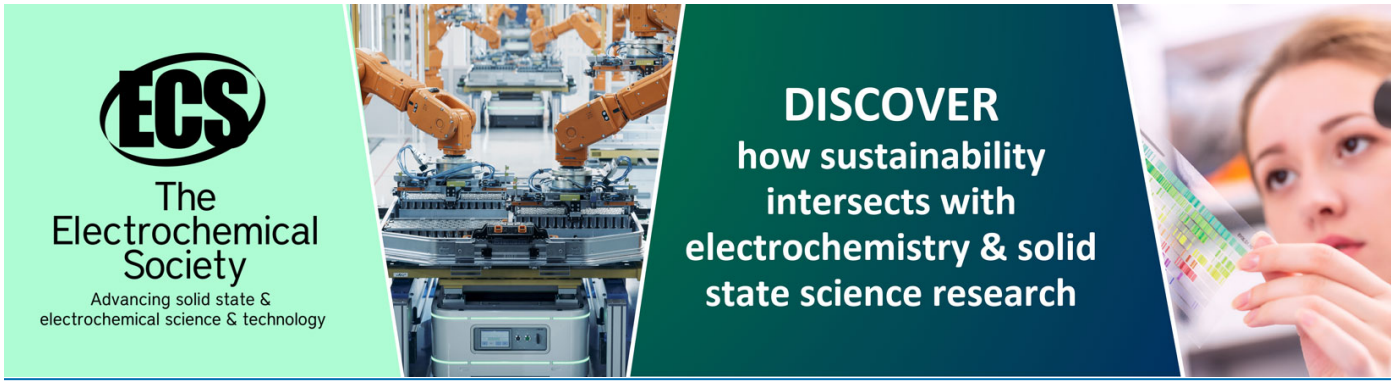
# On the role of solidification modelling in Integrated Computational Materials Engineering “ICME”





# On the role of solidification modelling in Integrated Computational Materials Engineering "ICME"

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**Abstract.** Solidification during casting processes marks the starting point of the history of almost any component or product. Integrated Computational Materials Engineering (ICME) [1-4] recognizes the importance of further tracking the history of microstructure evolution along the subsequent process chain. Solidification during joining processes in general happens quite late during production, where the parts to be joined already have experienced a number of processing steps which affected their microstructure. Reliable modelling of melting and dissolution of these microstructures represents a key issue before eventually modelling 're'-solidification e.g. during welding or soldering. Some instructive examples of microstructure evolution during a joining process obtained on the basis of synthetic and simulated initial microstructures of an Al-Cu binary model system are discussed.

## 1. Introduction

Segregation of alloy elements in a component is not only important for the properties of this component (e.g. solid solution hardening or formation of secondary phases etc.) but also for its further processing. Especially welding processes - typically happening at later stages of the production sequence of a component – strongly depend on the initial conditions for the materials to be joined. Scopes of the present paper are (i) to demonstrate effects of initial segregation patterns on microstructure formation during a typical laser welding process and (ii) to assess effects of simplifying assumptions for the segregation in the initial microstructure on the simulation of melting and solidification.

## 2. Simulation settings and materials data

Microstructure simulations were performed using MICRESS (- the MICRostructure Evolution Simulation Software) [5] version 6.154. MICRESS is based on the multi-phase-field concept [6, 7] and allows for online-coupling to thermodynamic and mobility databases [8].

The simulation domains are two dimensional using a cubic grid with 2000x500 grid points. The grid spacing is 0.5 µm. Boundary conditions for temperature were either defined as isothermal holding when generating the initial microstructures or using the 1-D thermal field functionality of MICRESS [13] for modelling the solidification and laser-welding conditions.

### *2.1. Materials data*

Numerical simulations require data on both the materials and the process conditions. For the materials, especially the phase-diagram data, the interfacial energies between the phases involved, the diffusion constants of the components in the individual phases, and thermal conductivities are required. A

binary Al-Cu alloy has been selected as a simple example in order to demonstrate the different effects on melting, grain growth in the liquid and eventually nucleation during re-solidification.

