Materials Science Forum Vols. 558-559 (2007) pp. 3-12
online at http://www.scientific.net

Recent Advances in the Simulation of Recrystallization and Grain Growth

Günter Gottstein[1,a], Lasar S. Shvindlerman[2,b], Mischa Crumbach[3,c], Luis A. Barrales-Mora[1,d]

[1] Institute of Physical Metallurgy and Metal Physics, RWTH Aachen, 52056 Aachen, Germany
[2] Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow Distr., 142432 Russia
[3] Novelis Technology AG, Badische Bahnhofstr. 15, 8212 Neuhausen, Switzerland

[a]Gottstein@imm.rwth-aachen.de, [b]shvind@imm.rwth-aachen.de,
[c]Mischa.Crumbach@novelis.com, [d]barrales@imm.rwth-aachen.de

Keywords: Simulation, nucleation, grain boundary junctions, grain growth kinetics.

Abstract. Modeling and simulation of recrystallization, grain growth, and related phenomena are important tools for the fundamental understanding of microstructural evolution and prediction of engineering properties. In particular for ultra fine grained and nanocrystalline materials proper account of microstructural evolution is essential for the optimal processing of these materials. It is shown that for modeling of softening phenomena it is important to discriminate between discontinuous primary recrystallization and discontinuous grain growth owing to their quite different underlying physics. Recent developments in recrystallization modeling and simulation of grain growth are addressed, in particular nucleation of recrystallization and junction effects in grain growth. Major progress is also expected from atomistic modeling and quantum-mechanical computations for making available specific material properties.

Introduction

Recrystallization and grain growth are softening mechanisms driven by the energy gain associated with the removal of lattice defects [1,2]. Both can occur as a continuous or discontinuous process. In fact, the phenomena of discontinuous grain growth have similarity to discontinuous recrystallization, and discontinuous grain growth is, therefore, also referred to as secondary recrystallization. On the other hand, continuous recrystallization is not a recrystallization process but essentially controlled by recovery. Owing to the ease of observation of recrystallization phenomena and the typical trend in materials science to coin a new term for every observed phenomenon there is a confusing abundance of terms for the same physical phenomenon which

i) unnecessarily complicates the understanding of the observed phenomena because they convey the impression of a large number of different processes that have to be explained separately,
ii) obscures the view on the underlying physics which are necessary to understand to adequately model the phenomena.

A pertinent recent example is the literature on the thermal stability of severely plastically deformed materials, for instance by equal channel angular extrusion (ECAP). In an orientation micrograph obtained by electron back scatter diffraction (EBSD) the microstructure appears like a perfect polycrystal [3,4], and the microstructural coarsening observed during annealing is throughout referred to as grain growth. A look into the specimen by transmission electron microscopy (TEM) readily reveals that the microstructure after ECAP is still a heavily deformed structure with a high dislocation density and a high fraction of cell boundaries which by definition will undergo recrystallization upon annealing [4]. One could argue that the terminology is not so important, since the phenomena of recrystallization and discontinuous grain growth are very similar. However, the underlying physics are quite different, because discontinuous grain growth is driven by grain boundary curvature whereas recrystallization is driven by the stored energy of cold work and in this case the grain boundaries of a growing nucleus frequently move locally opposite to their curvature.

Correspondingly, a respective model will be quite different, depending on what kind of microstructural process has been assumed. In essence, there are three different softening phenomena to be discriminated for modeling:

a) recovery on the basis of dislocation theory in conjunction with the behavior of low angle grain boundaries;
b) primary recrystallization on the basis of the generation of mobile grain boundaries and their migration at the expense of the deformed microstructure;
c) grain growth on the basis of curvature driven migration of grain boundaries with all implications due to the constraints of connected boundary systems.

Humphreys [5] tried to combine these three very different physical phenomena in a unified approach. However, this is only possible for a structure consisting exclusively of grain boundaries, comprising low angle boundaries and high angle boundaries. In such case nucleation of recrystallization could be modeled as discontinuous subgrain growth and primary recrystallization would be identical with discontinuous grain growth. It cannot be ruled out that such cellular structures exist, but TEM micrographs of deformed materials usually reveal a microstructure very different from a perfectly granular arrangement. Being aware of the fact that reality is more complex we will not further consider this concept in the following.

Nucleation of Recrystallization

A variety of approaches have been proposed to model primary recrystallization. A recent review can be found elsewhere [6]. The aim of recrystallization modeling is the prediction of recrystallization kinetics as well as microstructure and texture evolution for a given material and processing condition. Recrystallization comprises nucleation and growth of nuclei. Virtually all current recrystallization models are growth models, and substantial progress has been made by introduction of adaptive subgrid algorithms that allow to track minute details of microstructure evolution during recrystallization [7] However, nucleation of recrystallization is equally important to quantitatively predict recrystallization phenomena. Nucleation models require to include the processing prior to recrystallization annealing, because the recrystallization nuclei are contained in the as deformed microstructure or may be generated from orientations in the deformed structure, e.g. via twinning. Textbook knowledge postulates three necessary conditions [2] for the formation of a viable recrystallization nucleus (also referred to as the 3 instability criteria of the deformed microstructure)

a) supercritical nucleus size (thermodynamic instability),
b) directional driving force (kinetic instability),
c) mobile grain boundary (kinetic instability).

