Proceedings of the 1st World Congress on Integrated Computational Materials Engineering (ICME)

Edited by
John Allison
Peter Collins
George Spanos
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Proceedings of the

1st World Congress
on Integrated Computational Materials Engineering (ICME)

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John Allison, Peter Collins and George Spanos

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Preface

This book represents a collection of papers presented at the 1st World Congress on Integrated Computational Materials Engineering, a specialty conference organized by the The Minerals, Metals, and Materials Society (TMS) and the three conference organizers, and held at Seven Springs Mountain Resort, PA, USA, on July 10 - 14, 2011.

Integrated Computational Materials Engineering (ICME) is an emerging field with tremendous potential for developing advanced materials, manufacturing processes, and engineering components more quickly and cost-effectively. The major goal of this conference was to help unlock that great potential by bringing together scientists and engineers working in ICME-related areas to share information, stimulate creative ideas and discussion, and identify opportunities for collaboration of computational and experimental efforts. To that end, more than 200 authors and attendees contributed to this conference, in the form of presentations, lively discussions, and the papers found in this volume. As emphasized in a 2008 National Academies study on ICME, successful ICME efforts typically involve nearly 50 percent experimental components for critical development, testing, validation, and enhancement of the computational models, so it was critical to bring together both experimentalists and modelers at this ICME World Congress. In that regard, the presentations included both computational- and experimental-based research representing a wide range of programs related to ICME.

The specific topic areas (sessions) of the conference were: Modeling Processing-Microstructure Relationships - I & II, Modeling Microstructure-Property Relationships - I & II, The Role of ICME in Graduate and Undergraduate Education, Information infrastructure, and ICME Success Stories. The conference included 10 Keynote talks from prominent international speakers working in ICME, 40 contributed podium talks, and an exceptional poster session (>140 posters) seamlessly embedded into the main conference hall. International representation was certainly a hallmark of this “World Congress”, in that five materials societies outside of the US promoted the conference within their countries, and an international advisory committee representing 14 countries was active in advising and promoting this conference worldwide. This resulted in speakers from 11 different countries, and a third of the podium speakers were from outside of the US. The single session format and intimate setting were specifically planned to promote stimulating discussions and rich interactions amongst the attendees.

The 35 papers in this proceedings are divided into three sections: (1) Modeling Processing-Microstructure Relationships, (2) Modeling Microstructure-Property Relationships, and (3) The Role of ICME in Graduate and Undergraduate Education, Information Infrastructure, and Success Stories; these articles
represent a cross cut of presentations from this conference. It is our desire that this First World Congress on ICME, and these proceedings, will not only create opportunities to sustain, support, and enhance on-going ICME activities and evolving ICME strategies, but will additionally provide a greater awareness of ICME worldwide, and result in a recurrence of this ICME World Congress for many years to come.
Acknowledgements

The organizers/editors would like to acknowledge a number of people without whom this ICME World Congress, and the proceedings, would not have been possible.

First, thanks to a number of people on the TMS staff who worked tirelessly to make this a first rate event and proceedings; these include (in alphabetical order): Becky Arnold, Michael Bazzy, Marla Boots, Maureen Byko, Adrianne Carolla, Margie Castello, Patricia Dobranski, Trudi Dunlap, Christina Raabe Eck, Beate Helsel, Warren Hunt, Colleen Leary, Robert Makowski, David Rasel, Jim Robinson, Lynne Robinson, Elizabeth Rossi, Marleen Schrader, Dan Steighner, Louise Wallach, and Chris Wood.

Secondly we want to thank the international advisory committee of their input during planning and promotion of this conference world-wide. This committee included: John Agren, KTH - Royal Inst. of Technology, Sweden; Dipankar Banerjee, Indian Institute of Technology, India; Yves Brechet, Institute National Polytechnic de, Grenoble, France; Dennis Dimiduk, USAF Research Lab, USA; Masato Enomoto, Ibaraki University, Japan; Juergen Hirsch, Hydro Aluminum, Germany; Dorte Juul Jensen, Riso National Lab., Denmark; Nack Kim, Pohang University of Science and, Technology, Korea; Milo Kral, University of Canterbury, New Zealand; Peter Lee, Imperial College, UK; Baicheng Liu, Tsinghua University, China; Jianfeng Nie, Monash University, Australia; Tresa Pollock, UCSB, USA; Gary Purdy, McMaster University, Canada; Antonio J. Ramirez, Brazilian Synchrotron Light Lab., Brazil; K.K. Sankaran, Boeing Company, USA; Katsuyo Thornton, University of Michigan, USA; James Warren, NIST, USA; Deb Whitis, GE, USA.