Thermodynamic data for the system Al-Cu have been taken from a binary subset of the COST507 database [9]. The material being considered for this basic study is a binary Al-Cu alloy with a nominal composition of 3 at.% Cu. The system reveals the liquid, the FCC and the θ phase ($Al_2Cu$). Equilibrium calculations using Thermo-Calc Software [10] predict a fraction of approx. 0.8% of the θ phase in equilibrium at room temperature. The diffusion coefficient for Cu was assumed to be constant at $D= 2*10^{-4}$ $cm^2/s$ in the liquid phase and to be $D= 1*10^{-8}$ $cm^2/s$ in FCC. No diffusion was assumed in the θ-phase. Thermal conductivities were estimated as $\lambda_{liquid}$ =1.2 W/cmK and $\lambda_{solid\_phases}$ = 1.3 W/cmK. Data for specific heat and latent heat were determined from the thermodynamic database.

The properties of the interfaces relevant for the simulation are listed in table 1. They were either identified from literature or have been estimated. Details on the exact specification of these different entities in MICRESS can be found in [11, 12].

**Table 1.** Physical properties of the interfaces.

| phase-pair | interfacial energy ($J/cm^2$) | interfacial mobility ($cm^4/(Js)$) | anisotropy |
|---|---|---|---|
| Liquid/FCC | $10^{-5}$ | 0.2 | kinetic: 0.2<br>static:0.2 |
| Liquid/ θ | $1.2*10^{-4}$ | 0.05 | isotropic |
| FCC/θ | $1.2*10^{-4}$ | $10^{-8}$ | isotropic |
| FCC/FCC* | $10^{-5}$ | $5*10^{-3}$ | isotropic |

*to allow also description of grain growth phenomena

*2.2. Generation of initial microstructures*

Different initial microstructures were generated as input for the subsequent simulations of a typical laser welding process:

- an as solidified microstructure
- a solidified and heat treated microstructure
- a synthetic microstructure
- a recrystallized microstructure

Nucleation of the FCC and θ phases in all simulations was allowed in the bulk liquid using the seed density model being implemented in MICRESS [14] and a typical but arbitrary seed density distribution. Further, nucleation was also allowed at interfaces with a critical nucleation undercooling of $\Delta T_{crit}$= 4 K for both the FCC phase and the θ- phase.

The as solidified microstructure (#1) was generated by simulating an equiaxed solidification process starting from the homogeneous and isotropic melt at T = 950 K. Heat has been extracted at 1.5 $W/cm^2K$ from the simulation domain leading to full solidification after approx. 0.5 s. An iterative homoenthalpic approach [13] has been used to obtain a realistic equiaxed microstructure with an average grain size of approx. 150 µm and to assure self-consistency between heat extraction and release of latent heat.

The heat treated microstructure (#2) was generated by using the as solidified microstructure (#1) and subjecting it to an isothermal holding for 5h at 800K.

A synthetic microstructure (#3) was generated from microstructure #1 by a heat treatment at a higher temperature (5h at 850K). At this temperature the θ-phase dissolves. The resulting microstructure thus only contains grains of the FCC phase. Due to the treatment at higher temperatures and accordingly faster diffusion no residual segregation can be observed in this microstructure. Note that the secondary dendrite arms disappear during this process. This type of microstructure – i.e. grains with constant concentration – could also have been generated by a kind of Voronoi tessellation and

this microstructure thus has been called "synthetic". The procedure used here to generate this synthetic microstructure additionally provides the same topology of the grains as the microstructures #1 and #2 and thus allows for a better comparison of the results.

A recrystallized microstructure (#4) was simulated on the basis of the solidified microstructure (#1). The recrystallization functionality of MICRESS® was used to generate a recrystallized fine grained microstructure. Values for a stored elastic energy originating e.g. from a forming process and revealing typical values of 0-10 J/cm$^3$ were assigned to the different FCC grains in this microstructure for this purpose. During the re-crystallization process new grains nucleate and the grain growth is driven by stored elastic energy. It should be noted that grain boundaries are pinned by the θ-phase particles during the simultaneous recrystallization/homogenization process, and that the recrystallization process does not affect the segregation pattern. The homogenization heat treatment parameters were identical with those used for microstructure #2