The driving force p for recrystallization of heavily deformed materials is typically of the order $p \leq 10$ MPa. Therefore, the driving force per atom much smaller than the thermal energy even at 0.4 T_m (T_m − melting temperature) where typically recrystallization occurs in a reasonable time (order of 1h or so). Hence, the recrystallization nuclei cannot be generated by thermal fluctuations but must preexist in the deformed microstructure waiting to be activated by local recovery processes during annealing [2]. For a successful modeling of nucleation of recrystallization it is, therefore, indispensible to model already the evolution of the deformed state. TEM micrographs reveal the tremendous complexity of this microstructure, and one is tempted to say that it will be impossible to correctly model the deformed microstructure in detail. This may not be necessary, however, since not each and every detail of the deformed microstructure matters for the nucleation of recrystallization. In principle, the locations with high propensity for nucleation are known, and once their density in the microstructure is determined predictions can be made on the statistics of nucleation from such type of nucleation sites. Recently respective simulation tools have been developed to predict the essential features of the deformed structure e.g. crystal plasticity FEM [8] or cluster-type Taylor models like GIA [9,10] or Lamel [11]. In the following we will utilize GIA in conjunction with the dislocation based work hardening model 3IVM [12] to predict texture evolution and to provide information on slip distribution, dislocation density, local shear relaxation, and liability to recovery,

which can be utilized to characterize nucleation sites and to assess their nucleation potential. This will be outlined in the following (Fig. 1).

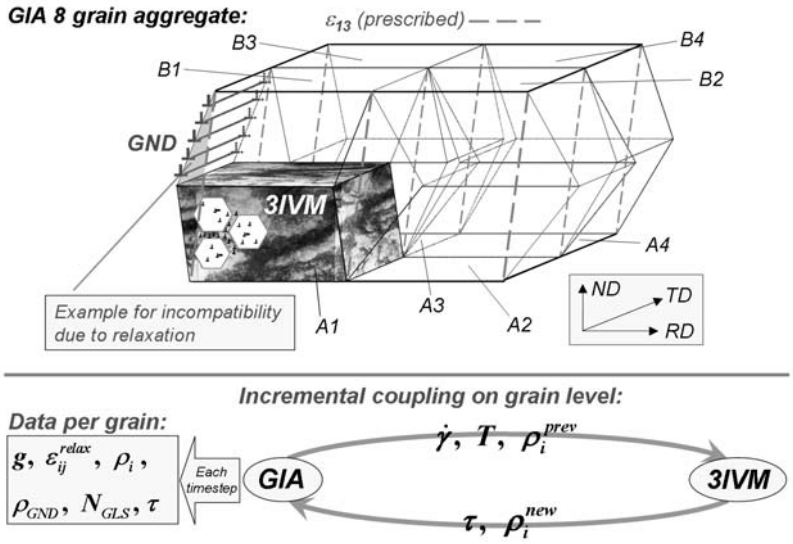


Fig. 1. GIA-3IVM: In GIA an 8 grain aggregate has to comply with the imposed strain state at its surface but can partition the deformation among the 8 grains at the internal interfaces. The coupling with 3IVM renders information on the dislocation density in the grains. See text for details.

In single phase materials nucleation usually is preferred at grain boundaries, in deformation inhomogeneities, and orientation gradients like transition bands [1]. To determine how often such nucleation sites will occur in a deformed microstructure the dislocation density distribution, the in-grain orientation gradients and the liability to shear band formation has to be known. This information is provided by models that probe the occurrence of these nucleation sites during deformation of a polycrystalline assembly. The respective models GIA-split-up and ReNuc will be introduced in the following.

Taylor type deformation texture models including the GIA model assume that each grain deforms homogeneously internally. The GIA model derivative, the *GIA-Split-Up model* [13] was developed to predict, whether grains tend to form in-grain orientation gradients during plastic deformation. It is based on the concept that in grains with a high Taylor ambiguity, i.e. many energetically equivalent possible solutions for the activation of slip systems, in different regions of the grain different sets of slip systems can be activated. This can potentially lead to the fragmentation of a grain, although not necessarily. In the GIA-Split-Up model a grain is subdivided into 8 initially identically oriented regions, and with a random selection of one of the equivalent solutions in case of Taylor ambiguity the orientations of these regions can develop differently due to the activation of different slip system combinations, which are computed according to standard GIA model procedures. The scheme is outlined in Fig. 2 for two examples of grains with different starting orientations. Their split-up behavior is studied under plane strain deformation but imposing locally the microscopic strain rate tensor as obtained from a GIA-texture simulation.

