

MatCalc

Engineering

Metallurgical Process Simulations

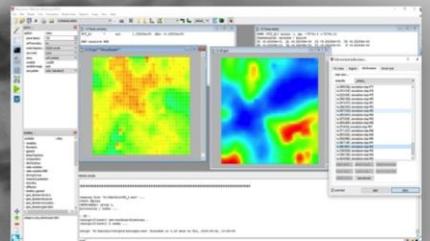
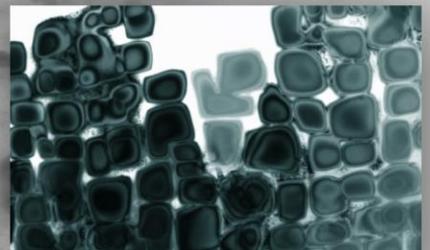
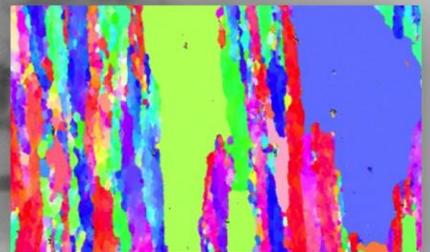
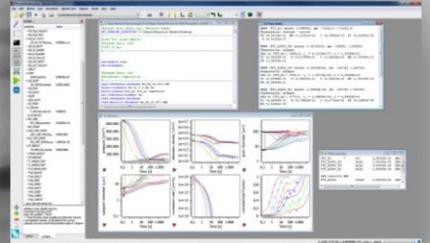


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Foreword

Dear partners, dear associates, dear customers,

MatCalc Engineering GmbH is a spin-off company from Vienna University of Technology, with many years of computational material engineering, materials testing and material characterization experience.

Our mission is to provide state of the art computational software, data and expertise in the field of materials engineering for more efficient, faster, cheaper and sustainable innovation, development and production of both materials and components.

Our team consists of multidisciplinary experts bridging the gap between science and practical manufacturing solutions seeking to offer viable step-change improvements in your materials design and your fabrication process. Our services include supporting your R&D projects, material consulting, optimization of your material processing route, material selection or assessment of your new materials, as well as materials testing.

We provide computational metallurgical technology solutions built on the application of the advanced and sophisticated software package “MatCalc” - Materials Calculator. MatCalc models the whole materials design and fabrication process, covering the three main areas of multicomponent thermodynamics, precipitation kinetics and microstructural evolution.

Customers and partners can benefit from the full range of the available know-how to capture opportunities and assure long-term competitive advantage. A general description and samples of our services are detailed below.



Prof. Dr. Ernst Kozeschnik
Chief Scientific Advisor



Dr. Ahmad Falahati
Chief Executive Officer

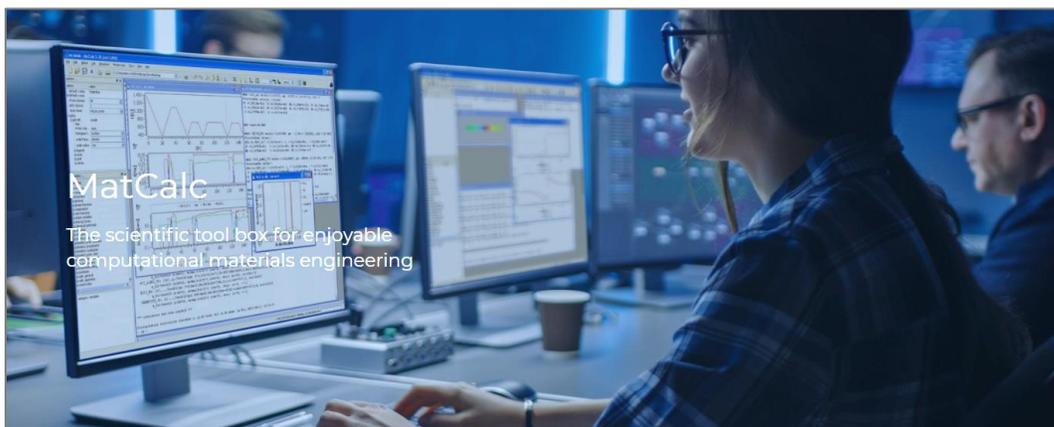
Our competences

Rising numbers of international competitors enforce companies to optimize their production process routes and offer high-quality products to be able to stay competitive in the global market. From our experience throughout the last decade, the market urgently seeks for higher efficiency of production lines, which cannot be achieved by empirical try and error methods anymore but requires the predictive capability of materials modeling and simulation. Twenty years of intensive development of MatCalc software provide us with a tool to fulfill these needs of our clients and to help them to stay ahead in their global competitiveness.

MatCalc Engineering GmbH offers consulting in metallurgical process engineering and performs custom simulations to help solve your materials technology problems. In addition, it is your professional partner for MatCalc licensing, technical support, user training and database development.

MatCalc Engineering GmbH provides services in the following areas:

- Consultancy
- Computational Engineering
- Materials characterization and testing
- MatCalc software licensing
- Database development



The combination of both experimental investigations in the laboratory and simulations, build the special strength in our services.

Services overview of MatCalc Engineering GmbH



Consultancy

The scientific and technical consulting of MatCalc Engineering GmbH assists in business and institutional decisions. Often working behind the scenes, we offer resources that clients cannot provide themselves. Usually, one of the resources is expertise - in the form of knowledge, experience, special skills, or creativity; another resource is time and/or personnel that the client cannot spare. By scientific and technical consulting services we assure long-term competitive advantage for our clients.

Computational Engineering

Computational material engineering is an emerging method that has proven to play a very important role in providing successful technology solutions. From materials property modeling and material process optimization to development of new high performance alloys and finding specific answers to sophisticated materials-related technological problems of our real-world industries. Finding the solutions at lower cost and much faster than via traditional trial and error methods shortens the development process of materials-enabled products.

A major pillar of our company is to provide technology solutions, as well as services building on the application of the software solutions integrated in MatCalc. Our expert team maintains continuous interaction with the MatCalc development group and can customize algorithms and create new technological solutions for emerging problems in the framework of MatCalc.