A summarizing overview of the initial microstructures is depicted in figure 1. Note the almost similar microstructures of #1 and #2 (two phase structures differing essentially in their Cu concentration fields) and the strong differences of #3 (FCC phase only, no Cu segregation) and #4 (small grains, Cu-concentration field same as #2)

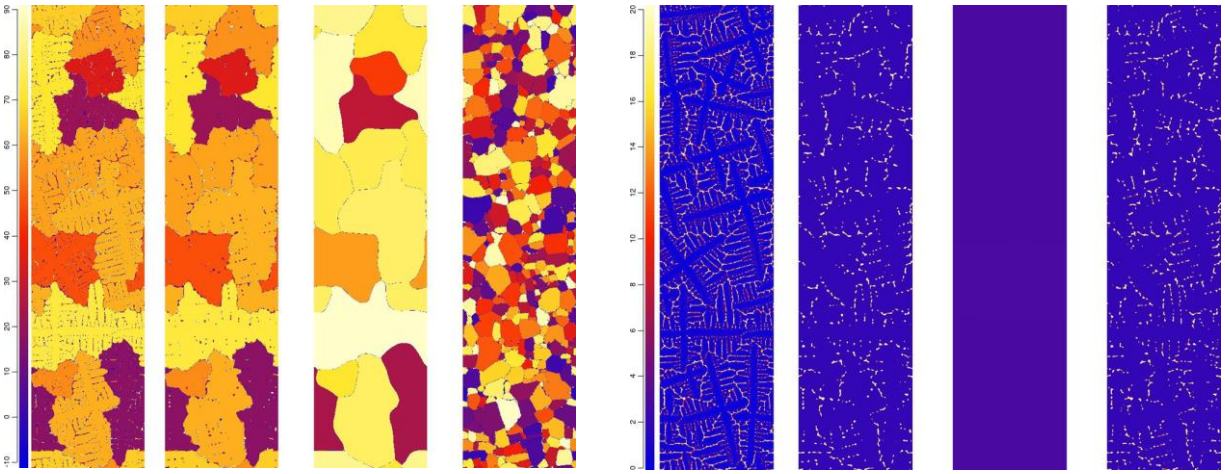

**Figure 1.** Overview of the four different initial microstructures (#1- #4 ; from left to right) for the grain orientations resp. grains (left) and for the Cu-concentration fields (right).

*2.3. Modeling laser welding*

The thermal boundary conditions for the subsequent simulation of the joining process - being identical for each of the initial microstructures - qualitatively correspond to a laser welding situation and were realized using the 1D-thermal field functionality of MICRESS®. The laser process was modelled as a heat flux boundary condition to the 1D temperature field as depicted in figure 2. This simulation setting leads to a partial melting and re-solidification of the microstructures as shown in figure 3 for the example of microstructure #1. Nucleation of the liquid phase inside the bulk solid phases and at grain/phase boundaries was allowed where a local overheating of 2 K was reached.

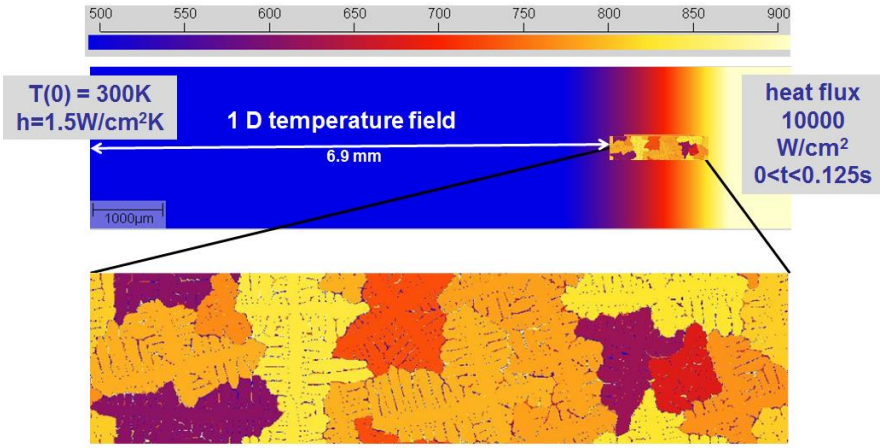


**Figure 2.** Schematic sketch of the 1D temperature field at t=0.13 s, its initial and boundary conditions and its relative position with respect to the 2D microstructure domain.

