Light Metals 2014
Edited by: John Grandfield
TMS (The Minerals, Metals & Materials Society), 2014

MODELING TEXTURE EVOLUTION OF PURE FCC ALLOY DURING ANNEALING

Shiyao Huang[1], Ruijie Zhang[2], Mei Li[1]
[1]Research and Advanced Engineering Laboratory, Ford Motor Company, Dearborn, MI 48121, USA
[2] School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, PR China

Keywords: Static recrystallization, Annealing, Texture, Phase field model, Crystal plasticity model

Abstract

During the annealing process of deformed materials, static recrystallization is an important phenomenon which can lead to significant texture changes in pure FCC alloy. In this paper, an integrated model was developed to describe the deformation and annealing process. The deformation process was firstly simulated in ABAQUS/Explicit, where crystal plasticity model was implemented into the FE package by developing the user subroutine. Then, a phase field model was proposed to simulate grain growth and texture evolution during annealing process. The outputs parameters of the deformation simulation, such as the orientation and deformation energy of each individual grain, were used as the inputs for phase field models. The nucleation of new grains was assumed to take place at grains which have the lowest deformation energy. This integrated model was applied to calculate the texture distribution of pure FCC sheet after annealing. The predicted texture distribution qualitatively matches the experimental results.

Introduction

Material anisotropy has significant influence on the mechanical properties, which can be attributed principally to the presence of texture. As a result, simulation of texture evolution during deformation and subsequent annealing process is crucial for predicting mechanical property of end products.

Crystal plasticity has been widely applied to predict deformation texture because of its ability to relate the plastic behavior of material to the microstructure. One of the difficulties in the crystal plasticity simulation is that the boundary condition during deformation is unknown. This problem could be solved by coupling the crystal plasticity model with finite element method (FEM) analysis. Since crystal plasticity constitutive theory is not available as standard in the commercially FE software, it's necessary to implement crystal plasticity model into FE software by writing the user-defined material module. The deformation texture distribution predicted by crystal plasticity based finite element method (CPFEM) was in correlation with experimental results [1].

But, in contrast, modeling texture evolution during annealing process is still rare. Static recrystallization occurs during annealing of the deformed material. It was Cyrell Smith who first recognized that the phenomenon of recrystallization during annealing must be subdivided into two consecutive processes, namely nucleation and grain growth [2]. To explain microstructure evolution during static recrystallization, the theories of oriented nucleation [3] and oriented growth [4] have been proposed. Recently, several other theories [5] [6] have been proposed. But there is still much debate about these theories up to now. On the other hand, with increasing capability of high power computers, various modeling methods have been employed to simulate microstructure development during static recrystallization, including Monte Carlo Potts model, vertex model, front tracking, Voronoi tessellation, surface evolver, cellular automata, level set, finite element method and phase field approach. Among these methods, phase field approach has a major advantage that it does not explicitly need to track the moving grain boundary or interface [8]. Although modeling static recrystallization has attracted a lot of interests, we should note that the aforementioned models were mainly employed to simulate grain growth rather than texture evolution.

In this paper, an integrated model was developed, where texture evolution during deformation process and annealing process were simulated by CPFEM and phase field model respectively. The outputs parameters of CPFEM, such as the orientation and deformation energy of each individual grain, were used as the inputs for phase field models. This integrated model was applied to calculate the texture distribution of pure FCC sheet after annealing. The influence of nucleation on texture distribution was also studied.

Model description

The integrated model

In 1974, Dillamore and Kato [7] became the first to realize that modeling of recrystallization has to commence with the modeling of the prior deformation. However, it is almost impossible to capture every feature of deformation microstructure, and passed them to the simulation of annealing process. It would be more realistic to select one or several parameters from deformation simulation results, which have predominant effects on nucleation and grain growth. A vast body of experimental work have showed that static recrystallization was influenced by low stored energy nucleation [9][10][11]. It is also well recognized that grain growth is driven by grain boundary curvature and the stored energy. Hence, the stored energy and orientation of each individual grain is selected to represent the deformation microstructure in this integrated model.

Figure 1 presents the diagram of the integrated model. In this model, the deformation process was simulated in the commercially FE software ABAQUS. ABAQUS provides an interface, where ABAQUS/Explicit users can define the constitutive behavior of a material with the user subroutine VUMAT. In CPFEM, each element in the FEM model can represent a set of grains (100 grains in the current study). ABAQUS/Explicit solution process involves large numbers of increments. The stress, grain orientation, hardening parameters, and the stored energy of each grain are passed in at the beginning of each increment, and then updated at the end of increment. At the end of FEM simulation, grain orientation and the stored energy of each individual grain were passed to the annealing simulation.