Our modeling competences include:

Phase equilibria

- Identification of stable and metastable phases
- Phase compositions
- Evaluation of state parameters phases (heat capacities, molar entropies, chemical potentials, etc.)
- Evaluation of driving forces for the phase formation

Cast structures

- Chemical composition of primary precipitates
- Evaluation of microsegregation in the solidified structures

Precipitation kinetics

- Amount of precipitated phase
- Precipitate sizes and number densities
- Precipitate composition
- Temperature-Time-Precipitate (TTP) diagrams

Microstructure evolution

- Vacancy concentration
- Dislocation density
- Subgrain sizes
- Grain sizes
- Recrystallization and recovery processes

Evaluation of thermo-mechanical treatments

- Homogenization
- Solution treatment
- Ageing, annealing
- Material deformation

Mechanical property estimation

- Yield strength predications
- Flow-curve modeling

Through process modeling

- Optimization of each process step by simulating the consequences on the final product

Cell simulation

- Long-range diffusion
- Coupled precipitation / diffusion

Materials characterization and testing

MatCalc Engineering GmbH has the technology, the expertise, and the background to perform different experimental methods to provide answers to our customers. Generally, the techniques used for a given problem are selected based on the information needed.

Our materials characterization and testing capabilities include:

Microscopy

- Optical light microscopy
- Scanning electron microscopy
- Transmission electron microscopy
- Electron backscatter diffraction

Mechanical testing

- Tensile tests
- Dilatometer
- Hot deformation tests (Gleeble)
- Hardness measurements

Thermal analysis

- Differential scanning calorimetry
- Thermogravimetric analysis
- Thermomechanical analysis



We cover also characterization methods that are not given here in detail and can develop custom material testing procedures based on our client needs. If you are not sure about your required type of characterization feel free to contact us: info@mceng.at

MatCalc software licensing

Since 2015, MatCalc Engineering GmbH is an exclusive license distributor for the MatCalc software package. It also handles all customer relations, user support, as well as training and workshop organization.

MatCalc is a software package for computer simulation of phase transformation and microstructure evolution in metallic systems. Since its origins in 1993, MatCalc established itself among both the academic and industrial institutions (over 70 users in 17 countries) as useful tool in the understanding and optimizing the nature of the metallic materials. It was used in the preparation of ~200 publications where also detail on the models used in the software were given.



For more information, please visit our website:

<https://www.matcalc-engineering.com/index.php/matcalc-software/matcalc-software-sub>

Database development

MatCalc utilizes standard CALPHAD-type databases for thermodynamics, diffusion and thermo-physical properties, which contain data for both, stable and metastable phases that are especially optimized for kinetic simulations. They are the pre-requisite for predictive kinetic simulations of precipitation and microstructural evolution. MatCalc Engineering GmbH tailors multi-component, multi-phase databases to your field of interest. We offer professional state-of-the-art databases for the following material classes:

- **ME-Fe steel database**

Elements: Fe, Al, B, C, Co, Cr, Cu, H, Hf, La, Mn, Mo, N, Nb, Ni, O, P, Pd, S, Si, Ta, Ti, V, W, Y

Some standard applications: Calculations of multi-component phase equilibria and thermokinetic precipitation simulations in tool steels, micro-alloyed steels, 9-12% Cr-steels, PH maraging steels, austenitic stainless steels.

Special simulations e.g.: Coupled nitride/sulfide precipitation in micro-alloyed steels, early precipitation of carbon clusters in tempered martensite, γ' -precipitation in Ti-alloyed irradiated austenitic steels.

- **ME-Al aluminum database**

Elements: Al, Cr, Cu, Fe, Hf, Li, Mg, Mn, Ni, Sc, Si, Sn, Ti, Y, Zn, Zr

Some standard applications: determination of solvus temperatures of metastable co-clusters and precipitates, determination of stabilities of AlFeMnSi dispersoids, thermokinetic precipitation simulations in AA2xxx, AA6xxx and AA7xxx alloys.

Special simulations e.g.: Phase equilibria and thermo-kinetic precipitation simulations of special aluminum alloys: AA-Li, AA-Sc, AA-Sn.

- **ME-Ni superalloys database**

Elements: Ni, Al, B, C, Co, Cr, Cu, Fe, Ge, Hf, La, Mn, Mo, N, Nb, O, Re, Ru, S, Si, Ta, Ti, V, W, Y, Zr

Some standard applications: Determination of gamma' solvus temperatures as a function of alloying in multi-component wrought and cast polycrystalline Ni-base superalloys, thermokinetic precipitation simulations in Fe-Cr-alloyed Ni-base superalloys.

Special simulations e.g.: Determination of phase relations and precipitate evolution in a variety of single-crystal Ni-base superalloys, bimodal to multimodal precipitate distributions.

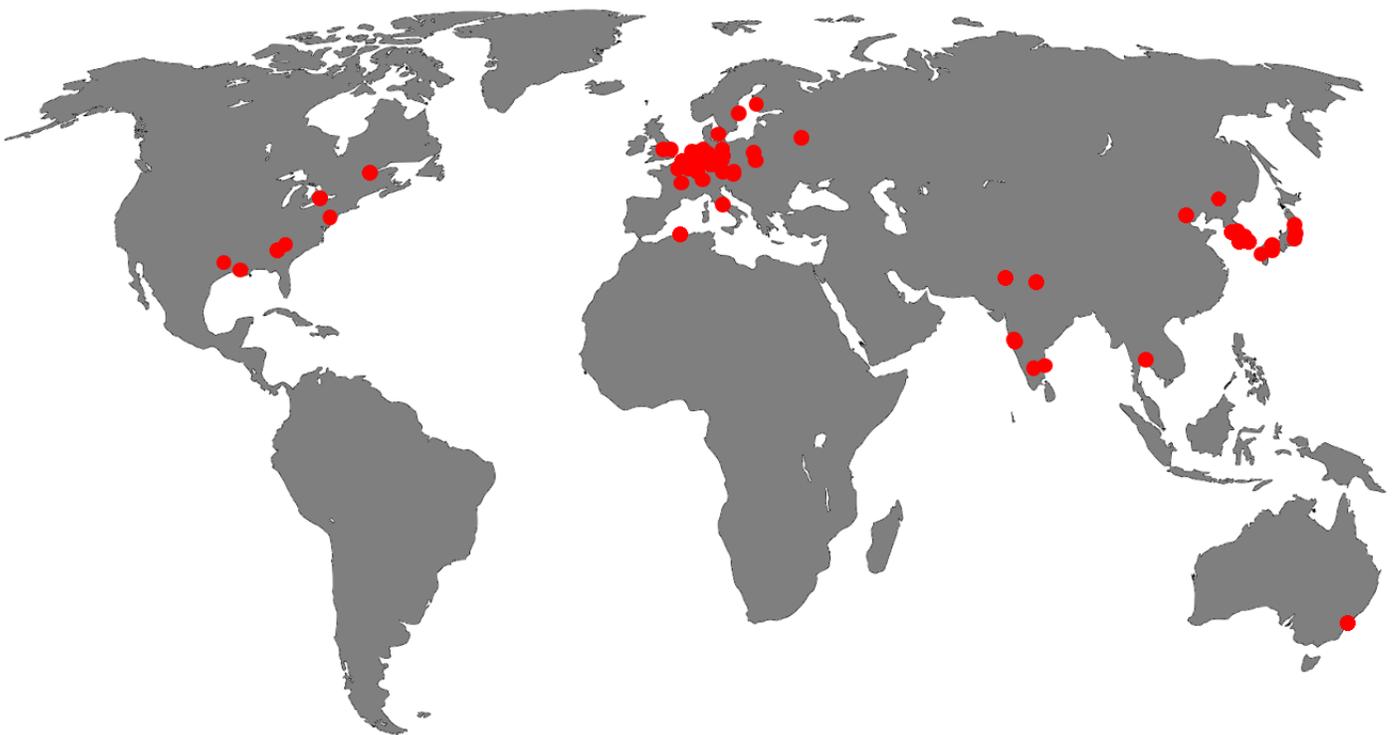
These databases are constantly optimized and represent the up-to-date knowledge in the field of thermodynamics.