After deformation the average in-grain misorientation (IGM) between the 8 regions in the aggregate was approximated by the average of the misorientations of all 28 different combinations of the 8 regions. This IGM value is not meant to be the exact absolute value for the orientation gradient inside a grain, since the subdivision into 8 regions is artificial. Rather it was taken as a measure for the *tendency* of a grain to split up. The IGM-distribution function (IGMDF) of 3744 initially randomly oriented grains after plane strain deformation of 88% is plotted for the *initial* orientations of each grain in Fig. 3. For the computation material data based on AlMg4.5Mn0.4 [14] was used with a grain size of 50µm. It can be seen that under plane strain conditions and pure {111}<110> slip system activity the Cube orientation has the highest IGM values, followed by orientations next to {011}<110> (Inverse Goss). By contrast, all β-fiber texture components show very low IGM values. These results are in good agreement with most experimental findings [15-17], and very similar

to recent analytical approaches and CPFEM simulations [7,15,17,18]. Details are given elsewhere [10,13].

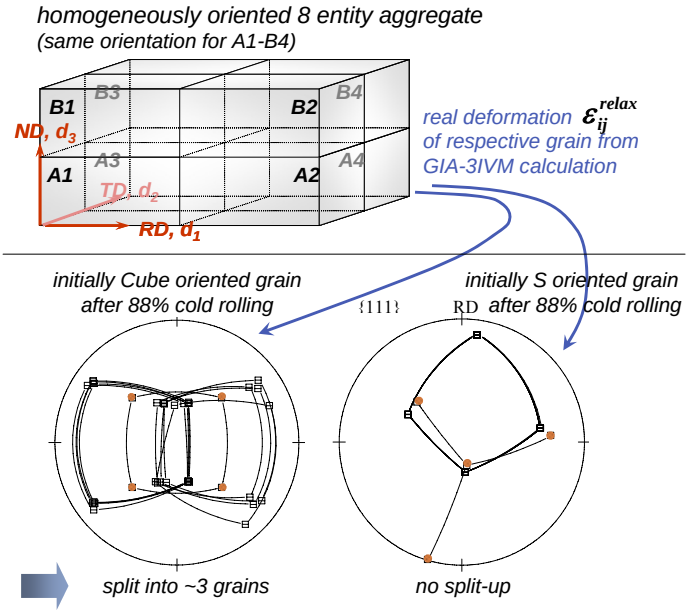


Fig. 2. GIA-split-up simulation for cube and S-orientation.

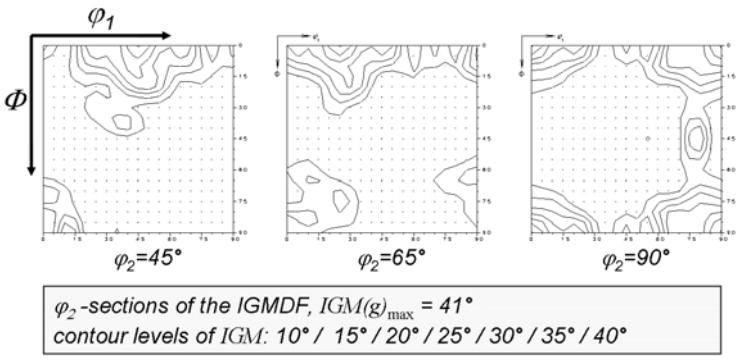


Fig. 3: In-grain misorientation distribution function after 88% plane strain deformation of an AlMg4.5Mn0.4 alloy.

The GIA and the GIA-Split-Up model in conjunction with a dislocation based work hardening model (3IVM) delivers the essential information for the three different types of nucleation mechanisms in single phase alloys: random nucleation at shear bands, nucleation due to subgrain growth at grain boundaries (GB-nucleation), and nucleation in orientation gradients or transition bands (TB-nucleation). The following important deformation (sub-) structure quantities are known for each individual modeled grain: orientation g, total dislocation density ρ_{tot}, number of different active slip systems during the entire deformation N_{GLS}, amount of shear relaxation $\varepsilon_{vM}^{shear-relax}$ in a grain, and IGM value. From this information the nucleus density of the considered nucleation mechanisms is computed by the *ReNuc* code.

Nuclei originating from shear bands are usually found to have an almost random orientation distribution. Shear banding is promoted by an increasing Zener-Hollomon parameter Z and increasing strain [19]; i.e by a higher flow stress. In the GIA model the difference between the local deformation ε_{ij}^{relax} and the macroscopic prescribed deformation ε_{ij}^{macr} shows exactly the same dependencies: the higher the flow stress of the material or the larger the initial grain size, the more relaxes the local deformation of the single grains. A ε_{ij}^{relax} very different from ε_{ij}^{macr} indicates that homogeneous deformation purely by slip is energetically unfavorable. In such case the GIA model introduces many GNDs into the grains, real crystals will additionally react with local shear band formation. To assess whether a grain is liable to form a shear band we defined the value $\varepsilon_{vM}^{shear-relax}$ that represents the amount of shear relaxation in each grain in the GIA model, summed up over the entire deforma-

tion. If $\varepsilon_{vM}^{shear-relax}$ reaches a critical value $\varepsilon_{vM}^{shear-relax^c}$, which depends, of course, on grain orientation shear band formation is considered to take place in the respective grain. In that case random nucleation is assumed to happen in this grain during recrystallization, although not exclusively, because other nucleation mechanisms might contribute to the nucleus orientations in this grain as well.