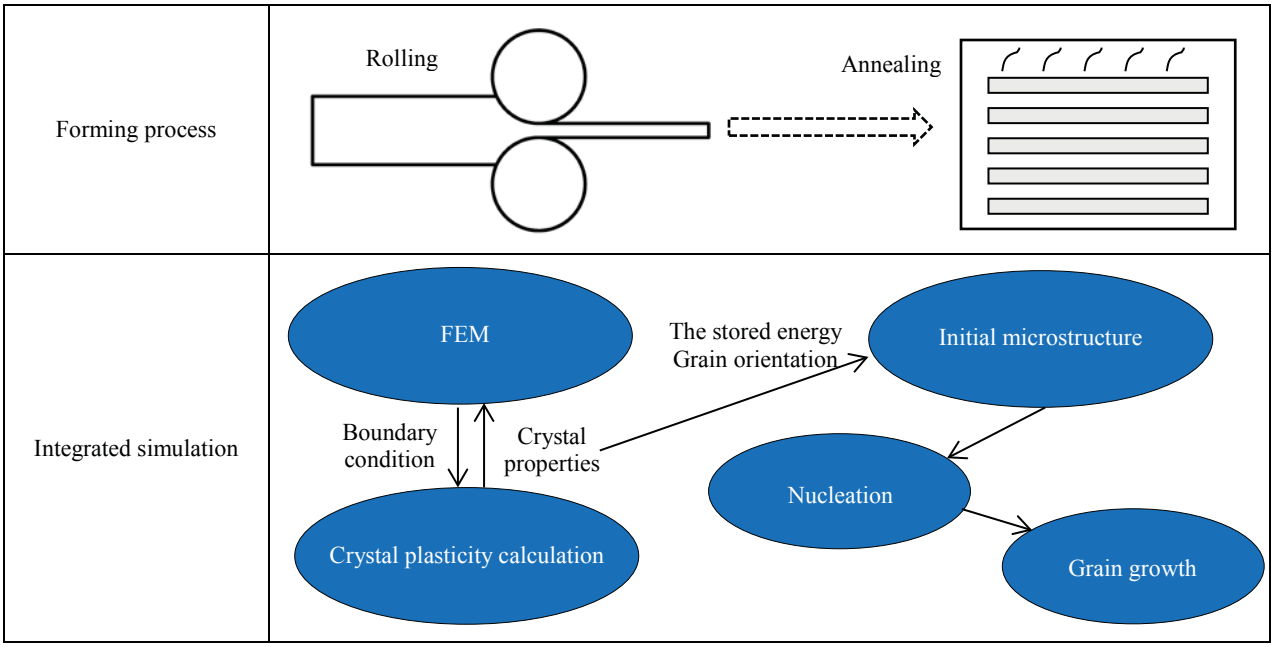


Figure 1. The diagram of integrated model

As shown in Figure 1, the annealing simulation was categorized as two steps: generating strain-free nuclei and its growth at the expense of the deformed matrix. Grain growth is modeled with a developed phase field model, which will be introduced later. As a result, the completion of integrated simulation relies on the nucleation modeling.

The main problems in nucleation simulation include nucleation timing, location and nucleus orientation. It is generally accepted that there are three different nucleation mechanisms [13]: random nucleation, nucleation at shear bands and nucleation at grain boundaries. The prominent and often observed nucleation mechanism in FCC alloy is the formation of nuclei at pre-existing grain boundaries [2]. The orientations of such nuclei have an orientation close to the parent grain.

Li et al. [12] found that most nuclei were formed in the early stage of recrystallization. To simplify the modeling procedure, current study assumes nucleation to be site saturated, which means all nuclei are created at the beginning of annealing simulation. The nucleus is assumed to be strain free, suggesting that the stored energy is zero.

However, not every grain but only a portion of grains with low stored energy are capable of generating the nuclei [14]. In this study, only 5 grains have lowest stored energy are allowed to generate nuclei. The number of nucleus of each parent grain is assumed to be around 5.

