

Assessment of parameters for precipitation simulation of heat treatable aluminum alloys using differential scanning calorimetry



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Abstract: Differential scanning calorimetry (DSC) has been used extensively to study different solid state reactions. The signals measured in DSC are associated with the growth and dissolution of different precipitates during a specific heat cycle. The time–temperature dependence of heat cycles and the corresponding heat flow evolution measured in the sample by DSC provide valuable experimental information about the phase evolution and the precipitation kinetics in the material. The thermo-kinetic computer simulation was used to predict the DSC signals of samples taken from 6xxx and 2xxx alloys. In the model, the evolution of different metastable and stable phases and the role and influence of excess quenched-in vacancies in the early stage of precipitation were taken into account. Transmission electron microscopy (TEM) and high-resolution TEM were used to verify the existence of precipitates, their size and number density at specific points of the DSC curves.

Key words: differential scanning calorimetry; aluminum alloys; precipitation kinetics; simulation; vacancy; MatCalc

1 Introduction

Understanding and simulating properly the precipitation kinetics during heat treatment of aluminum alloys are critical for achieving optimal materials microstructures. Over the last decade, with the increase of computational power, availability of thermodynamic databases especially for metastable phases, which depend on ab initio calculations [1] and existence of numerical solutions, we have the fundamental requirements to achieve reliable simulation of complex heat-treatment in aluminum alloys [2].

Before attempting to simulate complex heat treatment or calculation of their mechanical properties, a basic prerequisite is to get correct input parameters and to fine-tune the non-equilibrium kinetic parameters set for that specific material. A good methodology is to perform a non-isothermal continuous heating differential scanning calorimetry (DSC) experiment and to compare the experimental result with its DSC simulation curve

and to obtain the required set of precipitation kinetic parameters. To get a reliable parameter set, at least verified qualitative knowledge about the phases, which exist at different important points on DSC curve, is necessary. Using a non-isothermal DSC has two important advantages. First, from experimental point of view, it is an effective, easy to use and rapid tool to measure with good precision for the energy absorbed (endothermic peaks) or released (exothermic peaks) during phase transformation by a well-defined small sample. Second, the energy absorbed or released is the overall effect of the evolution of precipitates and the composition of Al-matrix. DSC simulation is directly correlated to the phase fraction of metastable and stable phases and the state of the solid solution in the multi-component matrix as a function of time.

In the present work, a computational tool, MatCalc [3], for thermo-kinetic simulation of phase transformation based on CALPHAD-type multicomponent thermodynamics is applied. Simulated DSC curves are calculated numerically as the first derivative of the

system enthalpy with respect to temperature as given by

$$Q = (c_p^{\text{sys}} - c_p^{\text{Al}}) \frac{\Delta T}{\Delta t} = \frac{d(H^{\text{sys}} - H^{\text{Al}})}{dT} \cdot \frac{\Delta T}{\Delta t} \quad (1)$$

where Q is the heat flow; c_p^{sys} and c_p^{Al} are the specific heat capacities of the alloy and pure reference aluminum, respectively; H^{sys} and H^{Al} are the specific enthalpies of the alloy and pure Al, respectively; $\Delta T/\Delta t$ is the heating rate.

A proper physically-based predictive precipitation kinetics model approach can deliver a correct DSC simulation and as a result a correct precipitation kinetic parameter set, the same parameters set can be used for complex heat treatments and/or mechanical properties calculation. In the following, two industrial heat treatable aluminum alloys types 6xxx (Al–Mg–Si) and 2xxx (Al–Cu–Mg–Si) are chosen for demonstration of the simulation method and explaining important parameters in the precipitation kinetics simulation that should be taken into account. We assume that the reader has the fundamental knowledge about the experimental aspects of DSC [4].