On request, MatCalc Engineering GmbH can also tailor multi-component, multi-phase special databases for cutting-edge new materials to your specific needs.

Examples & References

Most of our works for commercial customers are confidential. Below are just few typical generic examples of our works.



Our customers around the world

(© 2021)

Project examples

MatCalc Engineering GmbH is involved in various projects for our customers in different private sectors such as alloy producers, automotive industries, energy suppliers, medical industries, nuclear industries and semiproduct producers. However, most of our works for commercial customers are confidential. Below are few typical generic examples of our works applied for a variety of different material classes. Each solution is applicable to other materials too.

Our material characterization capabilities show what the real microstructure of the material is and our modeling tools help to understand why a given microstructure appears and how to influence its further evolution.

Regardless of the type of your project; a concept formulation and evaluation, realization or optimization and / or through process modeling the benefits of our simulation works is obvious. We help plant engineers to analyze and solve practical problems much easier, optimizing each process step in view of the consequence on final product and increases industrial process variability and at the same time material quality. Our results have positive impact on waste management by reducing defects and decreases significantly time and cost for development.

Some generic examples:

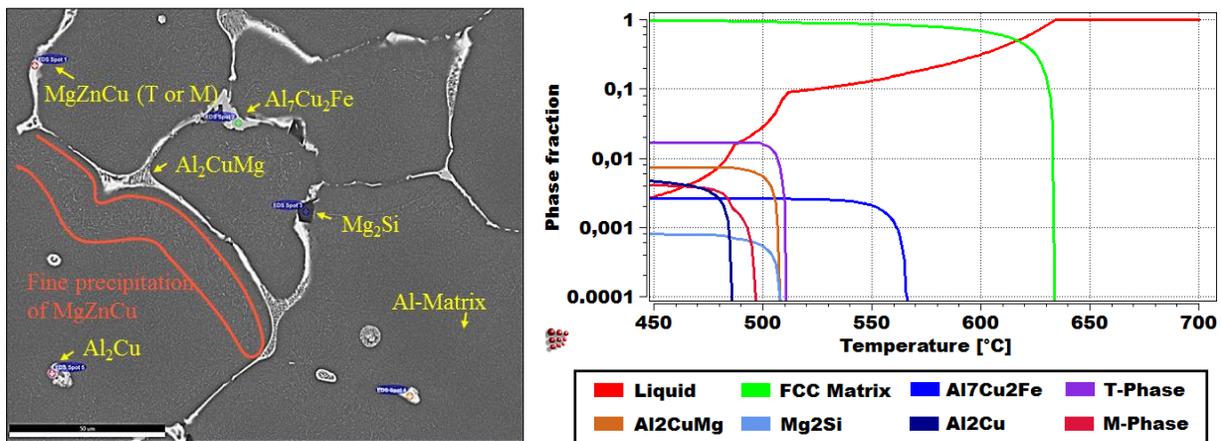
- Modeling of solidification processes
- Material homogenization simulations
- Precipitation kinetics calculations
- Microstructure modeling
- Modeling of mechanical properties
- Simulation of welded materials
- Through-process modeling

Modeling of solidification processes

Solidification of the alloy is usually the first stage in the metallurgical process chain. The properties of the solid material are created here and will be the subject of the subsequent process stages. The extent of the compositional inhomogeneity and the presence of the precipitates formed directly from the liquid phase will influence the further microstructure evolution.

Our solution: Scheil-Gulliver analysis utilizes the thermodynamic data to the simulation of the liquid alloy transformation toward the solid phases. It gives information about the number, the amount and the chemical composition of the created phases over the relevant temperature range. With this insight, various system compositions might be tested to find the optimal properties of the solidified material.

Typical applications; Identification of the solidification temperature range, Study of the composition gradients between the dendrite core and the interdendritic region of the alloy (microsegregation), Examination of the occurrence of the amount and the chemical compositions of primary precipitates



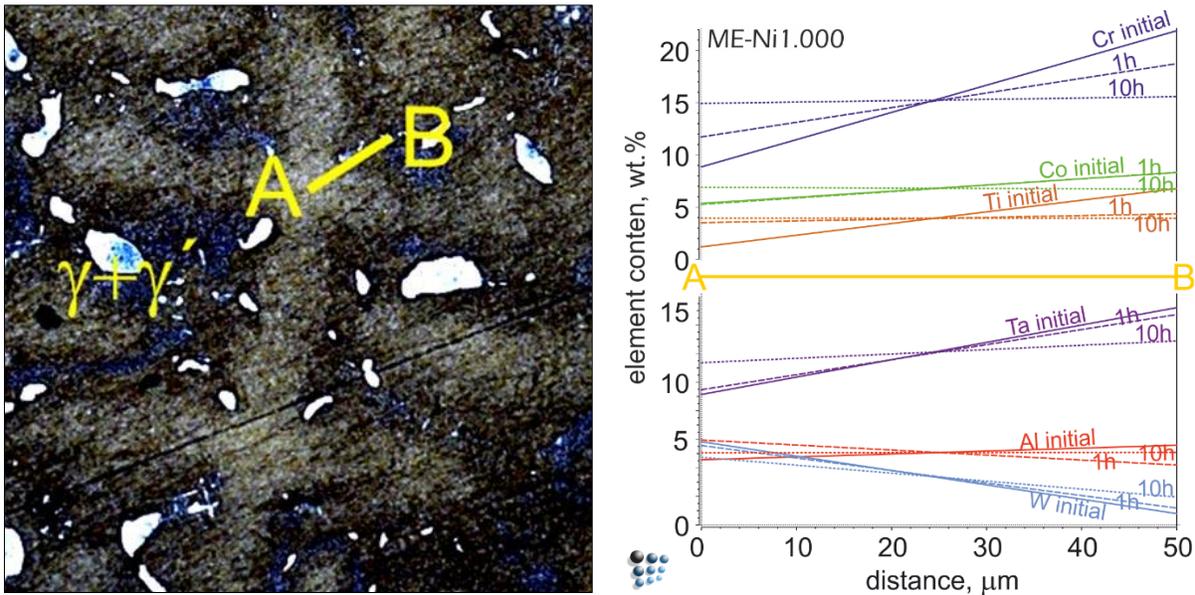
On the left, a scanning electron microscope picture of the as-cast structure of AA7050 is shown with numerous primary precipitates. On the right, the results of the Scheil-Gulliver calculation relevant for this system are displayed, which show good agreement with the experimental measurements and the predictive power of the calculations.