Finally, we would especially like to acknowledge the financial support of our US government sponsors: the Air Force Materials Laboratory, the Army Research Office, the National Institute of Standards and Technology, the National Science Foundation, and the Office of Naval Research. We likewise are grateful for the support of the congress' various corporate sponsors and exhibitors.
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Professor John Allison is a Professor of Materials Science and Engineering at The University of Michigan. He joined the faculty in September 2010. Prior to that he was a Senior Technical Leader at Ford Research and Advanced Engineering, Ford Motor Company in Dearborn, Michigan, where he was for 27 years. At Ford he led teams developing Integrated Computational Materials Engineering (ICME) methods, advanced CAE tools and light metals technology for automotive applications. Dr. Allison was the 2002 President of TMS and served on the US National Materials Advisory Board from 2001-2007. He is a member of the National Academy of Engineering, Fellow of ASM and has received numerous awards including two Henry Ford Technology Awards. Dr. Allison received his PhD in Metallurgical Engineering and Materials Science from Carnegie-Mellon University, his MS in Metallurgical Engineering from The Ohio State University and his BS in Engineering Mechanics from the US Air Force Academy.

Professor Peter Collins joined the faculty at the University of North Texas in September 2010. Prior to this, Collins has served as the Deputy Director – Director of Technology for the Quad City Manufacturing Lab (QCML), a not-for-profit manufacturing laboratory and center of excellence in the production and manufacturing of advanced materials, specifically titanium alloys for non-aerospace applications and as the Associate Director for the Center for the Accelerated Maturation of Materials (CAMM). His research has focused on the development of 2D and 3D characterization techniques across length scales, the development of mechanistic understanding of the role of microstructure on tensile and fracture toughness properties in Ti-based alloys, the development of combinatorial techniques to rapidly assess microstructure-property relationships, the use of advanced manufacturing techniques for the production of novel materials, and the use of advanced transmission electron microscopic techniques (including aberration corrected scanning TEM) to probe the most fundamental aspects of a materials microstructure. Collins received his MS and PhD in Materials Science and Engineering from The Ohio State University and his BS in Metallurgical Engineering from The University of Missouri-Rolla.
Dr. George Spanos is TMS Technical Director. He received his B.S., M.E., and Ph.D. degrees in Metallurgical Engineering and Materials Science from Carnegie Mellon University. In 1989 he joined the Naval Research Laboratory (NRL) as a staff scientist, in 1994 was promoted to Section Head at NRL, and in 2010 he joined TMS. Dr. Spanos is author/co-author of 92 technical publications in the fields of 3D materials analyses, phase transformations, processing-structure-property relationships, and ICME. Some of his past and present professional affiliations include: member of the Board of Governors of Acta Materialia Inc., chairman and member of the Joint Commission for *Metall. and Materials Trans.*, Chairman and Key Reader of the Board of Review of *Metall. and Mat. Trans. A*, and member of a number of TMS technical committees. Some of his awards include: Fellow of ASM-International, the Marcus A. Grossman Award for best article in *Metall. and Mat. Trans.* in 2001 for authors under 40, two Technology Transfer Awards at NRL, and the NRL 2009 Commanding Officer’s Award for Achievement in the Field of Equal Employment Opportunity.
1st World Congress
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Modeling
Processing-Microstructure Relationships
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CORRELATED NUCLEATION OF PRECIPITATES IN MAGNESIUM ALLOY WE54

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Keywords: Magnesium alloys, Precipitation hardening, Microstructure evolution, Interaction energy, Phase field approach.

Abstract
Magnesium alloy WE54 has been used commercially for fabricating components for aerospace and aircraft applications. Its useful mechanical properties are achieved via a precipitation process. β₁ and β' are the two strengthening precipitate phases when this alloy is peak-aged at 250°C. The β₁ precipitate plates often form with β' particles attached to their end facets. The aim of this study is to understand the correlated nucleation of the β₁ and β' phases. The equilibrium shapes of coherent β₁ and β' precipitates are simulated using the phase field method. The preferential nucleation site of a nucleating precipitate at the interface of pre-existing particle/Mg matrix is analyzed through the calculation of the elastic interaction energy between the nucleating precipitate and the pre-existing particle. The evolution sequence of the β₁ and β' phases are also simulated in this work. Our results indicate that the coherency elastic strain energy can be reduced significantly if a β' particle forms at an edge facet of a pre-existing β₁ plate, and that the preferred nucleation sites of the β' particles are at the two end-facets of the β₁ plate. Under the assumption that the β₁ phase nucleates first, the microstructure evolution sequence is proposed in this work.