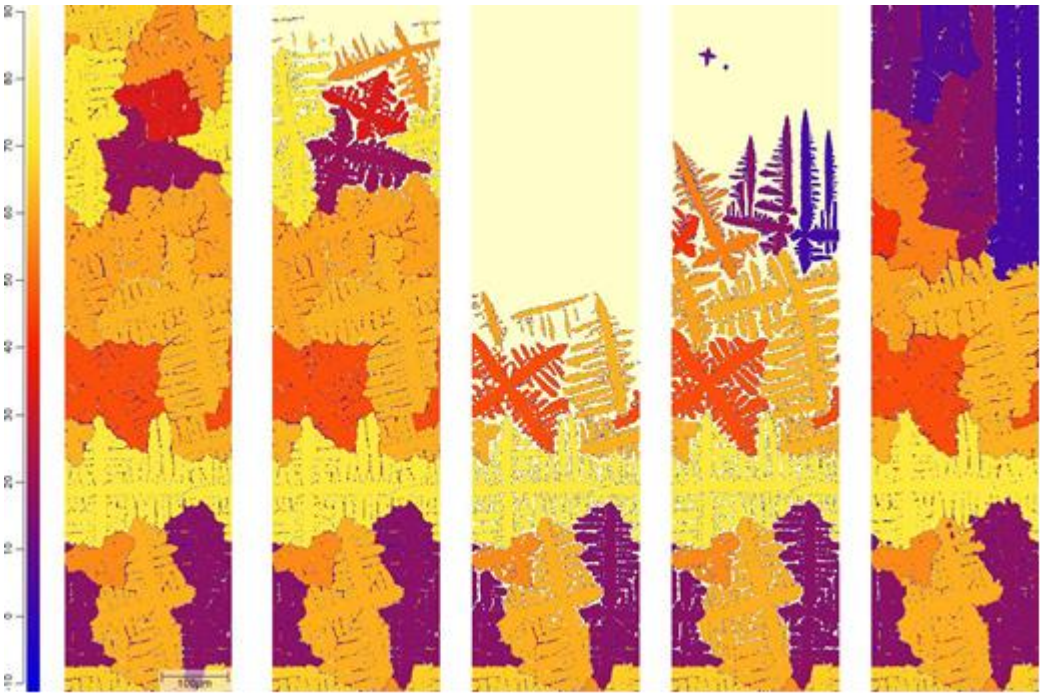

**Figure 3.** Melting and re-solidification of microstructure #1 as a time sequence (after 0, 0.124, 0.19, 0.26 and 2 seconds). Shown is the grain orientation. Note the directional dendritic structure in the re-solidified upper region.

### 3. Results and discussion

An overview of the phenomena occurring in the different initial microstructures, which will be discussed with respect to melting, grain growth in the mushy region, nucleation and subsequent re-growth in the following, is depicted in figure 4.

In the as solidified microstructure #1 melting as to be expected proceeds along the interdendritic regions, which solidified last during the generation of this microstructure and thus reveal the lowest melting point. The result is a continuous liquid film extending quite far into the bulk of the sample.

For the heat treated sample #2 in contrast no coherent liquid film is created, but different liquid regions are formed which also extend into the bulk of the sample.

Melting of the synthetic microstructure #3 significantly differs from samples #1 and #2. The homogeneous concentration field of Cu and its single phase FCC structure lead to a sharply localized

melting front with no extension into the bulk of the sample. Upon melting a large number of small fragments of the initial grains are created.

The recrystallized microstructure #4 does not melt along its grain boundaries. Its melting behaviour is essentially determined by the original Cu-segregation which was not altered during the recrystallization process. Molten areas are also here found in the bulk phases of the sample.