Material homogenization simulations

On some occasions that the material is not homogeneous or by typical examples of the cast materials with microsegregation, the existing composition gradients in the system can be disappeared with various time-temperature process cycle(s). Depending on the target, it might bring advantages or disadvantages for the material. It is possible to predict in advance the outcome and consequence of the process cycle(s).

Our solution: With available data for chemical potentials and mobilities of the system components, the diffusion processes leading to the microstructure homogenization can be simulated. The concentration profiles for various annealing times at various temperatures can be estimated. Moreover, it is possible to perform the precipitates kinetics simulation in this changing environment to realize the consequential microstructural evolution.

Typical applications: Time and energy cost optimization of the homogenization treatment of the cast structures, Microstructure development in the welding joint environment.



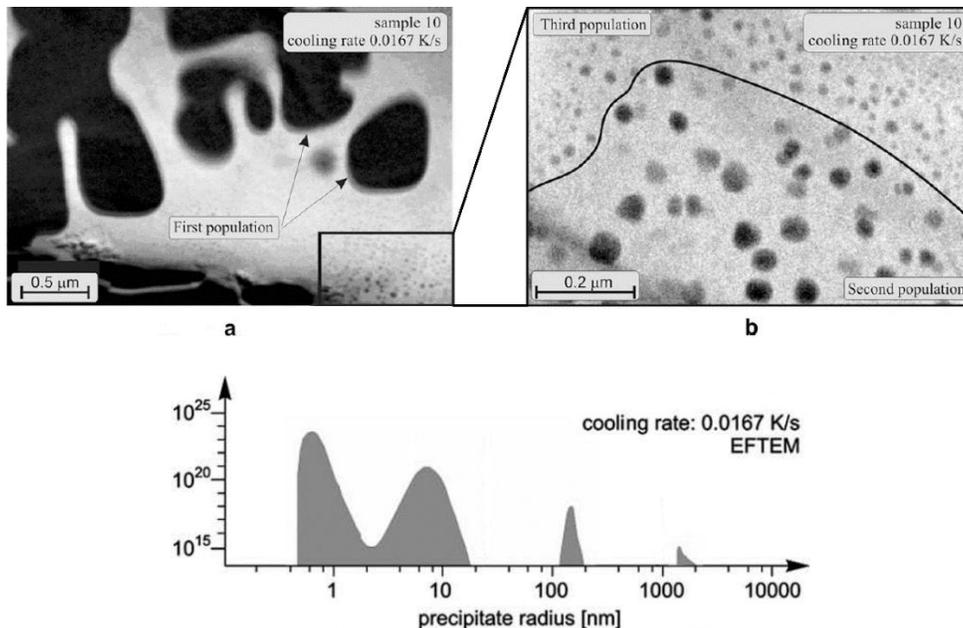
On the left, the metallographic picture of PWA 1480 alloy with an etched dendrite structure is shown. Simulated one-dimensional composition profiles along the A-B cross-section for the sample homogenized at 1300°C are shown on the right. As is demonstrated in the figure, this alloy is homogenized after 10 hours.

Precipitation kinetics calculations

Precipitates appear frequently in processed alloys. On some occasions, these are introduced intentionally to improve material strength. In other cases, the appearance of precipitates might be disturbing, e.g. intermetallics in specific welded parts. Undoubtedly, an insight into the precipitation evolution during the process is of a great value.

Our solution: With over 20 years of experience on this specific topic, our models have proved their realistic functionality of prediction in different applications. Our developed solutions and the approach for the prediction of the precipitate/matrix interfacial energy and the size evolution of the precipitates are broadly recognized in the scientific community. We are able to track the precipitates sizes, numbers and compositions of them during the whole thermomechanical process chain.

Typical applications: Estimation of temperature-time-precipitate (TTP) diagrams, Processing of the alloys aimed for the proper precipitate distribution (e.g. heat-treatable alloys of Al, Ni-based superalloys, microalloyed steels), Long-term simulations of materials in service (e.g. Z-phase formation in 9-12%Cr steels).



On top, the energy filtered transmission electron microscopy picture of the precipitate populations with different sizes in UDIMET 720 Li are shown. MatCalc simulation result is confirmed by the observed size distribution as shown on the bottom.

