5Ga_2 (a = 13.6935 Å; b = 7,0220 Å; c = 6.0284 Å);
- 67,5 wt.% Mg (a = 3.1941 Å; c = 5.1879 Å).

From the fundamental positions [4–9] we know that the effect of strengthening during doping is associated with an increase in the density of atoms and their ordering after the crystallization of the alloy. The foreign atoms in the crystalline lattice of the base metal are the centers of the

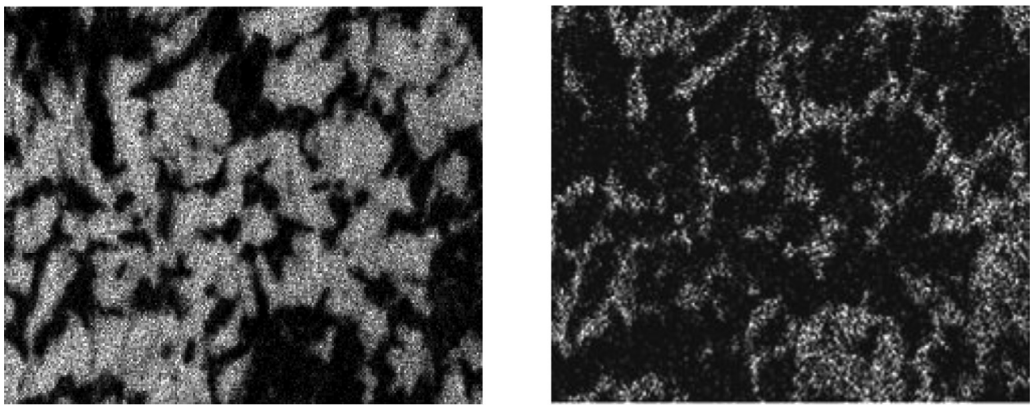


Fig. 3. SEM maps of the Ga (a) distribution in Mg alloy (b).

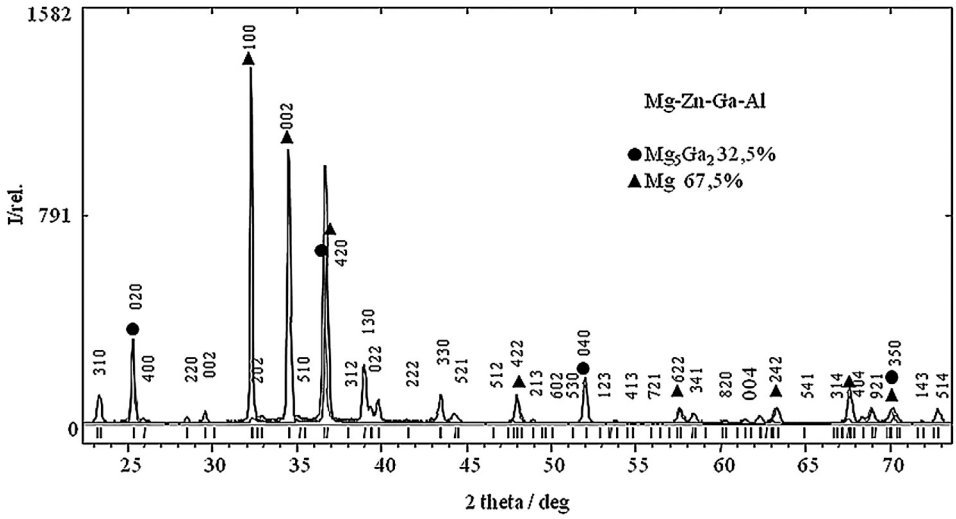


Fig. 4. Mg-Ga alloy X-ray diffraction.

deformation which creates an elastic field of stress around them. More precisely, the effect of compaction of the crystal lattice is due to the difference in the size of the atoms and the increase in the frictional forces between them.

3. Modeling

From the chemical point of view atom is the smallest electroneutral chemically indivisible particle of a substance that can be observed using electron microscopes. For atoms that form solid crystals the distance between adjacent nodes of a crystalline lattice can be approximated by their size. As a rule, it is difficult to fix the exact configuration of the crystalline structure by experimentally obtained diffraction due to the presence of plenty of areas with sufficient atomic density to represent X-rays, which can cross the plane at different angles and fix the distorted diffraction image. Therefore, imaging of the Mg_5Ga_2 phase which provides for the strengthening of the diffusion zone was carried out using the computer program ChemSite3.1, the theoretical and mathematical provisions of which are described by base physical law.

