Cellular Automaton Finite Element Method 
Applied for Microstructure Prediction of 
Aluminium Casting Treated by Laser Beam

J. Hajkowski *, P. Popielarski, Z. Ignaszak
Poznan University of Technology, CAD/CAE of Material Technology and Foundry Laboratory,
3 Piotrowo Street, 60-965 Poznan, Poland
* Corresponding author: Email address: jakub.hajkowski@put.poznan.pl

Received 16.06.2019; accepted in revised form 01.08.2019

Abstract

What is the limit of improvement the structure obtained directly from the liquid state, with possible heat treatment (supersaturation and aging)? This question was posed by casting engineers who put arbitrary requirements on reducing the DAS (Dendrite Arm Spacing) length to less than a dozen microns.

The results of tests related to modification of the surface microstructure of AlSi7Mg alloy casting treated by laser beam and the rapid remelting and solidification of the superficial casting zone, were presented in the paper. The local properties of the surface treated with a laser beam concerns only a thickness ranging from a fraction to a single mm. These local properties should be considered in the aspect of application on surfaces of non-machined castings. Then the excellent surface layer properties can be used. The tests were carried out on the surface of the casting, the surface layer obtained in contact with the metal mould, after the initial machining (several mm), was treated by the laser beam. It turned out that the refinement of the microstructure measured with the DAS value is not available in a different way, i.e. directly by casting. The experimental-simulation validation using the Calcosoft CAFE (Cellular Automaton Finite Element) code was applied.

Keywords: Cellular automaton, Dendrite arm spacing, Remelting by laser beam, Aluminium alloys, Tribology

1. Introduction

The aluminium alloys are widely used in the automotive and aerospace industry. The products made of these alloys should be characterized by good mechanical and tribological properties, effective wear resistance resulting from structure compactness. One of the special features of the casting is the structure gradient and thus the gradient of the mechanical properties [1]. These different properties are obtained by mould materials diversification (e.g. chills application).

Currently, the requirements of casting customers regarding the high compactness of the structure are increasing and there is a demand for the finer structure (expressed by low DAS – Dendrite Arm Spacing). Unfortunately, often these values cannot be achieved only by adapting conventional industrial casting methods. It is therefore necessary to explore other tools/methods to achieve the desired good properties. One of techniques that meets these expectations is a laser remelting of the thin surface zone, e.g. described by [3-5].

The tests related to laser modification of the local casting structure by rapid: remelting and solidification (due to fast cooling) of A356 (AlSi7Mg) alloy casting were performed. The
microstructure of the laser treated casting was characterized by DAS value of a few microns (one order of magnitude lower with respect to the origin casting structure). The microstructure studies were supplemented with microhardness tests in remelted and non-remelted zones. A satisfactory increasing of the microhardness was achieved in the laser treated zone and it confirms the improvement of cited characteristics, including the tribological properties.

2. Experimental procedure

The scheme of sample preparation to carry out the laser beam treatment is shown in the Fig. 1 and 2. The following laser was applied during the test: Trumpf TruLaser Cell 3008 with laser generator TruDisk 1000. An ingot made of AlSi7Mg alloy in the laser treated surface is characterized by the DAS value decreasing in order of magnitude (from few tens to few microns). This type of the structure modification and improvement of the local properties is unique as a kind of heat treatment with remelting.

Fig. 1. Gravity die-casting process (a) and sample preparation for the laser beam treatment (b)

The sample cut from the gravity die-cast made of the AlSi7Mg alloy and treated using a laser beam remelting was subjected to additional experimental tests, namely the microhardness tests. For the selected bead of the laser beam treatment using the polished cross section, the load of 0.025 kg and 0.050 kg during 15 seconds was applied, both in the remelted area and, comparatively, in the non-remelted casting zone. Authors consider two selected beads i.e. no.1.2 and 5.2. The laser value parameters were as follow for bead no1.2: laser power - 600 W, collimation beam = 10, diameter of laser spot - 1,09 mm, feed rate - 5,5 mm/s, energy per surface - 100,1 J/mm² and for bead no 5.2: laser power - 600 W, collimation beam = 10, diameter of laser spot - 1,09 mm, feed rate - 7,5 mm/s, energy per surface - 73,4 J/mm². The distance between singular beats was 1 mm.

Fig. 2. Samples cut from the casting and arrangement of individual beads
The microstructures and microhardness results are shown in the micrographs (Fig. 3-5). On this basis it can be stated that microhardness values are higher in the remelted zone than in the non-remelted zone. This is a result of the better structure compactness in this zone. Approximately a tenfold decrease of the space between the dendrite arms, i.e. from 30÷40 µm to 2÷3 µm (DAS 2) occurred due to an extremely rapid heat transfer from the remelted layer to non-remelted zone.