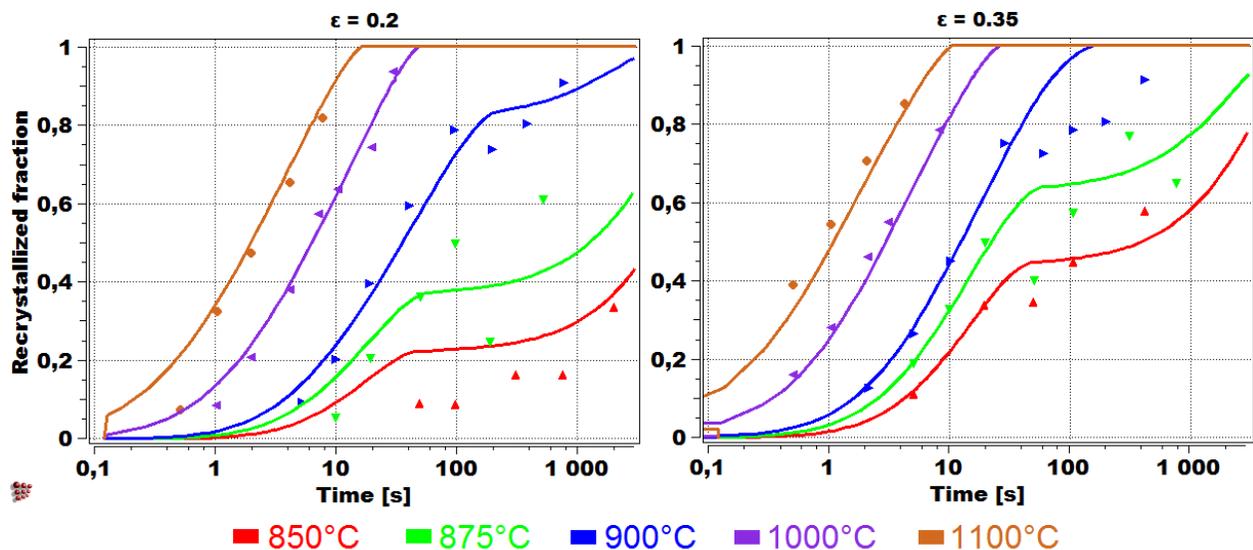
Microstructure modeling

Microstructure features like precipitates distributions, dislocation density, grain/subgrain sizes, as well as vacancy concentration are decisive for the material properties. Capability of microstructure evolution modeling gives us a great advantage in understanding, planning and optimizing of the process parameters.

Our solution: Instead of a bunch of independent models, we succeed to develop a coupled framework considering the mutual interactions of the microstructure elements and as a consequence a solution for the microstructure evolution simulations.

With our available modeling technique, the microstructure parameters of material can be calculated during and/or after various thermomechanical operations, such as deformation and/or annealing.

Typical applications: Deformation simulation of different alloys (e.g. rolling, forging), Annealing treatments, Analysis of the recrystallization process, Ageing treatments of aluminum alloys (including the influence of instantaneous vacancy concentration)



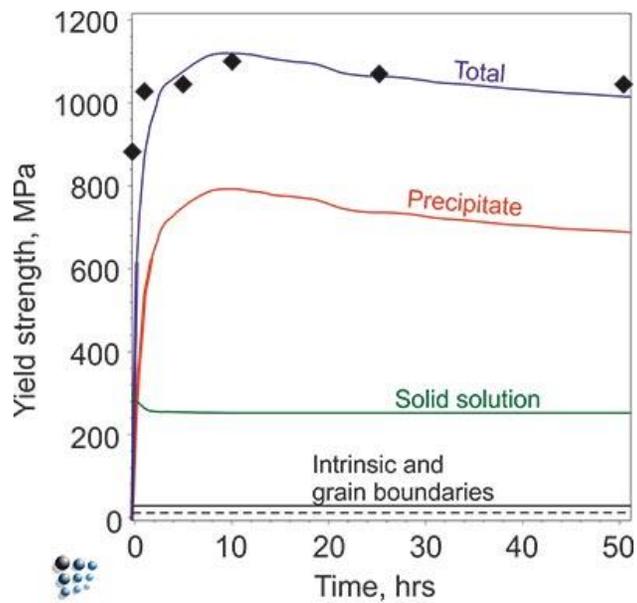
A simulation of the recrystallization progress in V-microalloyed steel for two strain values of 0.2 (left) and 0.35 (right) in compare with experimental findings (points). Recrystallization retardation by small precipitates of vanadium nitride is predicted for lower temperatures.

Modeling of mechanical properties

Mechanical properties of a material are controlled by the microstructure of the material. Microstructural evolution of a material during technological processes can be calculated by our software simulation capabilities. Therefore, it is possible to determine the mechanical properties during the process and to estimate the impact of different process modifications on the final material properties.

Our solution: Our yield strength model takes in to account the contributions of work hardening, grain and subgrain sizes, solid solution and precipitation strengthening effects based on the simulated microstructure evolution. Furthermore, the flow stress can be calculated at various temperatures.

Typical applications: Analysis of composition variation effect on the mechanical properties, Estimation of the optimal heat treatment parameters to achieve the maximal strength but avoid overageing, Prediction of flow curves for the deformed materials



Evolution of the total yield strength of a solution-treated Ni-base superalloy Allvac 718Plus. The evolution of γ' -phase precipitates during isothermal ageing is a critical factor for this material property. As is demonstrated overageing starts after ~10 hours.

Simulation of welded materials

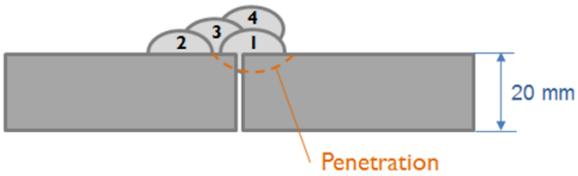
Welding is a popular method to join materials. Local application of a heat source on a material for a short period of time can have a tremendous effect on the microstructure of that material. If the heat source is strong enough or a filler material is used, there exist melting, solidification and heat treatment at the same time and the process can be much more complex. Our physically based simulations can shed light on the complexity of the welding process microstructural evolution.

Our solution: Thermodynamic and precipitation kinetics models allow us to predict the formation and growth of intermetallic phases. Furthermore, the microstructure evolution models give information about the grain size development. These results combined with the diffusion modeling allow simulating the various regions of the material with no uniform composition. Finally, the mechanical properties of the selected product part can be estimated.

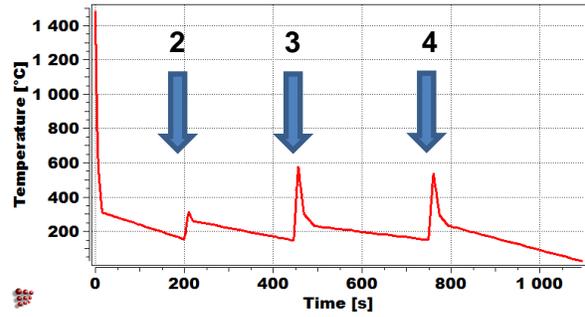
Typical applications: Analysis of the base and filler material properties after welding, Prediction of the weld microstructure evolution in specific service conditions, Welding simulation of dissimilar material parts



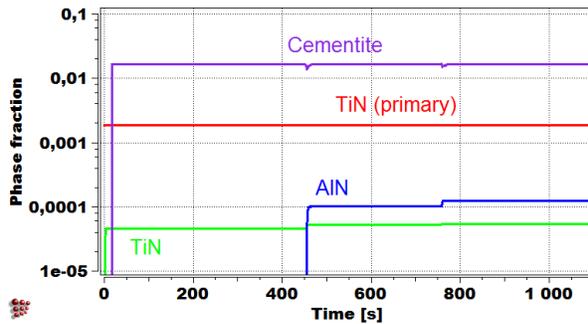
Yield strength simulation of the first weld droplet