2 Thermo-kinetic computational analysis

MatCalc version 5.52 (rel. 0.031) was used with the corresponding thermodynamic [5], mobility and physical databases [6] for Al alloys. Thermodynamics and mobility databases are CALPHAD-types. The thermodynamic database contains solid solution phases as a function of temperature and chemical composition and optimized Gibbs energy functions of stable and metastable compounds as a function of temperature [1]. The mobility database contains assessed self-diffusion and impurity diffusion data. The physical database contains optimized polynomials that describe the densities of phases as a function of temperature. Our simulation is based on multicomponent solid-state nucleation, which has been developed on the basis of classical nucleation theory (CNT). According to CNT, transient nucleation rate depends on the exponential expression of critical nucleation energy [7]. Individual nucleation events occur on a stochastic nature, but once a supercritical nucleus has formed, the deterministic laws of particle growth, dissolution and coarsening govern its further evolution.

In MatCalc, a mean-field approach to derive evolution equations for the growth and dissolution of spherical precipitates in multicomponent systems, which is based on the thermodynamic extremal principle (TEP), is used [8]. The numerical method implemented to follow up precipitates evolution (nucleation, growth and coarsening) is the numerical Kampmann–Wagner (NKW)

model. The key quantity when evaluating precipitate nucleation rates in kinetic simulations model is the Gibbs free energy change of forming a critical nucleus. The total energy change due to nucleus formation, ΔG_{nucl} , can be separated into the following three contributions:

$$\Delta G_{\text{nucl}} = \Delta G_{\text{bulk}} + \Delta G_{\text{vol}}^{\text{el}} + \Delta G_{\text{surf}} = \frac{4}{3} \pi \rho^3 \Delta G_{\text{bulk}}^0 + \Delta G_{\text{vol}}^{\text{el}} + 4\pi \rho^2 \gamma \quad (2)$$

where ΔG_{bulk} is the chemical bulk free energy; $\Delta G_{\text{vol}}^{\text{el}}$ is the coherency elastic strain energy; ΔG_{surf} is the total interfacial free energy; Chemical bulk free energy (ΔG_{bulk}) is associated with structural change from matrix to the precipitate phase; ρ is the radius of the precipitate and ΔG_{bulk}^0 is the specific bulk energy, which is evaluated from the assessed CALPHAD-type free energies of the matrix and precipitate phases.

Nucleus formation is generally accompanied by a typical mismatch between the lattice parameters of the precipitate and the surrounding matrix. For a completely coherent interface, the strain energy ($\Delta G_{\text{vol}}^{\text{el}}$) plays a crucial role since it is proportional to the total volume, whereas the interfacial energy is only proportional to the area of the nucleus. A simplified model for a solid spherical inclusion inserted into a spherical hole of an isotropic elastic matrix is a classic elasticity problem and the energy contribution coming from volumetric misfit stress is given by

$$\Delta G_{\text{vol}}^{\text{el}} = \frac{E}{9(1-\theta)} (\nu^*)^2 \quad (3)$$

where E is the elastic modulus; θ is Poisson ratio; ν^* is the misfit volume strain [2]. Considering an isotropic elastic matrix, the linear elastic misfit is given as $\epsilon^* \approx \theta^*/3$. This energy contribution is taken into account in the present simulation. If a precipitate nucleates coherently in the bulk crystal, the entire misfit energy, as given in Eq. (3), is theoretically operative in the nucleation process. If the volumetric misfit is large enough, the stress fields can be relaxed to some extent due to matrix plasticity. For precipitates located at dislocations, a certain portion of the elastic misfit is compensated for by either the compressive or tensile component of the dislocation stress field. The effective elastic misfit used in the simulations is therefore smaller than the value for homogeneous bulk nucleation. For precipitates nucleating at grain boundaries, we assume that there is no elastic misfit involved during nucleation, since stresses are quickly relaxed by fast diffusion of vacancies and atoms along the grain boundaries [9].

The total interfacial free energy contribution (ΔG_{surf}) is equal to the specific interfacial energy (γ) multiplied with the surface area of the nucleus. The interfacial

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