The formation of nuclei at pre-existing *grain boundaries* (GB) in the as deformed structure is attributed to a subgrain size advantage across the GB. The orientations of respective nuclei have the same orientation as the deformed parent grain, usually slightly changed due to a small orientation scatter within a deformed grain or next to a GB. This means that the overall texture of all potential GB-nuclei is the same as the deformation texture but somewhat weaker. But there is another important aspect of GB-nucleation. Not all potential nuclei will grow and contribute to the recrystallization texture, otherwise RX textures would be similar to the preceding deformation textures, which is generally not the case. Only those nuclei which are located in grains which recover fast and thus form larger subgrains will become active first and grow. The extent of orientation dependent recovery (ODR) can be related to the number of activated slip systems N_{GLS} [10,13], so that fast and slowly recovering orientations can be determined directly from the GIA model output. Orientations in the spectrum with a number of active slip systems exceeding a critical value were assumed to recover fast and to form viable recrystallization nuclei. The other nucleus orientations were deleted from the nucleus spectrum.

Grains with large in-grain orientation gradients, especially grains which discontinuously split into differently oriented regions, are preferred sites for nucleation, since such regions comprise mobile high angle boundaries and inhomogeneously distributed stored energy. Respective grains often contain transition bands (TB) as already proposed by Dillamore and Kato [20], i.e. are an important source of Cube oriented nuclei in cold rolled aluminum. During the formation of a TB, the orientation inside the band remains (almost) unchanged, but the surrounding grain volume rotates away. TB-formation results from constraints of crystallographic slip by deformation symmetry. Cube oriented grains are prone to TB formation, whereas grains with rolling texture orientations more frequently form shear bands. The GIA-Split-Up model renders the IGM for single grains of a deformed polycrystal, i.e. information on their in-grain orientation gradient. If the IGM in a grain exceeded a critical value, this grain was considered to form a TB in which the initial orientation of the grain was preserved. The nucleus orientations inside a TB were associated with a slight scatter around the initial orientation to obtain many similarly oriented nuclei. It is noted that, of course, all grain orientations are liable to subdivision and formation of local inhomogeneities in addition to the effect of grain interaction, which, however, are not considered here.

In the absence of other nucleation sites like large particles we assume the total number of nuclei N_{tot} per unit volume as

$$N_{tot} = N_{rand} + N_{GB} + N_{TB} \tag{1}$$

with N_{rand}, N_{GB} and N_{trans} being the numbers of random nuclei, GB-nuclei and TB-nuclei respectively.

The nucleation fractions (F_{rand}, F_{GB}, and F_{TB}) were calculated according to

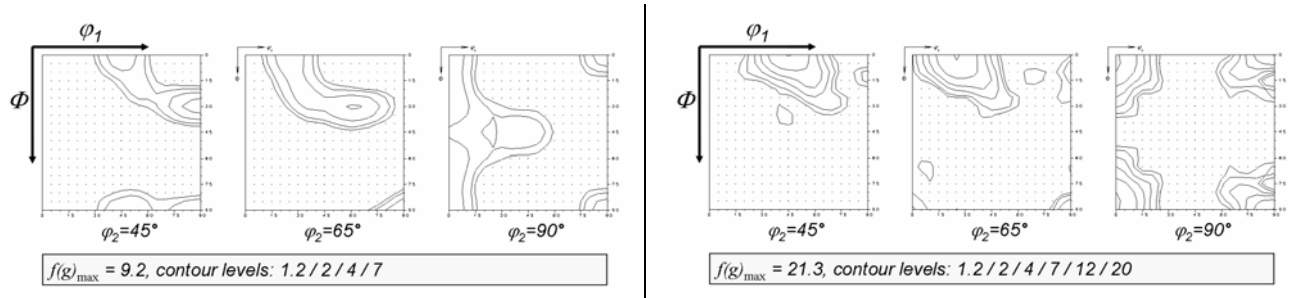
$$F_i = \frac{n_i}{\sum_{k=1}^{3} n_k} \quad with \quad i,k = 1,2,3 \quad and \quad 1 = rand,\ 2 = GB,\ 3 = TB \tag{2}$$

and with n_{rand}, n_{GB} and n_{TB} being the numbers of deformed grains forming random nuclei, GB-nuclei and TB-nuclei respectively, as extracted from the output of a GIA-3IVM simulation. Among all grains N_g^{tot} computed with GIA-3IVM, only those grains were selected and counted which met specific criteria. For example, to generate random nuclei at shear bands the shear relaxation of a grain had to exceed a critical value $\varepsilon_{vM}^{shear-relax^c}$, and n_{rand} is given by

$$n_{rand} = \sum_{i=1}^{N_g^{tot}} \Theta\left(\varepsilon_{vM}^{shear-relax^i} - \varepsilon_{vM}^{shear-relax^c} \right) \quad (3)$$