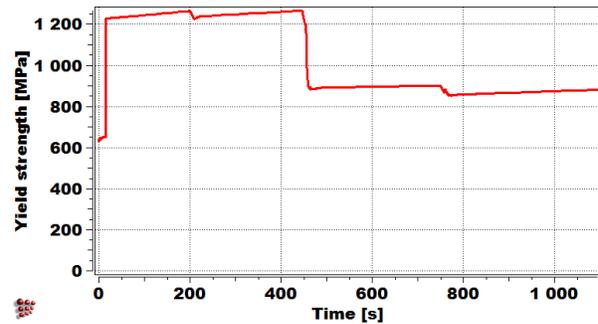
Weld bead configuration



First droplet exposed temperature profile

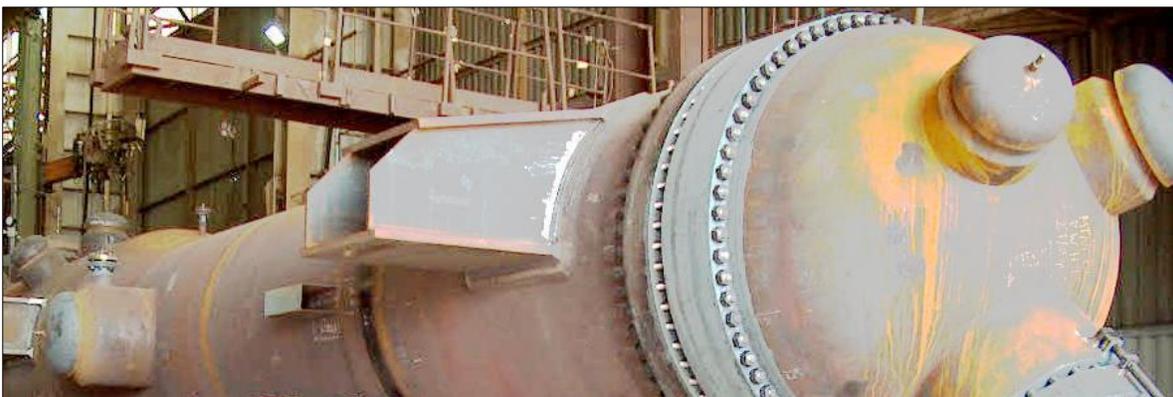


Evolution of precipitate phases in the first droplet

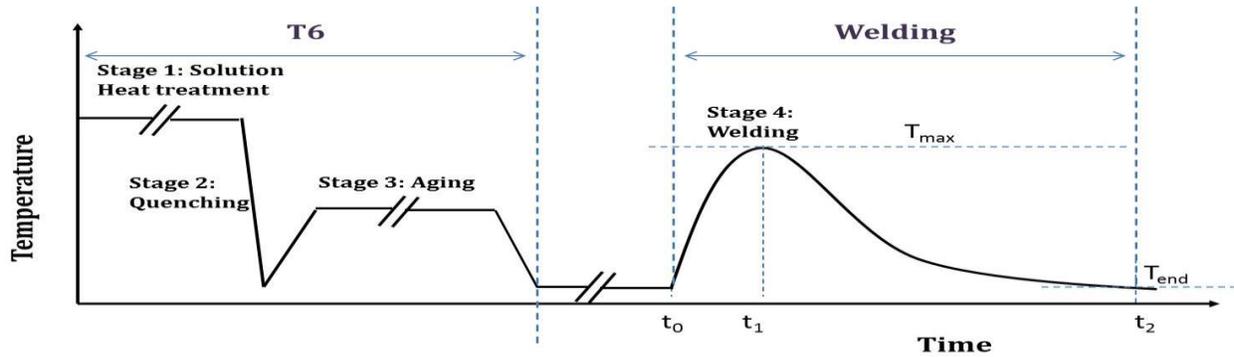


Yield strength of first droplet during welding

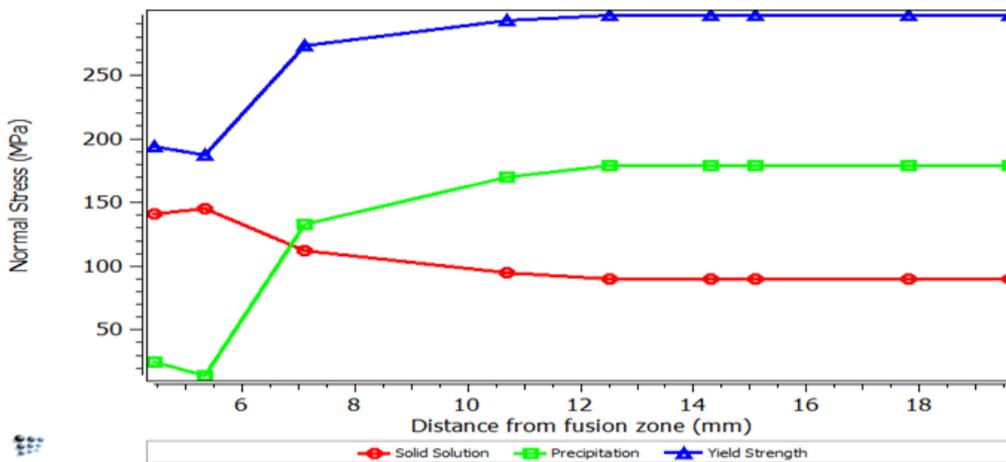
Simulation of the yield strength of the first droplet of the filler material (Cr-Mo microalloyed steel) exposed to heat treatment effect of the other covering droplets.



Yield strength simulation of the heat affected zone (AA 6061)



Scheme of the heat affected zone thermal history (T_{max} -value approaches T_{end} with the increasing distance from the fusion zone).



Yield strength within the heat affected zone as a function of the distance from the fusion zone. The contribution of the solid solution and precipitation hardening effects are visualized.

Simulation of the yield strength of the material (AA6061) within the heat affected zone. The contribution of various strengthening mechanisms is revealed.

Through-process modeling

Rising number of international competitors enforce producing companies to optimize their production process routes and offer high-quality products to be able to stay competitive in the global market. The number of influencing factors and parameters in the whole process-chain is tremendous. Any experimental investigation of the resulting material characteristics for optimization purpose or property prediction is highly time-consuming and cost-intensive with limited applicability.