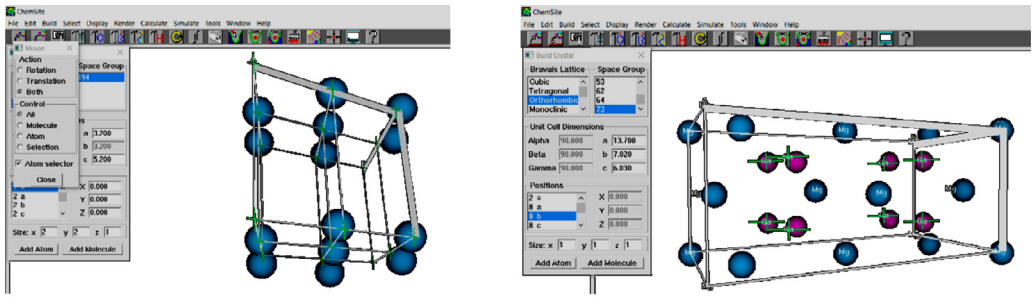
The program allows you to build images of two factors that contribute to strengthening:

1 – crystallographic parameters;
2 – growth of atomic structures of different volumetric-spatial type.

The main properties of the atoms considered in the system are known:

- Mg (Fig. 5a) – radius atom 160 pm, crystal lattice is hexagonal, Young's modulus 43 GPa;
- Ga – radius atom 141 pm, crystal lattice is orthorhombic, Young's modulus 40…50 GPa;
- Mg_5Ga_2 (Fig. 5b) – atoms ratio in orthorhombic crystal lattice [1] optimized to 8 atoms Mg and 4 Ga, Young's modulus 50…73 GPa.

Well known that the strength of pure metals is determined mainly by the electronic structure of atoms and the type of their interaction [4,5]. The effect of strengthening during alloying is associated with an increase in the density of atoms



a b

Fig. 5. Crystal cells: matrices - hexagonal (a) and phases - orthorhombic (b).

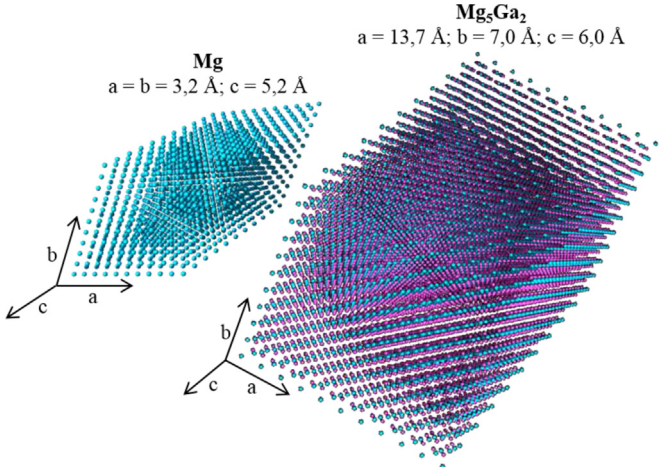


Fig. 6. Volume and density differences for 10 periodical crystal cells of Mg hexagonal and Mg_5Ga_2 orthorhombic phase after its compaction.

and their ordering after crystallization of the alloy. More clear description of the alloying effect - atoms compaction in the matrix crystal lattice by foreign atoms (Fig. 6) and the difference in atom size forms increase of friction between them which leads to a decrease in the mobility of atoms and constrains the mobility of dislocations. Therefore, foreign atoms are the centers of the deformation of the lattice and creates an elastic field of stress around them in the crystalline lattice of the base metal (Fig. 6).

For strengthening mechanism characterization of $67.5Mg + 32.5Mg_5Ga_2$ (% wt.) alloy it's should be considered the transition regions of the atomic structures of the matrix and phase. A completely arbitrary polycrystal without texture has a characteristic distribution of the orientations of boundaries, however, such cases are rare and most of the material will be different from this idealized representation to a greater or lesser side.

The boundary can be formed by single adjacent grains or crystallites [8,9]. It is likely that these boundaries are classified into a mixed type with an inclining component and torsion component. The thickness of the boundaries, as a rule, is estimated at 5 ... 20 interatomic distances (~100 Å). Fig. 7 shows a fragment of the consolidated boundaries of crystalline structures of Mg, Ga and Mg_5Ga_2.

Table 1
Ab-initio Young's modulus of Mg-Ga intermetallics [11].

Phase	Mg_5Ga_2	Mg_2Ga	MgGa	$MgGa_2$	Mg_2Ga_5
Young's modulus, GPa	56.5	52.1	52.9	50.2	74.8

Fig. 8 shows how formed the boundary between Mg hexagonal and Mg_5Ga_2 orthorhombic lattices with a significant angle of divergence, which occurs with the growth of crystals according to their volume-spatial type. The transition structure is formed by twin boundaries between the crystals when the atoms of one structure are on the surface of the partition. The twin layers at the coherent boundary of the reorientation of the crystal structure are very characteristic for a cast metal. The boundaries of two crystalline regions of different orientation are amorphous and contain fragments of atoms of both types.

On the contact surface of two different crystalline phases, the connection (cohesion) of crystalline lattices arises and remains. Areas with different spontaneous or proper deformations occurring in the solid phase when it is formed inside or on the surface of another solid phase are elastic domains. Due to the difference in the proper deformations of the phases, this surface is the source of internal stresses that extend over the distance, compared with the length of the contact surface (long-range field). Some another ab-initio result [10] confirm the mechanical stability against small distortions in such intrinsic twin boundary structures.