Introduction
The development of high strength, light-weight magnesium alloys for elevated temperature applications has experienced a rapid growth over the past 10 years [1-3]. One of the most successful magnesium alloys developed in this category is WE54 (5 wt% Y, 2 wt% Nd and 2 wt% heavy rare-earth elements). The strength of this alloy is achieved by conventional age-hardening treatments, i.e., a solution treatment for 8h at 525°C, followed by hot water quench and a subsequent ageing treatment of 16 h at 250°C [4]. The microstructure of such heat treated samples contains predominantly two precipitate phases: plate-like β₁ and globular β', Fig. 1[5]. The β₁ is metastable and has an f.c.c. structure with lattice parameter a = 0.74 nm. The orientation relationship between β₁ and the Mg matrix is such that (112)β₁//(1100)a and [110]β₁//[0001]a [5]. There are six different orientation variants of β₁ particles, which are shown in Fig. 1b. The β' phase is also metastable [6] and has an orthorhombic structure (a =0.667 nm, b = 2.351 nm, c = 0.521 nm). The orientation relationship between β' precipitates and the matrix phase has been determined as (100)β'//(1210)a and [001]β'//[0001]a. The β' phase has three variants which are related to each other by 120° rotation about the [0001]a axis [7].

Experimental results show that individual β₁ plate always forms with β' particles attached at its two ends [5] (Fig. 1a). This phenomenon is also observed in many other Mg-rare-earth based alloys. However, the reason behind this phenomenon is not clear. Apps et al. [8] claimed that the β' globules formed first and therefore acted as heterogeneous nucleation sites for the nucleation of β₁ phase. However, Nie and Muddle [5] suggested that β₁ formed directly from magnesium lattice via an invariant plane strain transformation, then the β' globules formed at the two end facets of individual β₁ plate as a consequence of shear strain.
accommodation.

The aim of this project is focus on the explanation of the reason why individual $\beta_i$ plate always forms with $\beta'$ particles attached at its two ends, and determine the formation mechanism of this structure by phase field simulation.

**Model Formulation**

Lattice Correspondences and SFTS (Stress Free Transformation Strain) Tensor

The lattice correspondences between the Mg matrix and $\beta_i$ is $[-1,-1,2,0] \rightarrow [1,-1,1]$, $[1,-1,0,0] \rightarrow [-1,1,3]$ and $[0,0,0,1] \rightarrow [110]$, and lattice correspondences between the Mg matrix and the $\beta'$ is $[-1,-1,2,0] \rightarrow [1,0,0]$, $[1,-1,0,0] \rightarrow [-1,1,3]$ and $[0,0,0,1] \rightarrow [0,0,1]$. The number of orientation variants of precipitates is determined by the number of symmetry elements in the intersection group of parent and product phases for a given orientation relationship [13]. There are 6 different orientation variants of $\beta_i$, but according to Fig. 1b, variant 1 and 6, 2 and 3, 4 and 5 have the same transformation strain and therefore there exists only three different types of SFTS. There are 3 different orientation variants of $\beta'$. To ensure that the phase transformations from Mg to $\beta_i$ and $\beta'$ can be reflected into one coordinate system, in this work, the $x$ direction corresponds to $[1,-1,0,0]_{\beta_i}/[1,-1,1]_{\beta_i}/[1,0,0]_{\beta_i}$, the $y$ direction corresponds to $[-1,-1,2,0]_{\beta_i}/[-1,1,1]_{\beta_i}/[0,1,0]_{\beta_i}$ and the $z$ direction corresponds to $[0001]_{\beta_i}/[110]_{\beta_i}/[0,0,1]_{\beta_i}$ for simulation system. Thus the SFTS tensors of different variant of $\beta_i$ and $\beta'$ are shown as follows:

$$\varepsilon_{\beta_i}^{1} = \begin{pmatrix} 0 & 0.0962 \\ 0.0962 & 0.1111 \end{pmatrix}, \varepsilon_{\beta_i}^{2} = \begin{pmatrix} -0.0556 & 0 \\ 0 & 0.1667 \end{pmatrix}, \varepsilon_{\beta_i}^{3} = \begin{pmatrix} 0 & 0.0962 \\ -0.0962 & 0.1111 \end{pmatrix};$$

$$\varepsilon_{\beta'}^{1} = \begin{pmatrix} 0.0217 & 0 \\ 0 & 0.036 \end{pmatrix}, \varepsilon_{\beta'}^{2} = \begin{pmatrix} 0.0323 & 0.0063 \\ -0.0063 & 0.0254 \end{pmatrix}, \varepsilon_{\beta'}^{3} = \begin{pmatrix} 0.0323 & 0.0063 \\ -0.0063 & 0.0254 \end{pmatrix};$$

With the particular form of the transformation strain given above, the microstructural evolution during the Mg$\rightarrow$$\beta_i/\beta'$ transformation can be effectively modelled in two dimensions without losing any essential physics. Furthermore, on the basal plane of the hexagonal lattice, the elastic constants are indeed isotropic.

**Elastic Energy Calculation**

In the present study, a homogeneous modulus is assumed throughout the system and the elastic energy is calculated via Khachaturyan and Shatalov’s microelasticity theory (KS theory) [9]. The modulus of the Mg matrix is selected as the reference, i.e. $C_{11}=63.5$ GPa, $C_{12}=24.85$ GPa, $C_{13}=20.0$ GPa, $C_{23}=66.6$ GPa and $C_{44}=19.3$ GPa, which are obtained by ab initio calculations [10]. Assuming that the precipitate and the matrix phases are coherent and considering a zero strain boundary condition (i.e. a grain embedded in a polycrystalline aggregate), a close form of the coherency elastic strain energy reads [9]:

![Fig. 1. (a) Transmission electron micrograph showing a WE 54 alloy aged at 250°C 8 hours, showing six variants of $\beta_i$ phase (arrowed) and the globular $\beta'$ phase, and (b) schematic representation of the six variants distinguishable in [0001], orientation [5].](image-url)
where

\[ \mathbf{B}_{pq}(n) = C_{ijkl} \varepsilon_i^j(n) \varepsilon_k^l(n) - n_i \varepsilon_j^k(n) \varepsilon_k^l(n) n_l. \]  

In Equation 1, to keep the stability of the programme, \( \{ \mathbf{P}[\eta_p(r)] \} \) is the Fourier transform of \( \mathbf{P} \) function, i.e. \( \mathbf{P}(r) = r|3(10-15r)+6r|^2 \), which is used to connect the transformation strain between product phases and matrix, \( \varepsilon^{0} \) is the STFS and \( \sigma^{0} = C_{ijkl} \varepsilon^{0} \) where \( C_{ijkl} \) is elastic constant, \( g \) is a vector in the reciprocal space and \( n_e = g/\|g\| \). The superscript asterisk indicates a complex conjugate.

**Bulk Chemical Free Energy Calculation**

In this study the WE54 alloy is simplified as Mg-5wt\%Y-4wt\%Nd. The Mg phase can be treated as a regular solid solution, and according to the CALPHAD database [11], its chemical free energy density as a function of concentrations of Y and Nd can be expressed in the following dimensionless form and the energy normalised factor is \( 10^4 J/mol \):

\[ G_{\text{Mg}} = -1.8989 - 5.1124x_{\text{Nd}} + 4.7448x_Y + 6.8855x_{\text{Nd}}^2 + 4.1893x_Yx_{\text{Nd}} + 8.2346x_Y^2 / l_0^3, \]  

where \( l_0 \) the length of one unit grid.

Since both \( \beta_i \) and \( \beta' \) are metastable phases, their free energy functions are not available from the CALPHAD database. In this work, the free energy of both \( \beta_i \) and \( \beta' \) phases are approximated by parabolic functions of solute concentrations. A tangent surface is drawn from \( G_{\text{Mg}} \) at the equilibrium Mg matrix concentration, which should be tangential to the free energy curve of both \( \beta_i \) and \( \beta' \) at their equilibrium compositions. Considering the effect of the curvature on the interfacial energy between the two phases, the following parabolic functions are used to describe the bulk chemical free energy densities (in reduced unit, i.e. \( /l_0^3 \)) of the \( \beta_i \) and \( \beta' \) phases, respectively, and the energy normalised factor is \( 10^4 J/mol \):

\[ G_{\beta_i} = -2.9084 + 2.1565x_{\text{Nd}} + 2.2180x_Y - 5.0x_Y^2 - 5.0x_{\text{Nd}}^2 - 7.50x_Yx_{\text{Nd}} / l_0^2, \]  

and

\[ G_{\beta'} = -2.5909 - 1.0738x_{\text{Nd}} + 1.1122x_Y - 5.0x_Y^2 - 5.0x_{\text{Nd}}^2 + 7.50x_Yx_{\text{Nd}} / l_0^2. \]  