Crystal plasticity model

Crystal plasticity model not only established the quantitative description of plastic deformation in single crystal, but also provided the ability to relate the response of individual grain to macro-response of the polycrystalline aggregate. In the single crystal plasticity, the velocity gradient L is expressed as

$$L = D + W \tag{1}$$

where D is the symmetric part of the rate of deformation and W is the skew symmetric spin tensor. The plastic parts D^P and W^P are related to the plastic shear strain rate as

$$D^P = \sum_{\alpha=1}^{n} P^\alpha \dot{\gamma}^\alpha$$
$$W^P = \sum_{\alpha=1}^{n} R^\alpha \dot{\gamma}^\alpha \tag{2}$$

P^α and R^α can be defined as

$$P^\alpha = \frac{1}{2}(n^\alpha \otimes m^\alpha + m^\alpha \otimes n^\alpha)$$
$$R^\alpha = \frac{1}{2}(n^\alpha \otimes m^\alpha - m^\alpha \otimes n^\alpha) \tag{3}$$

where the slip direction is designated by the unit vector m and the slip plane normal by the unit vector m, the superscript α is the number of deformation systems. A single crystal constitutive rule [15] which relates the grain level plastic strain rate $\dot{\gamma}^\alpha$ and shear stress τ^α is employed,

$$\dot{\gamma}^\alpha = \dot{a}^\alpha \left[\frac{\tau^\alpha}{g^\alpha}\right]\left[\left|\frac{\tau^\alpha}{g^\alpha}\right|\right]^{1/m-1} \tag{4}$$

where g^α denotes the critical resolved shear stress, which describes the current strain hardening state of the crystal, $\dot{a}^\alpha$ is the reference shear rate and m is the material rate sensitivity. The evolution of critical resolved shear stress g^α can be defined as:

$$g^\alpha = \sum_{\beta} h^{\alpha\beta}\left|\Delta\gamma^\beta\right| \tag{5}$$

with

$$h^{\alpha\beta} = h^\alpha q^{\alpha\beta} \tag{6}$$

where $h^{\alpha\beta}$ is hardening modulus, $q^{\alpha\beta}$ is introduced to describe the self and latent hardening, $q^{\alpha\beta}$ can be expressed as:

$$q^{\alpha\beta} = q + (1-q)\delta^{st} \tag{7}$$

where q is called latent-hardening ratio. For h^α, a power hardening law [16] is employed here

$$h^\alpha = h_0^\alpha \left(\frac{h_0^\alpha \gamma}{g_0^\alpha n^\alpha} + 1\right)^{n^\alpha - 1} \tag{8}$$

where h_0^α is the initial hardening rate, g_0^α is the initial CRSS, n^α is the hardening exponent and γ is sum of the slips on all slip systems at the current instant.

In ABAQUS/VUMAT, a co-rotational coordinate system in which the basis system rotates with material is considered. All stress and strain tensor quantities are defined with respect to the co-rotational basis system. In this formulation, a crystal orientation tensor, Q, is used to define the orientation of the crystal coordinate system with respect to the material co-rotational coordinate system. During deformation, the rigid body rotation matrix in an incremental form can be expressed as [17]

$$Q_n = Exp\left[\left(W - \sum_{\alpha=1}^{n} R^{\alpha}\dot{\gamma}^{\alpha}\right)\Delta t\right]Q_{n-1} \quad (9)$$

The stored energy in the individual grain is calculated as

$$E_n = E_{n-1} + \int d\sigma^E \cdot d\varepsilon^E \quad (10)$$

The single crystal quantities (D_c , W_c , $\dot{\sigma}_c$) are linked with polycrystalline quantities ($D_M, W_M, \dot{\sigma}_M$)as

$$D_c = D_M \quad W_c = W_M \quad \dot{\sigma}_M = \langle\dot{\sigma}_c\rangle \quad (11)$$

Phase field model

There are two main types of phase field models: one uses two order parameters to describe the degree of crystallinity and the crystallographic orientation [18][19], the other one uses a set of non-conserved order parameter fields with each of them representing a specific grain [20]. In this paper, the second one is adopted to simulate texture evolution by taking into account of the stored energy. The spatial and temporal evolutions of the order parameters are described by Ginzburg-Landau equations (also called the Cahn-Allen equations) [21]:

$$\frac{\partial\eta_i}{\partial t} = -L\frac{\delta F}{\delta\eta_i} \quad (12)$$