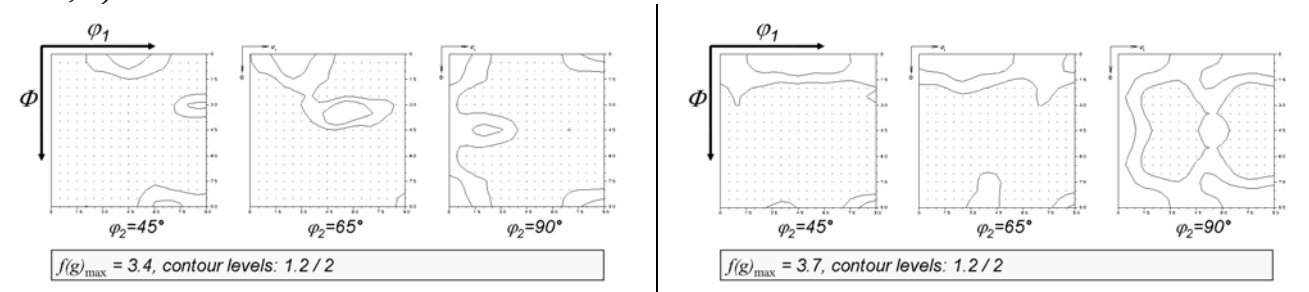
where Θ is the step function $\Theta(x) = 1$ $x > 0$, zero otherwise. Equivalent relations hold for n_{GB} with a critical number of slip systems N_{GLS}^c and for n_{TB} with a critical IGM-value M^c.

The modeling constants of the ReNuc model were tuned to a few measured recrystallization textures. Thereafter they were assumed to apply for all kinds of deformation conditions and a wide range of different aluminum alloys to enable truly predictive simulations. A computed nucleation texture for a rolled AlMg4.5Mn0.4 alloy is given in Fig. 4.



a) b)

Fig. 4. Nucleus textures computed for a 40% cold rolled AlMg4.5Mn0.4 alloy. a) GB nuclei after ODR; b) TB nuclei.



a) b)

Fig. 5. Simulated (left) and experimental (right) recrystallization texture of the alloy given in Fig. 4.

In summary, major progress has been achieved by incorporating information on the evolution of the deformed structure as provided by deformation texture models into recrystallization simulation codes. Evidently, this information is only rudimentary compared to the complexity of the deformed microstructure and does not yet take into account effects of secondary phases so that differences remain between experiment and simulation. Nevertheless, this approach marks a large step forward to truly predictive recrystallization modeling.

Junction Effects on Normal Grain Growth

The phenomena of grain growth have been subject of modeling much more often than recrystallization, probably owing to the much better defined microstructure, which specifies the initial conditions and allows to address the challenging mathematical problem behind the physical phenomenon. Analytical approaches which are typically confined to 2D geometry and which have touched both the kinetics and topology of grain growth have recently experienced a revival in several attempts to find an analytical solution to the 3D problem, in particular a 3D formulation of the so-called von Neumann-Mullins relation which ties the growth rate to the number of faces of a grain, respectively the number of sides in a 2D cellular arrangement [21,22].

In lieu of reliable experimental data of 3D grain structures and their coarsening behavior, numerical simulations are used to evaluate the predictions of analytical approaches. The classical

method of computer simulation of grain growth is the Monte-Carlo (MC) method [23] which finds a trajectory to a lower energy state of the granular system by evaluating the energy change associated with the exchange of elements of the MC grid. Another thermodynamic approach is the phase field method which is derived from the analytical theories of precipitation proposed by Cahn-Hilliard and Ginzburg-Landau [24]. The governing equations can be reformulated for grain growth, and the temporal evolution of the grain structure can be obtained by numerical integration.

A quite different approach is used by kinetics models, like the *vertex models* [25,26], which reflect our physical picture of curvature driven grain growth. In early versions the connected grain boundary system was reduced to its junctions and the equation of motion was solved for each junction in a time step to compute its displacements and thus, the new arrangement after this time step. This approach assumed an imbalance of grain boundary surface tensions at the junction which, however, is not in line with our understanding of curvature driven grain growth. This deficiency was amended by the introduction of virtual vertices on the grain boundaries, which segment the boundaries and determine the local curvature. The equation of motion is then solved for any grain boundary segment while the junctions can be left in equilibrium. Details can be found elsewhere in these proceedings [27].