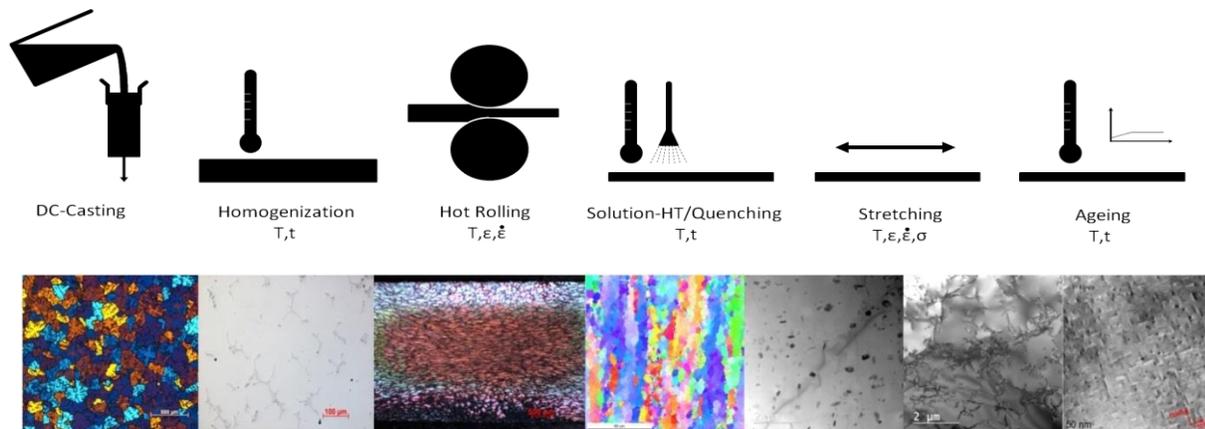
For through process modeling, the major issue is to track the evolution of microstructure throughout the manufacturing process chain from casting after solidification to the final product and the challenge is to integrate correctly different sub-models by properly defining their interactions. An overview of the material state resulting from each single operation is a key for process optimization and the creation of a cost-effective technological production line.

Our solution: We provide simulation package based on fully integrated models incorporated in the software MatCalc that be capable of a complete through-process modeling for each production route. Beginning with casting and ending with the simulation of the last thermomechanical operation of the final product. An intelligent optimization can only be reached when the combined influence of all the processing parameters during fabrication is known and is taken into account. After that various process- and material-related scenarios can be tested with an analysis of their impact on the material microstructure and properties.

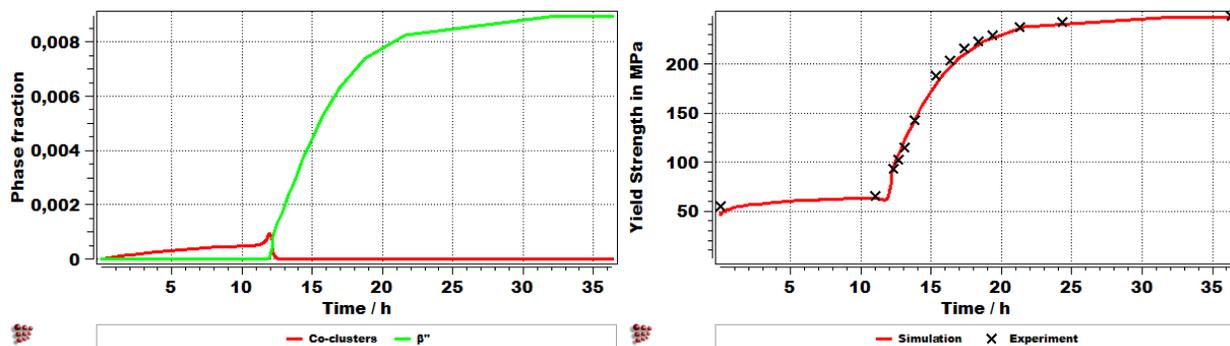
Typical application:

Optimization of aluminum sheet production route

Each processing step changes the microstructure and, therefore, affects the properties of the material. The final properties of aluminum plate depend not only on the chemical composition of the material but also on the microstructural evolution throughout the processing route.



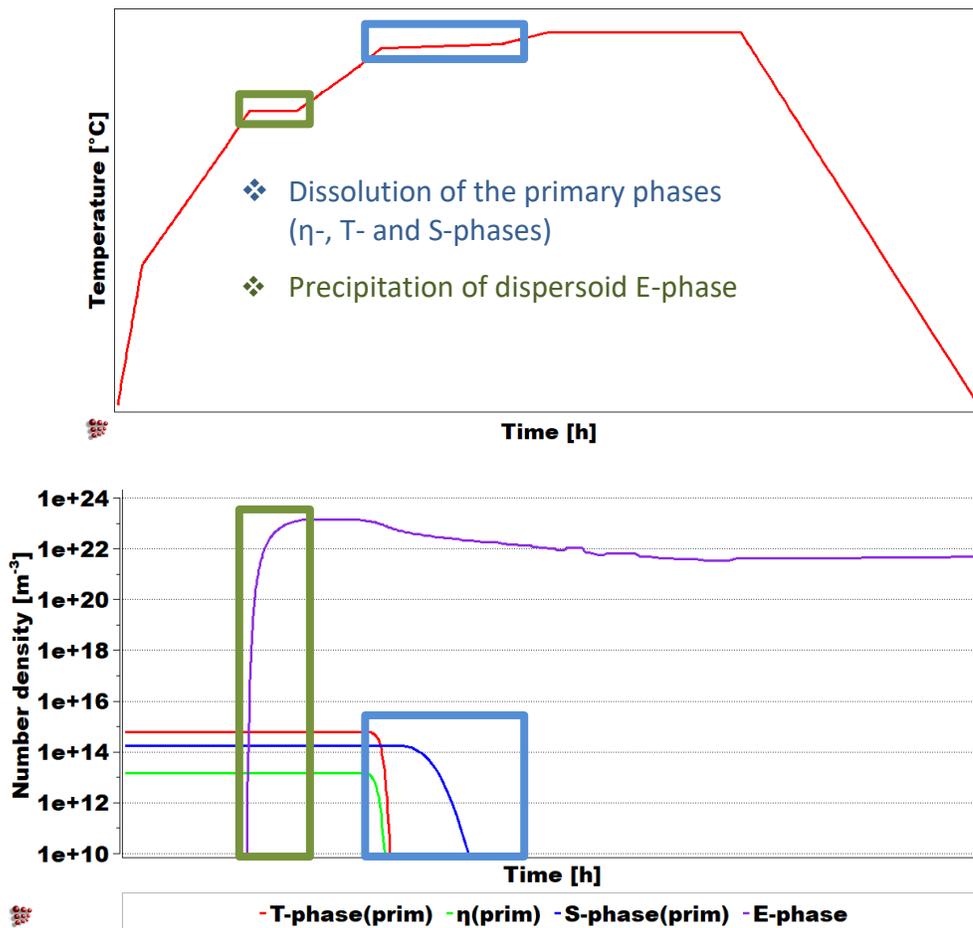
A scheme of the process chain for the production of aluminum alloy sheets and their relevant material characterization steps.