Also, obtained in an experimental part of our work results in good correlated with other researcher's data (Table 1), which predict the elastic and diffusion properties constants of Mg-based alloys using a stress-strain method.

Thus, 3d visualization of structures at alloying of magnesium alloy by gallium shows a significant reorientation of structural fragments (Mg and Mg_5Ga_2), significant density increases of the amorphous transition layer of interphase boundaries, which means contains a high level of internal stress and strengthening of the microstructure what was fixed experimentally by indentation method.

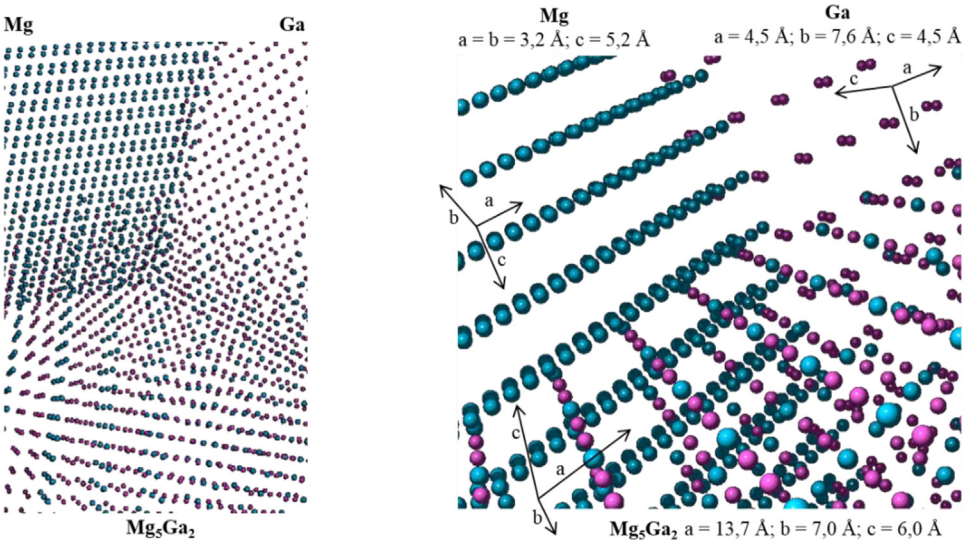


Fig. 7. A fragment of the consolidated boundaries of crystalline structures Mg, Ga and Mg_5Ga_2.

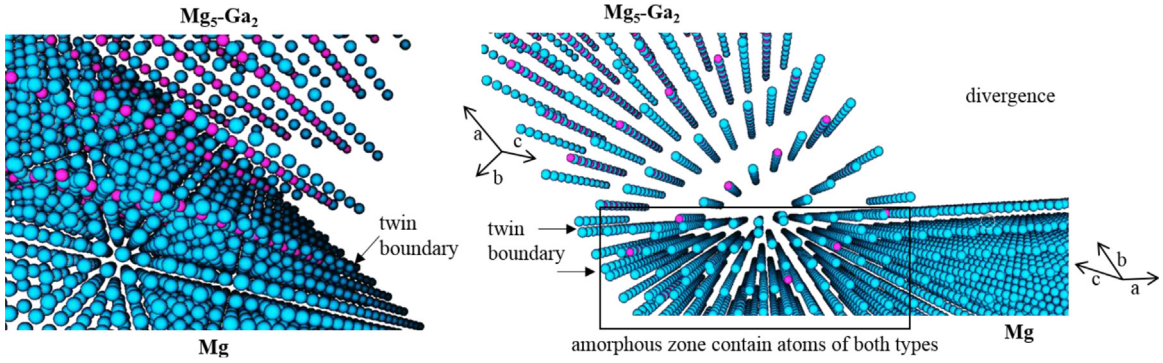


Fig. 8. Fragments of the amorphous boundary of the hexagonal crystalline structure of Mg and orthorhombic Mg_5Ga_2 with a significant angle of reorientation, which arises when the crystals grow according to their volume-spatial type.

4. Conclusions

Computer model allowed to visualize the effect of strengthening consisting of two main factors: 1 - the volume formation of the intermetallic phase Mg_5Ga_2 with the ordering and compaction of the crystalline structure of the Mg matrix at alloying by foreign Ga atoms; 2 - increasing the density of the amorphous transition layer at volumetric-spatial changes with significant angle of divergence which forms between boundaries of Mg hexagonal and Mg_5Ga_2 orthorhombic lattices according to their crystallographic characteristics.

Of course, obtained visualizations do not consider real and complex interactions at a distance (for example, electrostatic) and the laws of crystallization of multicomponent real chemical systems of the micro-macro levels. However, such results well explained fundamental key factors of experimentally obtained and studied alloying effect at crystallization Mg-Ga binary system.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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