The effect of junction drag on grain growth can be easily implemented into such model since each vertex is associated with a specific mobility. We have recently developed a 3D vertex code to particularly address junction effects and grain growth affected by external fields like a magnetic field. The latter will be addressed in a separate contribution and only the former will be outlined in the following. It has been shown by theory and experiments that grain boundary junctions (triple lines, quadruple points) can drag boundary motion if either their mobility m is low or the grain size a is very small [28-30]. The junction effects can be expressed in terms of dimensionless parameters Λ, namely

$$\Lambda_{tl} = \frac{m_{tl}}{m_b} a \text{ for a triple line; } \Lambda_{qp} = \frac{m_{qp}}{m_{tl}} a \approx \frac{m_{qp}}{m_b} a^2 \text{ for a quadruple point} \quad (4)$$

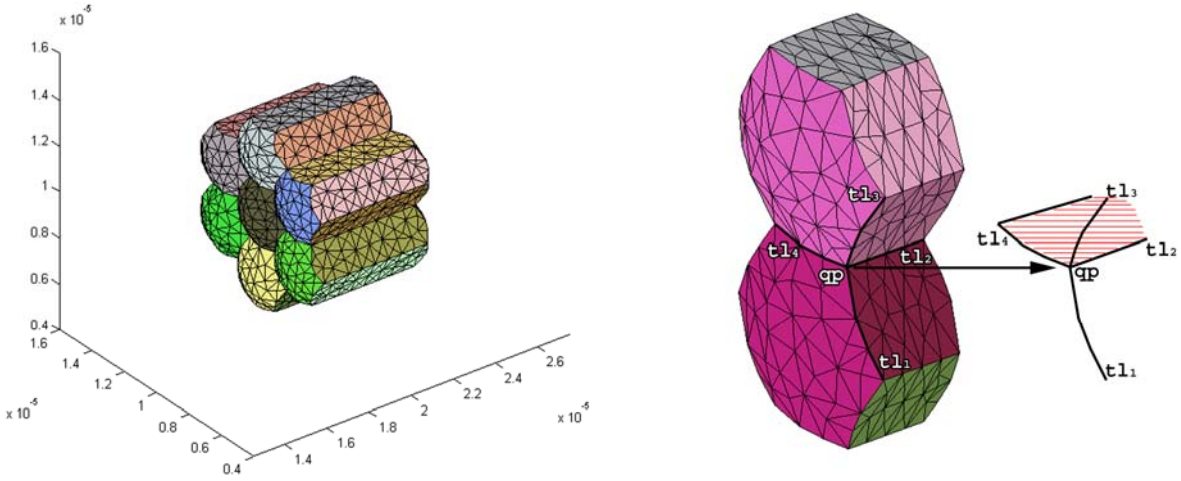
where m_b, m_{tl}, and m_{qp} are the mobilities of the grain boundary (GB), the triple line (TL), and the quadruple point (QP), respectively.

A special grain boundary arrangement is necessary to warrant a stationary motion of the junctions which is a prerequisite for the determination of Λ or the junction mobilities. Indeed there are specific configurations where a connected grain boundary system undergoes a change with constant junction velocity (stationary motion). In 2D systems there are two basic configurations which reflect the stationary growth or shrinkage of a grain [29]. In 3D an arrangement of four connected grains can be found which contains four triple lines that meet in a quadruple point (Fig. 6). In case of a hexagonal cross section of the adjoining grains, the quadruple junction moves with constant velocity, the corresponding parameter Λ can be determined, and the effect of Λ on grain microstructure evolution can be studied.

The temporal change of the volume of the central grain of the assembly in Fig. 6 for different Λ_{qp} is shown in Fig. 7a. A small but distinct retardation of the kinetics can be observed with a decrease of Λ_{qp}. For the simulations, m_{qp} was varied, whereas m_b and the grain boundary energy γ were held constant, and m_{tl} was considered infinite. From these simulations it is evident that QPs can drag grain boundary motion and thus, slow down grain growth.

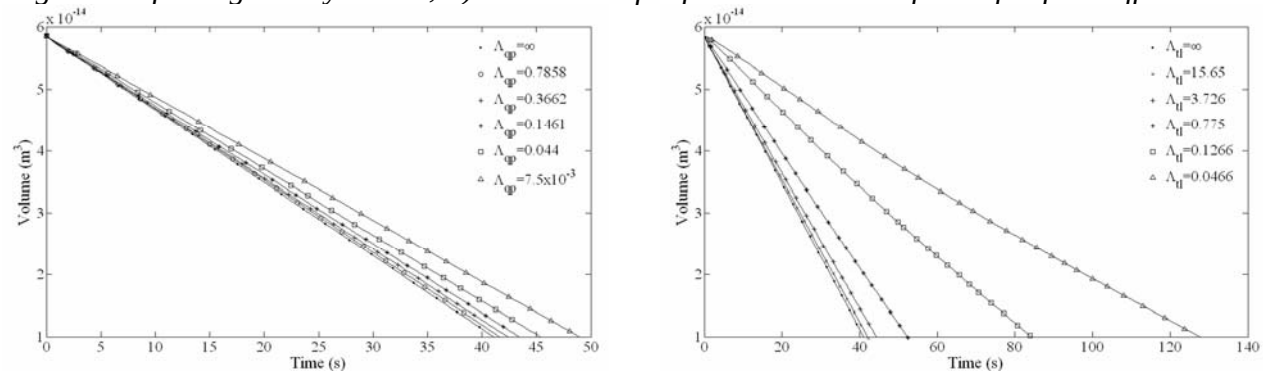
It has been demonstrated previously that TL drag can affect the kinetics of grain growth [28-30]. However, the influence of such junctions on the evolution of a 3D configuration has been studied here for the first time. In Fig. 7b, the volume change for different m_{tl} is represented. For this case m_{qp} was taken as infinite while other parameters had the same values as in the previous simulations. As in the case for a finite quadruple point mobility, the volume change is delayed with the decrease of Λ_{tl}. Note that for very low Λ_{tl} the volume change deviates from linearity, which means also that the system did not behave in a steady-state any more. This occurs because the grain boundaries become flat for small values of Λ_{tl}, i.e. the driving force due to the curvature of the boundary tends to

