Modeling and Simulation to Improve Quality and Efficiency

For several years, the AMAG has been cooperating with Prof. Ernst Kozeschnik from the Institute of Materials Science and Technology at the Vienna University of Technology, to adapt the software package MatCalc and the related databases to the specific alloying systems and processes of AMAG.

Before the age of computational material science, the development of alloys had been based on empirical correlations between the chemical composition, applied processes and the resulting product properties. Theoretical modeling is becoming increasingly important for understanding the behavior of polycrystals with different microstructures, the correct prediction of precipitation sequences and description of deformation mechanism. Numerical methods, based on physical laws, are time- and cost-saving in optimizing and development of materials of the future. AMAG uses the software package MatCalc, a thermo-kinetic modeling tool for the prediction of precipitation sequences, to evaluate process parameters [1-3].

Precipitation occurs by rapid quenching of a homogeneous solid solution. The crystals remain in single-phase supersaturated solid solution, even though the thermodynamic equilibrium will contain the alloy phase and an intermetallic phase. In addition to the supersaturation of solute elements, there is a high amount of empty lattice sites in the crystal. These quenched-in excess vacancies are inducted by the heat treatment of quenching. In contrast to these non-equilibrium vacancies, each material has a temperature-dependent amount of equilibrium vacancies, which are thermodynamically necessary for the diffusion of solute elements within the matrix. The equilibrium vacancy concentration increases with temperature. By quenching the material from elevated temperatures to room temperature, excess vacancies get frozen inside the crystal and increase the diffusion of the system. This increase of diffusion governs the precipitation of early metastable phases. Dependent on the subsequent heat treatment the metastable phases transform into more stable phases and finally the system reaches equilibrium condition.

For the first time there is an appropriate model implemented in MatCalc to describe the reactions based on the increase of diffusion by the excess vacancies [4]. This approach allows the prediction of the very early metastable coherent precipitates. Even these nano-scaled precipitates lead to a strength increase because the dislocation movement is retarded by a coherency strain field around the particles. The precipitation sequence of heat-treatable aluminium alloys after quenching from elevated temperatures is as follows: Tiny coherent precipitates up to a few nanometers with a very high number density at room temperature aging and less, larger and semi- to incoherent particles at artificial aging conditions. The properties of heat-treatable Al products can be influenced by suitable heat treatment design.

The classical T6 heat treatment includes the following process steps: Solution annealing – quenching – artificial aging at elevated temperatures. MatCalc is able to predict optimum time and temperature conditions for different alloy compositions to reach the required product properties. In the following example of an AA6016, kinetic simulations are carried out for a heat treatment (Figure 1) consisting of solution annealing, quenching, intermediate warming and artificial aging in order to predict the evolution of precipitation hardening.

In the first process step, solution annealing, all Mg and Si atoms are dissolved in the aluminium matrix. For complete solution, in a real process it is necessary to heat the system up to the single-phase region of cubic Al, and the system needs to be kept there for some time. In the simulations this step is not needed because the thermodynamic equilibrium condition at the start temperature for the quenching process keeps already all the solute atoms dissolved in a solid solution and the simulation can start from the end of the solution annealing process.

According to the AlMg2Si binary phase diagram just the Mg2Si phase would precipitate for a very slow cooling rate. Such a microstructure is not intended because it has unfavorable mechanical properties compared to very rapid quenching and