Here, η is order parameter, t is time, L is the kinetic coefficient that characterizes the grain boundary mobility, and F is the total free energy that can be written in the following form:

$$F = \int [f_0(\eta_i) + k(\nabla\eta_i)^2]dv \quad (13)$$

where f_0 is the free energy density and k the gradient energy coefficient. The free energy density is generally written in the form [20]:

$$f_0 = \sum_{i=1}^{p}(-\frac{a}{2}{\eta_i}^2 + \frac{b}{4}{\eta_i}^4) + c\sum_{i=1}^{p}\sum_{j>i}^{p}{\eta_i}^2{\eta_j}^2 \quad (14)$$

where a, b and c are positive constants. However, the above equations can only describe isotopic grain growth. According to previous research [22], grains with lower stored energy have higher ability to grow. Hence, the stored energy is introduced into the kinetic coefficient L to describe its influence

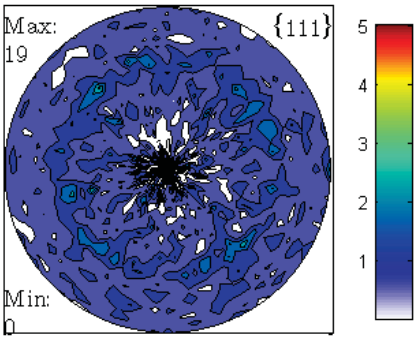
$$L = L_0(1-\bar{E}_i)^5 sign\left(\sum_{j\neq i}^{p}[(\bar{E}_j - \bar{E}_i)\eta_j]\right) \quad (15)$$

Here, E is the stored energy calculated by crystal plasticity model. $\bar{E}$ represents E is normalized by the maximum stored energy in the polycrystalline. This equation ensures that grains with lower stored energy can grow at the expense of grains with larger stored energy. The set of kinetic equations is solved using the simple Euler technique,

$$\eta_i(t+\Delta t) = \eta_i(t) + \frac{\partial\eta_i}{\partial t}\times\Delta t \quad (16)$$

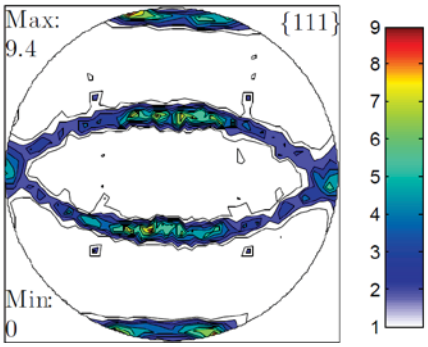
Results and discussion

A rectangular model is built to simulate the rolling process. The dimensions of the initial specimen were 6.35 mm in the compression direction, 9.53 mm in the free direction and 14.73 mm in the constraint direction. The geometry is meshed with 20 elements, type C3D8R. Each element in the FE model is initialized with 100 random grain orientations. The initial random texture distribution is plotted by MTEX [23], as shown in Figure 2. The predicted deformation texture is illustrated in Figure 3. The predicted texture is in qualitative agreement with typical experimental result (Figure 4) of rolled FCC alloy [1].



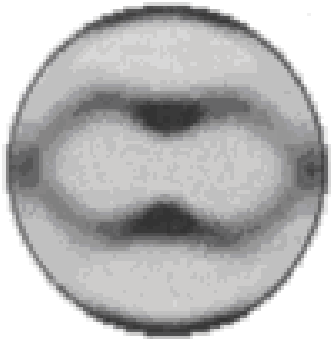
(111)

Figure 2. The initial random texture distribution



(111)

Figure 3. The predicted rolled texture



(111)

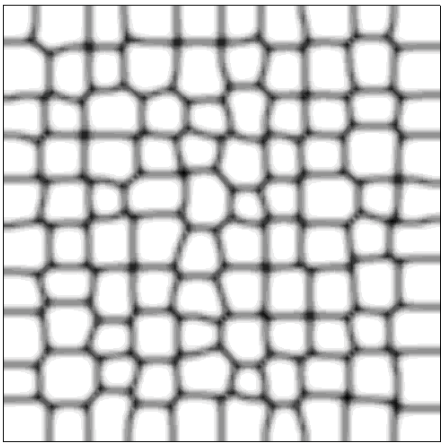
Figure 4. The typical texture distribution of rolled FCC alloy [1]

It is necessary to rebuild the deformation microstructure in order to perform phase field simulation for the annealing process. As discussed earlier, the stored energy is recognized as the most important parameter, and other features of the deformation microstructure are not considered in the integrated model. As a result, a homogeneous microstructure is produced as the initial microstructure.