zero, and the major source for the driving force becomes the deviation of the dihedral angles from equilibrium at the triple lines. From Figs. 7a,b we can conclude that TLs influence the kinetics during grain growth more effectively than quadruple points. This comparison is possible because the simulation parameters for both simulation cases were the same, the only independent variables were m_{qp} and m_{tl}, respectively.



a) b)

Fig. 6. Special 3D grain assembly that allows a steady state motion of the quadruple point. a) Arrangement of hexagonal cylinders; b) indication of triple lines tl's and quadruple point qp.



(a) (b)

Fig. 7. Volume change with time (a) for different m_{qp} and (b) for different m_{tl}.

Future Needs and Developments

Despite the obvious progress in modeling approaches of recrystallization and grain growth there are still major needs and deficiencies left which must be rectified for a more comprehensive and a more reliable simulation of these softening phenomena, like the evolution and structure of deformation inhomogeneities to more accurately account for nucleation of recrystallization. On the other hand there is a substantial lack of data on grain boundary thermodynamics and kinetics, like grain boundary and junction energies and mobilities.

The rapid development of high performance computers will not only allow us to address larger systems in a reasonable computational time frame but it will also make models accessible for materials physics issues that so far were only marginally considered in the context of recrystallization and grain growth. Such models are advanced molecular dynamics (MD) [31] codes to determine boundary and junction energies and mobilities and also quantum mechanical ab-initio computations via electron density functional theory (EDT) [32] for a calculation of interfacial and junction energies and for providing better interatomic potentials for MD simulations. Such computations are now

widespread in use also due to the public availability of respective codes. There is hope that this will eventually allow to conduct true multiscale simulations for a reliable prediction of engineering phenomena and properties on a macroscopic scale. It is evident that it will be impossible to validate all these simulations by experiment, in fact many material data are virtually impossible to obtain by experiment. In this respect we will increasingly rely on the computation of fundamental material constants to predict macroscopic material properties.

An example is the computation of grain boundary mobility by molecular dynamics simulations. Various approaches have been proposed in recent years to address this problem. Schönfelder et al. [33,34] proposed an artificial driving force to move flat boundaries without exposing the crystals to unnecessary constraints, which may render unstable configurations for certain types of boundaries. They were able to simulate grain boundary motion also for high Σ boundaries and to extract the thermodynamic parameters of grain boundary mobility (Fig. 8). Moreover, the simulations revealed that grain boundary motion and grain boundary diffusion are quite different atomistic processes so that boundary mobility cannot be associated with grain boundary diffusivity as frequently assumed in analytical approaches of grain boundary motion.

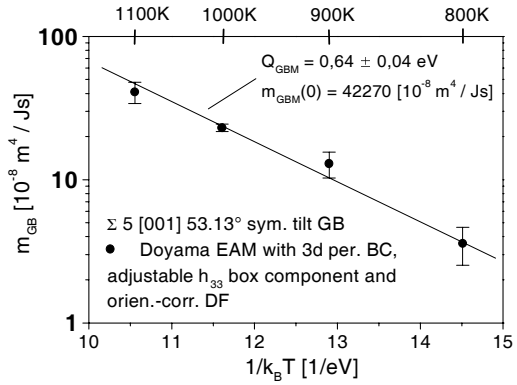


Fig. 8. Arrhenius plot of GB mobility of the Σ5 (210) symmetrical tilt GB with adjustable h_{33} variable and OCDF.

Conclusions

We have shown that advanced modeling tools are now at hand to address more complex issues of recrystallization (e.g. nucleation) and grain growth (e.g. junction drag). This allows a more comprehensive simulation of these softening mechanisms which become particularly important for ultrafine grained and nanocrystalline materials, but are also decisive for industrial product- and process optimization in e.g. aluminum and steel sheet fabrication. Major issues are still unsolved and need further attention like the evolution of deformation inhomogeneities and the availability of experimental data on boundary and particularly junction energies and mobilities which are difficult to determine experimentally but which can now be obtained from advanced atomistic models.

Acknowledgement

Financial assistance from the Deutsche Forschungsgemeinschaft (Grant Go/335/10) is gratefully acknowledged. The cooperation was supported by the Deutsche Forschungsgemeinschaft (DFG Grant 436 RUS 113/714/0-1(R)) and the Russian Foundation of Fundamental Research (Grant DFG-RRFI-05-02-04017)

References

[1]H.F Humphreys, M. Hatherly: *Recrystallisation and related annealing phenomena* (Elsevier, Oxford 1995).