\( P \) function, \( P(\eta) \), is used to connect the free energy of the two phases. Thus the chemical free energy can be expressed as follows:

\[ E^{\text{chem}} = \int [f(c, \eta) + \kappa[(\nabla c)^2 + (\nabla \eta)^2)] d^3r, \]  

where \( \kappa \) is the gradient energy coefficient. The numerical value (in reduced unit) used in the simulations in this project are \( \kappa = 0.4 \) to guarantee a diffused interface profile.

**Kinetic Equations**

The Cahn-Hilliard generalized diffusion equation [12] is used to describe the evolution of the concentration field \( c(r, t) \):

\[ \frac{\partial c(r, t)}{\partial t} = \nabla \left( \frac{M \delta (E^c + E^{\text{chem}})}{\delta c(r, t)} \right) + \xi(r, t), \]  

where \( M \) is the chemical mobility. \( M \) has its unit \( J^3 \text{mol}^2 \text{m}^{-4} \text{s}^{-1} \). In this study, due to the lack of data of inter-diffusion coefficient between Y and Mg, as well as Nd and Mg, the time step is used by reduced time step \( t \). The numerical value of \( M \) used in this study is 10. \( \xi(r, t) \) is the Langevin noise term which describes thermal fluctuation.

The time dependent Ginzburg-Landau equation [14] is used to describe the time evolution of the structural order parameter \( \eta(r, t) \):

\[ 5 \]
where L is the mobility of the order parameter, and the numerical value L used in this project is 5.0.

**Results and Discussion**

The system size used in the simulations is $256l_0 \times 256l_0$. The interfacial energy of a coherent interface between the Mg matrix and the precipitate phases is assumed to be 50mJ/m$^2$ and possible anisotropy in the interfacial energy is ignored. The corresponding length scale is $l_0=0.98$nm.

Figs. 2a and b show the simulation results for a single particle of $\beta_1$ and $\beta'$ respectively. The simulation result shows the habit plane between plate shaped $\beta_1$ particle and Mg matrix in the given orientation relationship is $<1,-1,0,0>$ Mg, which corresponds to the experimental results [5-7].

Fig. 2 2D Simulation results illustrate the growth and shape evolution process of one single (a) $\beta_1$ particle, and (b) $\beta'$ particle in h.c.p Mg matrix for $r=2000$. Interfacial energy is taken to be isotropic.

Fig. 3 (a, b and c) Interaction energy calculation results between a pre-existing $\beta_1$ particle and three different variants of $\beta'$ particles. The unit of interaction energy in this figure is $10^8$ J/m$^3$. (d) 2D Simulation result illustrates the growth and shape evolution process of $\beta'$ particles under the influence of stress field of the pre-existing $\beta_1$ particle in h.c.p Mg matrix.
values of the interaction energy between the pre-existing $\beta_i$ and the different variants of $\beta'$ are different, which means that for $\beta_1$ phase in each orientation relationship, it should have a preferred orientation relationship of $\beta'$. However, this preference hasn't been examined in experiments because the difference of elastic interaction energy values between a $\beta_i$ precipitate and different variants of $\beta'$ particles is very small.

Figs. 4a, b and c shows microstructure evolution by assuming that $\beta_1$ particles form first, which then act as heterogeneous nucleation sites for $\beta'$ particles. Fig. 4b shows the simulation obtained right after the Langevin noise terms in Eqs. (7) and (8) are turned off. It is readily seen that, under the influence of the stress field of the pre-existing $\beta_1$ particles, the preferred nucleation sites of $\beta'$ particles are the two ends of the pre-existing $\beta_1$ particles. This is good agreement with the experimental observations. These $\beta'$ particles keep growing until the equilibrium volume fraction is reached.