Fig. 3. Photographs of polished cross-sections with imprints from microhardness tests inside and outside of the remelting zone. Two loads were used. Distance from the remelting boundary approx. 400µm – 52 HV 0.025

Fig. 4. Photographs of polished cross-sections with imprints from microhardness tests outside of the remelting zone (distance from the remelting boundary – interface approx. 550 µm – 45 HV 0.025 and 850 µm – 55HV0.025)

Fig. 5. Distances between dendrite arms – DAS 1 (primary) and DAS 2 (secondary) a) remelted and non-remelted zone, b) remelted zone
3 Results and analysis

3.1 Energetic model validation of the laser remelting process

In order to conduct the energy validation, the simulation of the cast sample heating process by laser beam and its cooling was performed. The simulation results were compared with experiment of the laser surface impact (treatment) on AlSi7Mg alloy plate casting. The results of the experiment for the selected laser pass on the sample surface (bead no. 1.2), allowed to identify the geometry and dimensions of the remelted zone. The measured average depth was 0.21 mm and average width was 0.85 mm (Fig. 6).

As a typical procedure for a simplified solution of the inverse problem of heat transfer, a series of heating simulations were performed, in order to achieve conformity of the remelting boundary (interface) corresponding to the liquidus isotherm with the real boundary determined on the basis of the metallographic tests. The virtual melting profile, in principle, was assumed as the iso-liquidus line with the value of \( f_l = 1 \) (\( f_l \) – fraction of liquid; \( f_l = 1 \) corresponds to \( f_s = 0 \) as solid fraction). The time of sample exposure on the laser beam was 0.2 s (estimated value based on the kinematic analysis of the laser head movement).

The expected conformity of the simulation results with the experiment was obtained for the process of AlSi7Mg alloy sample heating under the assumption of a second type boundary condition (for the average Heat Flux = 105 W/mm\(^2\)). The simulation result with the display pattern of the laser energy distribution is shown in Fig. 7. In Fig. 8, the result of the heating process as a time-temperature curve for the points marked in Fig. 7 and the free cooling process are shown. After the time of 0.2 s, the boundary condition was changed from the second type (Heat flux = 105 W/mm\(^2\)) to the third type (Robin condition), describing the convective heat transfer with the ambient environment (\( T_{ambient} = 20 ^\circ C \); estimated Convection Heat Transfer = 100 W/m\(^2\)K) for the molten region, corresponding to the remelted zone.

The following final results of the heating process simulation (Thermal Module of Calcosoft system) are used subsequently to create the microstructure model calculations in the Calcosoft CAFE Module [6-9]. The CAFE module does not allow the re-computation with the delay in relation to the end of the process, that is, as assumed above, after time of 0.2 s with the modified boundary condition. In order to obtain the temperature field conformity at the beginning of the crystallization process using the CAFE module, and thus taking into account the initial temperature conditions corresponding to these assumed after laser heating, a layered geometry of the non-remelted sample was prepared in a way to re-create the temperature distribution in the whole sample after the impact of the laser beam in the individual constant temperature layers. The layers of the sample were assigned with the average initial temperature basing on the heating simulation result (Fig. 9).

In a similar way (comparing with no. 1.2 bead), an initial temperature distribution in the plate for the CAFE calculation for the next analyzed bead (no. 5.2) was prepared, where the higher remelting i.e. 0.46 mm deep and 1.4 mm width was obtained from the experiment. Layer-averaged initial temperatures for the CAFE calculation for the bead no. 5.2 are shown in the Fig.1.
Fig. 8. Temperature curves as a simulation results of the laser heating process and next rapid cooling

Fig. 9. Temperature distribution in the sample after heating, a – result of the heating simulation, b – layered average initial temperatures for CAFE calculations of structure

Fig.10. Averaged initial temperatures for the CAFE calculations of structure, laser pass no. 5.2
3.2 Prediction of the casting structure after laser re-melting

Consecutively, the validation of the CAFE model (nucleation and crystal growth) was performed for the two above selected beads (remelting pass) obtained using a laser beam i.e. 1.2 and 5.2. The variants of the best conformity of the virtual structure to the real one obtained for the laser beam transition is shown in Fig. 11 and Fig. 12. The resulting virtual structure contained solely the columnar crystals (simplified pseudo-dendrites). In the real structure, the equiaxed crystal zone was not visible on the metallographic cross section because of the specific heat conditions – forced high cooling flux (casting that has not melted is considered as a metallic mould, which is a kind of a “natural chill”). For this reason, in the validation procedure of Calcosoft system and its CAFE module, the hypothesis was stated about the need to suppress the algorithm responsible for the so-called volume nucleation (n_v=0). This led to formation of an exclusively oriented virtual structure (simplified pseudo-dendrites). Only this procedure allowed to achieve compatibility of the virtual structure with the real one.