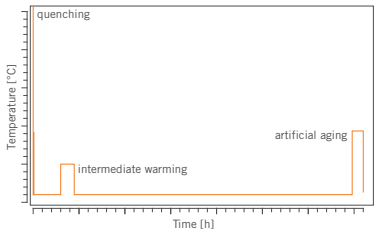

Figure 1: Temperature profile – precipitation hardening

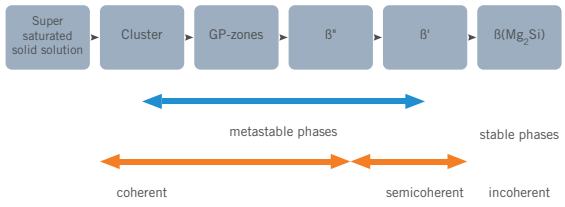

Figure 2: Precipitation sequence AlMgSi-alloy

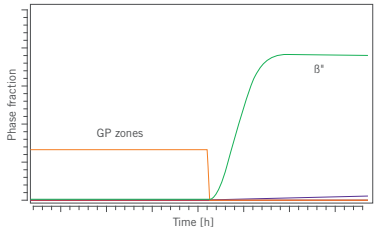

Figure 3: Phase fraction during heat-treatment

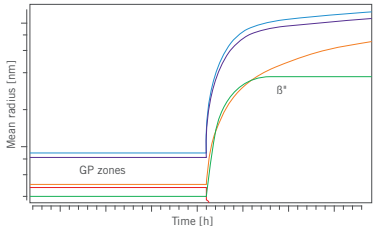

Figure 4: mean radii of precipitates

subsequent precipitation of metastable, finely distributed nanoparticles of MgSi co-clusters and GP zones. The generally accepted precipitation sequence for AlMgSi alloys is as follows (Figure 2):

Clusters and GP zones precipitate at room temperature already. The needle-like ß" phase succeeds in the temperature range from approx. 100°C to 220°C. This Mg5Si6 phase is known as the main hardening phase due to larger size and coherency strengthening characteristics. ß' precipitates form after ß" in the continuous ageing sequence. These precipitates are rod-shaped. The equilibrium phase Mg 2Si, and, in the case of excess Si, also Si precipitates are present. The later metastable precipitates ß' and the stable phases contribute little to the strength of AlMgSi alloys.

During the intermediate warming, co-clusters get dissolved and thus the ß" phase is stabilized. The precipitate fractions are shown in Figure 3. The dissolution of the GP zones and the considerable increase of the phase fraction of the ß" phase can be seen.

Figure 4 shows the mean radii of the precipitates. Late-stage semi- and incoherent precipitates are already present in the material together with the main evolution stage of ß", but with an order of magnitude less particles than the ß" phase, which beyond doubt is the most effective phase for strengthening.

Prediction of yield strength

Knowledge about number densities and mean radii of the individual precipitates and strengthening models implemented in MatCalc enables us to calculate the evolution of the yield strength for different temperature-time cycles for AlMgSi alloys [5] (Figure 5).

The complete yield strength σ total can be written as:

$$\sigma_{total} = \sigma_i + \sigma_{ss} + \sigma_p$$

σ_i - intrinsic yield strength of pure aluminium
σ_{ss} - solid solution strengthening
σ_p - precipitation hardening

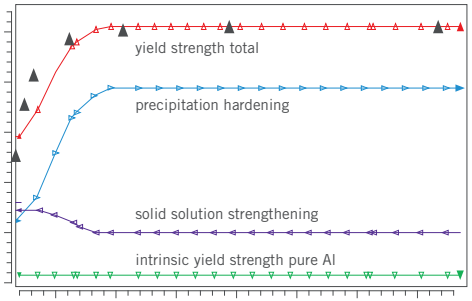

Figure 5: Evolution of the yield strength (simulation and experience)

LITERATURE:
[1] Svoboda J., Fischer F.D., Fratzl P., Kozeschnik E.; Mater. Sci. Eng. A 385 (1-2) (2004) 166
[2] Kozeschnik E., Svoboda J., Fischer F.D.; Calphad, 28 (2005) 379
[3] Kozeschnik E., Svoboda J., Fratzl P., Fischer F.D.; Mater. Sci. Eng. A 385 (1-2) (2004) 157
[4] Fischer F.D., Svoboda J., Appel F. and Kozeschnik E., Acta Mater, 59 (2011) 3463
[5] Lang P., Falahati A., Povoden-Karadeniz E., Ahmadi M.R., Warczok P., Kozeschnik E., Proceedings of the 12th International Conference on Aluminium Alloys (2010) 1443

The thermo-kinetic simulation is appreciably gaining importance. The combination of empirical experience and many years of research and development together with the possibilities of predictive simulations give us new and improved opportunities for fine-tuning of chemical compositions and optimized process parameters for the ongoing progress of AMAG products. Modeling can also help to increase energy efficiency by avoiding unnecessary processing times.

Professor Ernst Kozeschnik
member of the scientific advisory board of AMAG