Re-solidification for all cases starts from grains, which have not fully dissolved in the melt. Additionally the formation of some new nuclei in the bulk liquid can be observed in all cases. Major differences are identified for the recrystallized microstructure – revealing more and smaller grains as starting points for the re-solidification of dendrites. In case of the synthetic microstructure a large number of small fragments of the initial microstructure can be observed during melting. Each of these fragments should be assigned to become a new grain. In this case thus a very fine polycrystalline array of dendrites would have to be expected in contrast to what is depicted in figure 4.

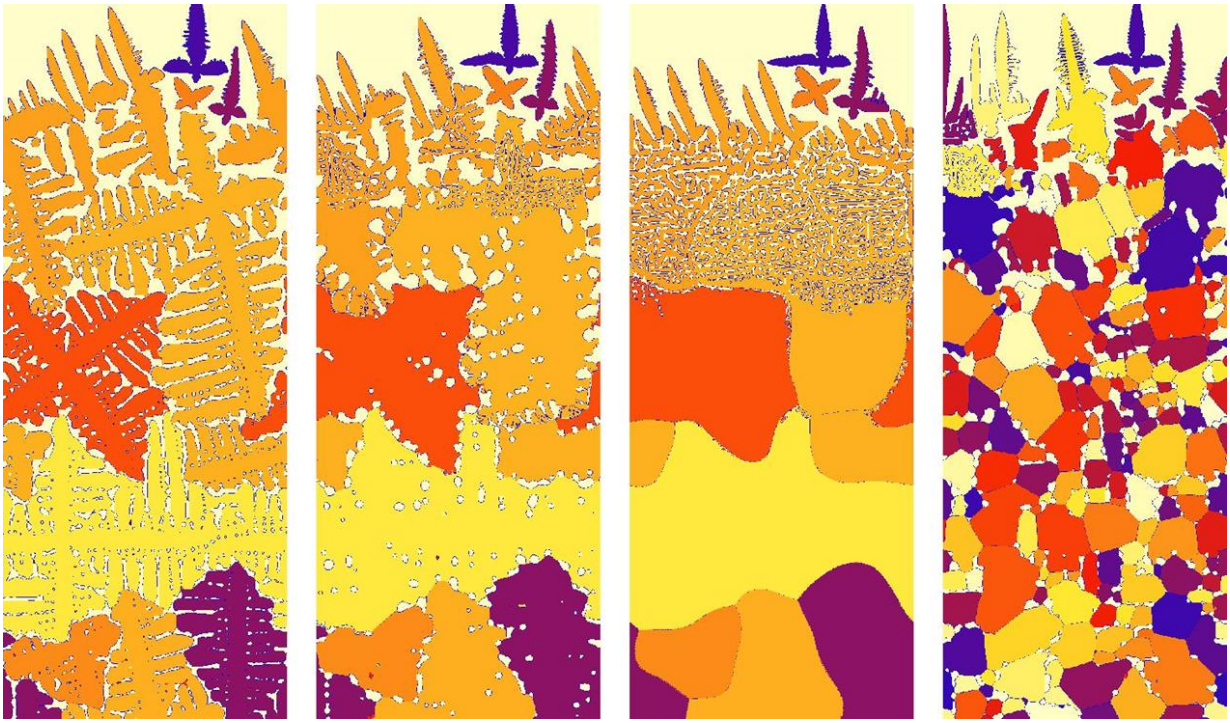

**Figure 4.** Melting and re-solidification of the four different initial microstructures (zoomed view #1 through #4; from left to right, width of each domain is approx. 200 µm) during a laser type process. Time step and process conditions are identical for all four microstructures. Depicted are the grain orientations respective grains.

## 4. Conclusions

In summary, modelling of melt based joining processes needs information about microstructures - especially segregation- which originates from the casting process and further evolved along the process chain. Modelling of segregation and its evolution along the entire process chain is highly important for both the properties of the materials but also for their further processing. Different segregation patterns lead to qualitative differences in the melting behaviour during thermal joining processes. Oversimplified assumptions - like e.g. a simple Voronoi type grain structure revealing a homogenous concentration of the alloying elements – will not be sufficient to correctly describe the melting process. In addition to modelling of solidification processes, the modelling of melting and

dissolution processes of heterogeneous microstructures is expected to become important in the near future. "Processing-microstructure" relationships can be refined as "initial microstructure- processing-final microstructure" relationships in the future.

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