The microstructure evolution by assuming that $\beta'$ particles form first, which then serve as heterogeneous nucleation sites for $\beta_1$, is shown in Figs. 4d, e and f. Fig. 4e corresponds to the moment when the Langevin noise terms are just turned off. As can be seen from this image, the preferred heterogeneous nucleation sites of $\beta_1$ particles are at the interface between the pre-existing $\beta'$ particles and Mg matrix. It is interesting to note that the heterogeneously nucleated $\beta_1$ particle shown in Fig. 4e has a tendency to grow towards a nearby $\beta'$ particle (Fig. 4f) due to their long-range elastic interactions. Fig. 4e, also shows a configuration that only one end of $\beta_i$ has $\beta'$ particle attached (see the white circle). Comparing these simulation

![Fig. 4 Nucleation sequence determination. (a, b, c) show the microstructural evolution by assuming that $\beta_1$ particles form first and then $\beta'$ particles nucleate under the influence of existing $\beta_1$ particles and the associated stress and concentration fields, while (d, e, f) show the microstructural evolution by assuming that $\beta'$ particles form first and then $\beta_1$ particles nucleate under the influence of existing $\beta'$ particles and the associated stress and concentration fields. Two different variants of $\beta_1$ phase can be seen in (f). (a) and (d) show the pre-existing $\beta_1$ and $\beta'$ particles, respectively, which are the initial condition for the two simulations. The interfacial energy is assumed to be isotropic.](image)
results to experimental observations, we may conclude that $\beta_1$ particles forms first during ageing followed by heterogeneous nucleation of $\beta'$.

**Conclusion**

The existence of an invariant plane provides a tendency for $\beta_1$ particles to grow along the invariant plane and form plate-shaped particles to minimise its elastic energy. The morphology of $\beta'$ particles is globular because all strains along principle directions are positive and the difference of elastic strain between different principle directions are not very large (2.17% in $x$ direction and 3.6% in $y$ direction). The interaction energy calculation results indicate that the coherency elastic strain energy can be reduced significantly if $\beta'$ particles forms at the two edge facets of $\beta_1$ particles, and that in this case the preferred nucleation site of the $\beta'$ particles is at the end-facets of the pre-existing $\beta_1$ particle. For microstructure evolution sequences determination, if $\beta'$ phase forms first and then act as heterogeneous nucleation sites for $\beta_1$ particles, only one $\beta'$ particle (the pre-existing one) can be observed attached at the end of the $\beta_1$ particles thus formed, which is not in consistent with the experiment observations. Therefore, our modelling work indicates that the $\beta_1$ phase may have formed first and then acted as heterogeneous nucleates sites for $\beta'$ particles.

**References**


FROM PROCESSING TO PROPERTIES: THROUGH-PROCESS MODELING OF ALUMINUM SHEET FABRICATION

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Keywords: Aluminum, Through-Process-Modeling, Deformation, Recrystallization, Texture

Abstract

The microstructure of a material rather than the processing condition is the state parameter of material properties. We report on activities of microstructural through-process modeling activities to predict the properties of a processed product from the knowledge of the processing conditions and the chemical composition of the material. The respective modeling tools are introduced. As an example we address aluminum sheet fabrication and material behavior during subsequent sheet metal forming. Using additionally atomistic modeling tools for the prediction of thermodynamic, kinetic and elastic data provides promising avenues for a comprehensive multi-scale modeling of materials processing.

The Problem

The control variables of a materials engineer for optimizing materials properties are overall chemistry and processing parameters. Therefore, it is desirable to derive processing-property relationships for cost-efficient production and property optimization. Such efforts have led in the past 20 years to the development of empirical models to predict properties of semi-finished products via closed form analytical functions, mostly power law relationships for monotonous dependencies. For a given material and processing route this is a very successful approach and the predictive power of such models is excellent so that many steel producers only computed final materials properties rather than measuring them.

This modeling approach fails, however, if the processing window or the composition of the material is changed. In that case a complete reformulation of the used empirical function is necessary which involves a large number of measurements. To avoid these time consuming and costly efforts, attempts have been made to put physical metallurgy to work, i.e. to apply our scientific understanding of the metallurgical phenomena for property predictions.

Unfortunately, these concepts prove that the processing conditions are not the state variables of materials properties so that there is no such thing like a processing-property relation. Rather, the processing parameters determine the microstructural development of a material and the microstructure constitutes the state variables of materials properties (Fig. 1.)
The properties of a part are measured on a macroscopic length scale, but they are controlled by the microstructure, which is defined on a much smaller length scale.