Last production step (ageing): A typical Al-Mg-Si alloy strengthening as a function of the precipitation kinetics during the last ageing treatment. In this simplified version just the evolution of β'' phase during ageing has been shown.

Optimization of homogenization process

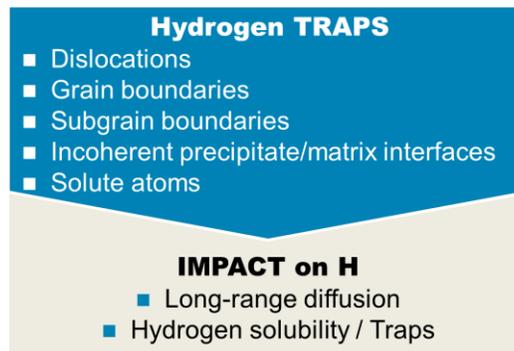
Homogenization process in Al-alloy processing route achieves multiple goals, including solution of primary precipitates of as-cast structure, removal of existing microsegregation and formation of dispersoid phases for a better grain size control. Within this project, the processing of AA7075 was improved to contain multiple isothermal steps aimed to realize each of the goals, one after another. This resulted in the maximal utilization of the material composition to reach the optimal microstructure for the further processing steps.



Scheme of homogenization schedule containing isothermal sections optimized for most efficient precipitation of dispersoid E-phase (within green rectangle) and dissolution of the primary phases (η -, T- and S-phases) present in the as-cast structure (within blue rectangle).

Steels and Hydrogen embrittlement

The development of steel, which is resistant against hydrogen embrittlement, is a major research focus and highly challenging since typical operation temperatures range from -150°C to 600°C . H embrittlement can occur during manufacturing, welding or from services in an aqueous, corrosive or gaseous environment that charge H into the steel. Depending on the prevalent mechanism, several influencing factors must be considered, such as the varying hydrogen diffusivity as a function of the number and strength of traps, the yield stress of the material, the fracture toughness and the hydrogen potential at the sample surface.



Different types of hydrogen traps

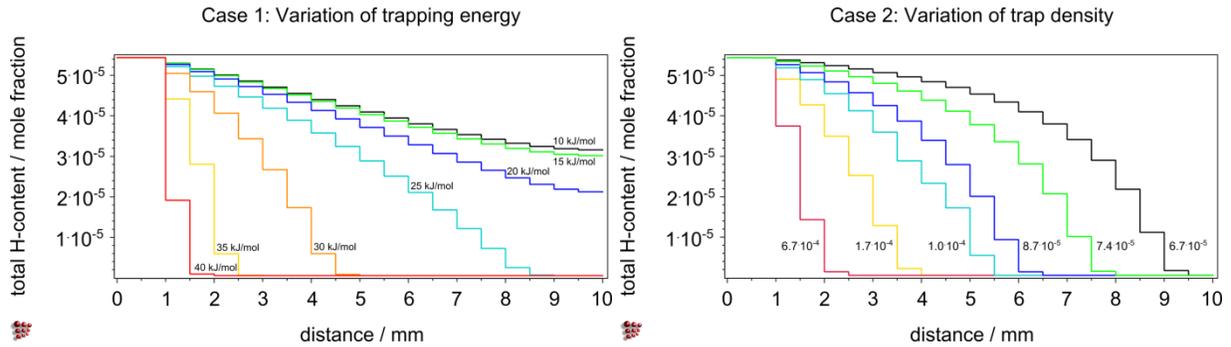
Our solution: A quantitative calculation of hydrogen redistribution would allow deeper understanding of hydrogen embrittlement in the materials and open the possibility of prediction and prevention of this type of material degradation.

By application of MatCalc it is possible to understand and analyze the evolution of the microstructure during processing and application. This, in combination with the cell simulation method gives us the opportunity to analyze the diffusion of H-atoms through the material and their trapping respectively. As a result, it is possible to optimize the production route, heat treatments and the alloying concept of the steels.

Typical applications: H-charging and –discharging behavior of different steels in the presence of traps, prediction of the optimal cooling rates from operating temperatures for maintenance to prevent H induced damage, parameter studies on the influence of trapping energies between H atoms and precipitate interfaces on the H-diffusion, evaluation of the relation between size and shape of precipitates and trapping capacity



Sketch of the simulation grid for the calculated hydrogen charging and discharging process



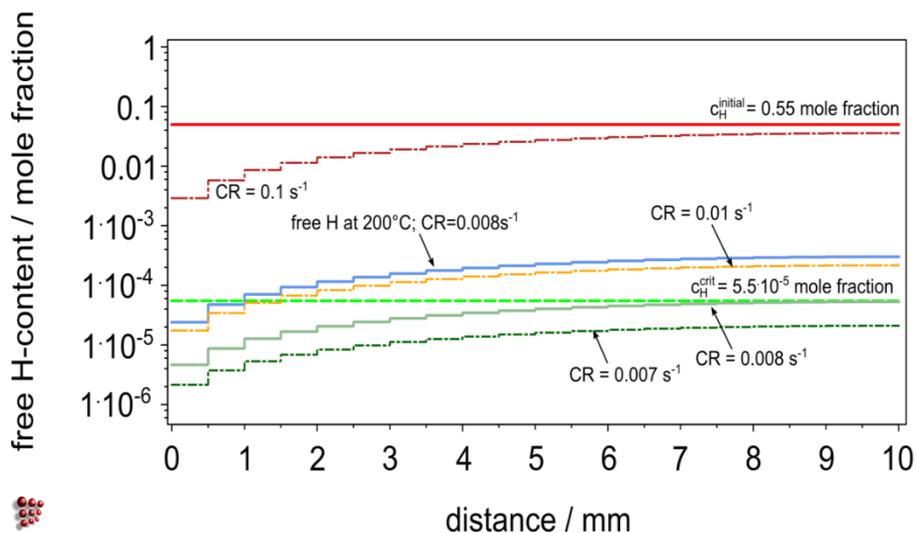
Parameter study: Case 1 – Influence of the trapping energy, Case 2 – Influence of a variation in the trap density

Example for vessel maintenance

Material: C-2.25%Cr-1%Mo – Mo₂C as active traps

Vessel in operation at 400°C, traps are filled during operation

Discharging from operating temperature to room temperature for technical service is simulated at different cooling rates until $c_H^{bulk} < c_H^{crit} = 1$ wtppm



Free H content after cooling at different cooling rates (CR)

Selected publications

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