[2]G. Gottstein: *Physical Foundations of Materials Science* (Springer Verlag, Berlin 2004).

[3]P.B. Pragnell, J.R. Bowen, M. Berta, P.J. Apos, P.S. Bate: Mater. Sci. Forum Vol. 467-470 (2004) 1261.

[4]X. Molodova, A. Khorashadizadeh, G. Gottstein, M. Winning, R. Hellmig: submitted to International Journal of Materials Research (2006)
[5]P.J. Hurley, F.J. Humphreys: Acta Mater. Vol. 51 (2003), p. 3779.
[6]G. Gottstein, in: *Virtual Fabrication of Aluminium Products*, edited by J. Hirsch, Wiley-VCH (2006) p. 157.
[7]P. Mukhopadhyay, M. Loeck, G. Gottstein: Acta Mater. (2006, in press)
[8]D. Raabe, M. Sachtleber, Z. Zhao, F. Roters, S. Zaefferer: Acta Mater. Vol. 49 (2001) p. 3433.
[9]M. Crumbach, G. Pomana, P. Wagner, G. Gottstein, in *Recrystallization and Grain Growth*, edited by G. Gottstein and D.A. Molodov, Springer-Verlag Berlin, (2001), p. 1053.
[10] M. Crumbach: Doctoral Thesis, RWTH Aachen, Der-Andere-Verlag Tönning, Germany (2005).
[11] P. Van Houtte, S. Li, O. Engler, in: *Continuum scale simulation of engineering materials*, edited by D. Raabe, F. Roters, F. Barlat, L.Q. Chen, Wiley-VCH (2004), p. 448.
[12] F. Roters, D. Raabe, G. Gottstein: Acta Mater. Vol. 48 (2000), p. 4181.
[13] M. Crumbach, M. Goerdeler, G. Gottstein: Acta Mater. Vol. 54 (2006), p. 3275.
[14] M. Crumbach, M. Goerdeler, G. Gottstein: Acta Mater. Vol. 54 (2006), p. 3291.
[15] L. Delannay: Ph. D. Thesis, KU Leuven, Belgium (2001).
[16] S. Zaefferer, T. Baudin, R. Penelle: Acta Mater. Vol. 49 (2001), p. 1105.
[17] M. Seefeldt, L. Delannay, B. Peeters, E. Aernoudt, P. Van Houtte: Acta Mater. Vol. 49 (2001), p. 2129.
[18] D. Raabe, Z. Zhao, W. Mao: Acta Mater. Vol. 50 (2002), p. 4379.
[19] A. Duckham, O. Engler, R.D. Knutsen: Acta Mater. Vol. 50 (2002), p. 2881.
[20] I.L. Dillamore, H. Katoh: Metal Sci. Vol. 8 (1974), p. 73.
[21] G. Gottstein, L.S. Shvindlerman: *Grain boundary migration in metals.* (CRC Press, *Boca Raton*, USA) 1999.
[22] W.W. Mullins: J. Appl. Phys. Vol. 27 (1956), p. 900.
[23] E.A. Holm, M.A. Miodownik, K.J. Healey, in: *Recrystallization and Grain Growth*, edited by B. Bacroix et al., Trans Techn. Publ.Zürich-Uetikon, Switzerland, (2004), p. 611.
[24] C.E. Krill III, L.-Q. Chen: Acta Mater. Vol. 50 (2002), p. 3059.
[25] C. Maurice, in: *Recrystallization and Grain Growth*, edited by G. Gottstein and D.A. Molodov, Springer-Verlag Berlin, (2001) p. 123.
[26] D. Weygand, Y. Bréchet, J. Lépinoux, W. Gust: Phil. Mag. B Vol. 79 (1999), p, 703.
[27] L.A. Barrales, L.S. Shvindlerman, V. Mohles, G. Gottstein: these proceedings (2007).
[28] G. Gottstein and L.S. Shvindlerman: Scripta Mat., Vol. 54 (2006), p. 1065.
[29] G. Gottstein, Y. Ma, L.S. Shvindlerman: Acta Mater., Vol. 53 (2005), p. 1535.
[30] D. Mattissen, A. Wær∅, D.A. Molodov, L.S. Shvindlerman, G. Gottstein.: Journal of Microscopy, Vol. 213 (2004), p. 257.
[31] M.P. Allen, D.J. Tildesley: *Computer simulation of liquids* (Clarendon Press, Oxford, 1990).
[32] G. Kresse, J. Hafner: J. Phys. Condensed Matter Vol. 6 (1994), p. 8245.
[33] B. Schönfelder, G. Gottstein, L.S. Shvindlerman: Acta Mater. Vol. 53 (2005), p. 1597.
[34] B. Schönfelder, G. Gottstein, L.S. Shvindlerman: Met. Trans. A Vol. 37A (2006), p. 1757.