The larger melting zone (bead no. 5.2) in relation to the bead no. 1.2 results from the higher initial temperature of the treated sample, which was caused by transfer of the heat energy during realization of laser beads with lower numbers (previous pass), occurring before imposition of the current bead (in this case no. 5.2).

Values of the parameters assumed for the simulation tests are shown in the Table 1.

Table 1. Values of parameters assumed for the simulation tests

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Name</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>λ_drop</td>
<td>drop thermal conductivity</td>
<td>Solid</td>
<td>130</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Liquid</td>
<td>90</td>
</tr>
<tr>
<td>α_casting-ambient</td>
<td>heat transfer coefficient casting-ambient</td>
<td>100</td>
<td>W/(m²K)</td>
</tr>
<tr>
<td>α_casting-mould-side</td>
<td>heat transfer coefficient mould-casting</td>
<td>100e6</td>
<td></td>
</tr>
<tr>
<td>α_casting-mould-bottom</td>
<td>heat transfer coefficient mould-</td>
<td>100e6</td>
<td></td>
</tr>
<tr>
<td>α_mould-ambient</td>
<td>heat transfer coefficient mould-ambient</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>L</td>
<td>latent heat of crystallization</td>
<td>1,13e+9</td>
<td>J/(m³K)</td>
</tr>
<tr>
<td>ΔT_mould</td>
<td>undercooling on drop surface from mould side</td>
<td>5</td>
<td>K</td>
</tr>
<tr>
<td>ΔT_mould-ambient</td>
<td>undercooling on drop surface from ambient side</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>ΔT_drop</td>
<td>drop volume undercooling</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>n_casting-ambient</td>
<td>nuclei number on surface from ambient side</td>
<td>1e6</td>
<td>1/m</td>
</tr>
<tr>
<td>n_casting-mould</td>
<td>nuclei number on surface from mould side</td>
<td>1e11</td>
<td>1/m</td>
</tr>
<tr>
<td>n_v</td>
<td>nuclei number in drop volume</td>
<td>0e0</td>
<td>1/m²</td>
</tr>
<tr>
<td>a3</td>
<td>kinetic coefficient</td>
<td>1e-4</td>
<td>ms⁻¹K⁻¹</td>
</tr>
</tbody>
</table>

Fig. 11. Real and virtual microstructure of melted zone - bead no. 1.2
4 Conclusions

Using the laser beam heating the superficial zone of Al-Si casting was remelted (pass by pass) and immediately cooled by non-remelted part of casting. According to the result of experimental metallographic and microhardness tests the high refinement of structure and significant increase of the microhardness values in remelted zone (comparing with non-remelted one) were observed. The improvement of mechanical properties is related to the structure being result of the intensive heat extraction (high heat flux) from the remelted zone.

Parallel to experimental tests the studies of validation remelting process using the laser beam heating were performed. In simulation test the conformity of the melting zone corresponding to the liquidus isotherm with the real interface determined on the basis of the metallographic tests was obtained. The significant influence on the simulation result of structure formation has the initial temperature distribution in the treated sample (resulting from previous multi-pass by laser beam). The estimation of temperature field was based on the heating simulation result (planned experimental acquisition of volumetric temperature field weren’t effective).

The final comparative tests of real casting microstructure related to microstructure predicted by Calcosoft-CAFE (Cellular Automaton Finite Element) simulation system were realized.

The microstructure has been validated and it should be stated that only columnar crystals (pseudo-dendrites) were virtually formed.

Based on the numerous simulation tests, the database containing the values of micro-model CAFE parameters were determined regarding the microstructure formation. The very high cooling rate and a relatively small remelting area as well the very small FEM mesh size (about 0.02 mm) reduced the simulation time increment drastically, to $10^8$ s. Also the appropriate parameter values for the microstructure virtualization in comparison with the conventional sand/gravity die-casting conditions in the past by our team, were modified. The next stage of planned study will be concern the tribological properties of remelted zones.

Acknowledgments

The research was partially supported by internal project financed by Polish Ministry of Science and High Education no 02/25/SBAD/4630.

References