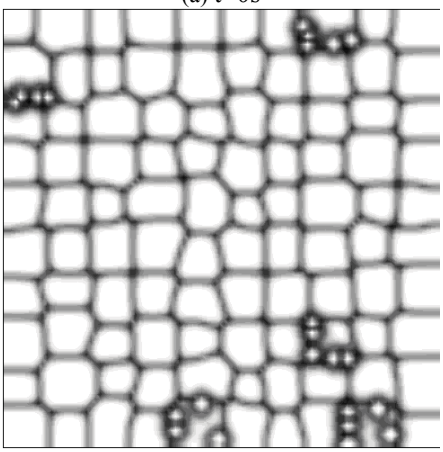
To increase the modeling efficiency, the phase field simulation is running with 100 grains each time. The grain orientation and

stored energy are retrieved from each element in the FEM model, and assign to grains in the initial microstructure randomly. As shown in Figure 1, the recrystallization simulation is divided as nucleation and grain growth. It is difficult to define a clear boundary between two steps. In the integrated model, nucleation takes place at the beginning of recrystallization simulation. Among the 100 grains, only 5 grains have lowest stored energy are allowed to generate nuclei. The number of nucleus of each parent grain is assumed to be around 5.

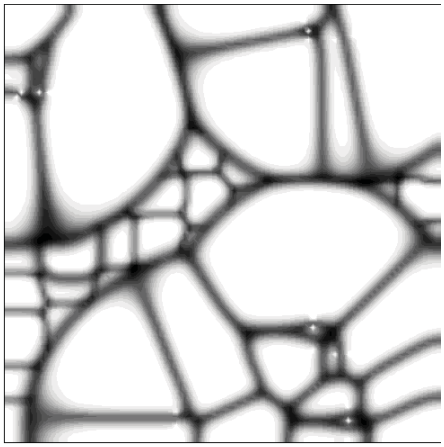
Grain growth is simulated by phase field model calculation. The values of input parameters are: L_0=0.1, k=0.1, a=0.2, b=0.2, and c=0.01. The simulation is increased in increments of Δt =0.05s. The total increment number is 24000. Figure 5 presents the evolution of microstructure during annealing process. It shows that the strain-free nuclei grow at the expense of deformed grains, and the initial microstructure is replaced by the annealed microstructure.



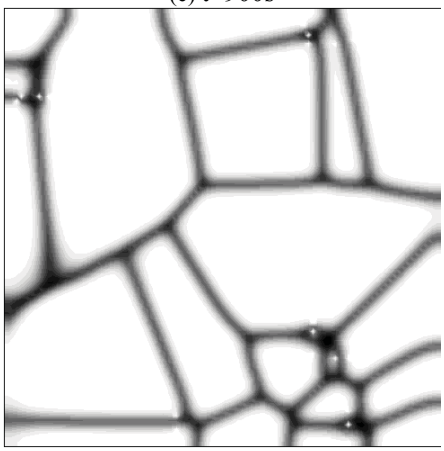
(a) t=0s



(b) t=100s



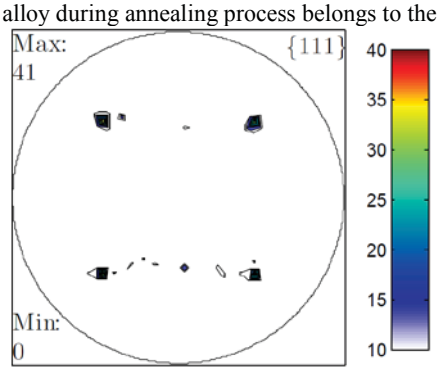
(c) t=900s



(d) t=1200s

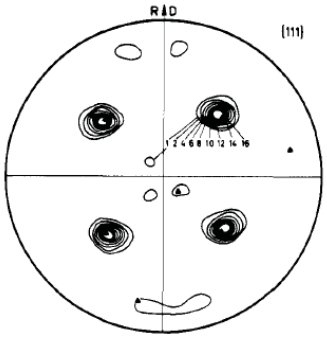
Figure 5. The evolution of microstructure during annealing

This simulation procedure is repeated 20 times until all deformed grains in the FEM model are examined. The grain orientations are retrieved from 20 pieces of annealed microstructures. Figure 6 plots the predicted texture, which is cube texture. Figure 7 shows the experimental annealed texture [24]. Cube texture component is insignificant in the rolled texture (Figure 4), but becomes predominant in the annealed texture. Literature [5] shows that static recrystallization can lead to three possible textural changes, namely, no significant changes, relative randomization of the deformation texture, and relatively insignificant components of the deformation texture become significant. Texture evolution in pure FCC alloy during annealing process belongs to the last type.