**The Modeling Approach**

Hence, there are highly non-linear relationships between processing and properties, and at most, one can establish a processing-property correlation that can be used as a database or for optimization procedures like neural networks.

In order to describe metallurgical phenomena the development of microstructure has to be known. We define microstructure as the spatial distribution of elements and defects in a material, hence comprising thermodynamic constitution, crystal orientation, crystal defects etc. [1].

For through-process modeling (TPM), i.e. the prediction of properties along a process chain, microstructure evolution through the entire process chain has to be modeled. The typical process chain for Al sheet production is given in Fig. 2.
It encompasses solidification, homogenization, hot rolling, cold rolling and annealing prior to sheet metal forming. Here, we want to restrict ourselves to solid state processing, starting with homogenization of a known (i.e. fully characterized) solidification microstructure. If we consider a specific volume element, it will undergo temperature changes $T(x,y,z,t)$ and will suffer deformation $\varepsilon(x,y,z,t)$ during processing which can be computed by finite element modeling (FEM). Hence, a computation of the processing history will provide the path line for microstructure development, i.e. the FEM model can serve as a process model. A given state of change of temperature or strain will cause microstructural changes. At first glance, this is a simple problem since there are only three metallurgical phenomena that cause microstructural changes, i.e. phase transformations, crystal plasticity, and recrystallization (including related processes like recovery and grain growth) [2]. The problem is the complexity of each of these metallurgical phenomena and their mutual interaction during processing. Therefore, in order to follow the microstructural development in a volume element, the microstructural changes caused by all phenomena have to be updated in a time increment, and the changed microstructure will serve as input to the computation of microstructure development in the next time step etc.

Microstructural processes like precipitation, dissolution, recrystallization, grain growth, plastic deformation have been extensively investigated in the past century and are most appropriately described on a microscopic scale. Accordingly, the metallurgical phenomena are adequately modeled by mesoscopic modeling tools, which utilize statistical information of a volume element, like solute content, precipitate size and volume fraction, dislocation density and arrangement or crystal orientation and grain boundary misorientation in conjunction with their change in space and time.

Several TPM exercises have been successfully conducted in the past [3-7]. Since a comprehensive microstructural characterization requires the knowledge of a large number of parameters, it is recommendable to first define the target quantities of a TPM run, in order to reduce the number of microstructural parameters to the minimum necessary set of variables.

**Through-Process Modeling**

**Modeling Tools**

In the following we will consider as an example a TPM exercise to predict the terminal strength and texture of a rolled sheet. The strength can be calculated with a dislocation based work hardening model if the nature and arrangement for dislocation motion is known, i.e. crystal structure, dislocation density, particle size and volume fraction, solute content, grain size and texture. The crystallographic texture is changed by plastic deformation and recrystallization, which in turn are affected by deformation and phase transformations. Hence, this is an intricate problem on top of the difficulty that the process of recrystallization itself proceeds by nucleation and growth of strain free grains in a deformed crystal, which are difficult to describe quantitatively and which are difficult to determine experimentally [8].
The modeling tools used for this exercise are given in Fig. 3. They comprise a dislocation based work hardening model, a precipitation, coarsening and dislocation model and a recrystallization model that accounts for nucleation and nucleus growth. Of course, all effects can mutually influence each other.

**Example: Recrystallization**

To give a feeling for the complexity we specifically want to consider recrystallization. The growth of a viable nucleus can be reasonably numerically modeled by discretizing the microstructure and tracking the location of the nucleus surface by solving the equation of motion for its grain boundaries under the given boundary conditions (dislocation density, particle distribution, misorientation etc.). This growth process can be successfully modeled with a variety of different approaches, like Monte-Carlo simulation, cellular automata or phase field methods. We will use cellular automata in the following [9].

The major problem for recrystallization modeling is to properly account for nucleation. Without quantitative information on the nucleation rate and nucleus orientation it is not possible to predict grain size, texture, and recrystallization kinetics. From a large body of experimental results on Al-alloys it is known that nucleation occurs preferentially at deformation inhomogeneities, grain boundaries and large particles (Fig. 4). To predict the microstructure at these preferred locations, microstructure development during deformation has to be simulated prior to recrystallization modeling to provide information on nucleation density, size and orientation. This can be accomplished by the code ReNuc [10].