(111)

Figure 6. The annealed texture distribution



(111)
Figure 7. The annealed texture distribution [24]

The initial microstructure shown in Figure 5(a) is homogeneous. It does not contain shear bands, elongated grains and other frequently observed deformation features. This does not hold true in reality, but the predicted texture verifies the assumption that the stored energy has predominant influence on the texture evolution.
The simulation result suggests that nucleation is easier to take place at the cube component than the non-cube component because of the lower stored energy in the cube component. This is in consistent with earlier study that cube component stores less energy than the other orientation component [25][26], and cube nuclei formation is easier[27].
On the other hand, nucleation parameters have great influences on texture evolution during annealing. In the current study, a simple assumption is made, where nucleation parameters were assumed to some particular values. Further study should be conducted to quantify the relationship between the stored energy, microstructure features and nucleation model.

Conclusion

In this paper, an integrated model was proposed to calculate the texture distribution of pure FCC sheet after annealing. The developed model predicted the formation of cube texture during annealing, which qualitatively matched the experimental results. The results verified that accounting for the stored energy was crucial for annealed texture prediction. The nucleation parameters were assumed to some particular values in the current study. An advanced nucleation model has to be developed to build the relationship between the stored energy, microstructure features and nucleation parameters.

Acknowledgement

The second author acknowledges the financial support from National Natural Science Foundation of China (No.51101014).

References

[1] C. A. Bronkhorst, S. R. Kalidindi, and L. Anand, *Phil. Trans. R Soc. Lond. A.*, 341 (1992), 443-477.
[2] C. Schäfer, M. Crumbach, and G. Gottstein, *Mater. Sci. Forum*, 550 (2007), 85-94.
[3] W. G. Burgers and P. C. Louwense, *Z. Phys.*, 61 (1931), 605-678.
[4] P. A. Beck, *Adv. Phys.*, 3 (1954), 245-324.
[5] I. Samajdar et al., *Mater. Sci. Eng. A*, 266 (1999) 146-154.
[6] Y. B. Park, D. N. Lee, and G. Gottstein, *Acta Mater.*, 46 (1998) 3371-3379.
[7] I. L. Dillamore and H. Katoh, *Metal Sci.*, 8 (1974), 73-83.
[8] G. Abrivard et al., *Philos. Mag.*, 92 (2012), 3618-3642.
[9] A. L. Etter et al., *Scripta Mater.*, 46 (2002), 311-317.
[10] T. Baudin et al., *Scripta Mater.*, 51 (2004), 427-430.
[11] J. Sidor et al., *Philos. Mag.*, 88 (2008), 3779-3792.
[12] X. L. Li et al., *Acta Mater.*, 55 (2007), 3531-3540.
[13] G. Gottstein, *Mater. Sci. Forum*, 408-412 (2002), 1-24.
[14] J. J. Sidor, R. H. Petrov, and L. A. I. Kestens, *Acta Mater.*, 59 (2011), 5735-5748.
[15] J. W. Hutchinson, *Proc. R. Soc. London*, Ser. A 348 (1976), 101-127.
[16] D. Peirce, R. J. Asaro, and A. Needleman, *Acta Mater.*, 30 (1982), 1087-1119.
[17] J. C. Simo and L. Vu-Quoc, *Comput. Methods Appl. Mech. Engrg.*, 58 (1986), 79-116.
[18] R. Kobayashi, J. Warren, and W. Carter, *Physica D*, 140 (2000), 141-150.
[19] M. Lusk, *Proc. R. Soc. London*, Ser. A 455 (1999), 677-700.
[20] L. Chen and W. Yang, *Phys. Rev. B*, 50 (1994), 15752-15757.
[21] S. M. Allen and J. W. Cahn, *Acta Metall.*, 27 (1979), 1085-1095.
[22] Y. Lü, D. A. Molodov, and G. Gottstein, *Acta Mater.*, 59 (2011) 3229-3243.
[23] R. Hielscher and H. Schaeben, *J. Appl. Cryst.*, 41 (2008), 1024-1037.
[24] U. Schmidt and K. Lücke, *Texture of Cryst. Solids*, 3 (1979) 85-112.
[25] M. C. Theyssier and J. H. Driver, *Mater. Sci. Eng. A*, 272 (1999) 73-82.
[26] M. Koyobayashi, Y. Takayama, H. Kato, *Mater. Trans.*, 45 (2004) 3247-3255.
[27] B. Radhakrishnan and G. B. Sarma, *Mater. Sci. Eng. A*, 494 (2008) 73-79.