AFRL-RX-WP-TP-2010-4140

MONTE-CARLO MODELING OF RECRYSTALLIZATION KINETICS OF COLD-ROLLED TITANIUM (PREPRINT)

Y.B. Chun

Monash University

S.L. Semiatin

Metals Branch
Metals, Ceramics & NDE Division

S.K. Hwang

Inha University

APRIL 2010

AIR FORCE RESEARCH LABORATORY
MATERIALS AND MANUFACTURING DIRECTORATE
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7750
AIR FORCE MATERIEL COMMAND
UNITED STATES AIR FORCE

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
April 2010	Conference Paper Preprint	01 April 2010 – 01 April 2010

4. TITLE AND SUBTITLE

MONTE-CARLO MODELING OF RECRYSTALLIZATION KINETICS OF COLD-ROLLED TITANIUM (PREPRINT)

5a. CONTRACT NUMBER
In-house

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
62102F

6. AUTHOR(S)

Y.B. Chun (ARC Centre of Excellence for Design in Light Metals)
S.L. Semiatin (AFRL/RXLMP)
S.K. Hwang (Inha University)

5d. PROJECT NUMBER
4347

5e. TASK NUMBER
RG

5f. WORK UNIT NUMBER
M02R2000

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Monash University
ARC Centre of Excellence for Design in Light Metals
Department of Materials Engineering
Clayton, Victoria 3800, Australia

Metals Branch (AFRL/RXLM)
Metals, Ceramics & NDE Division
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, OH 45433-7750
Air Force Materiel Command, United States Air Force

Inha University
School of Materials Science and Engineering
253 Yonghyun-dong
Nam-gu, 402-751
Incheon, South Korea

8. PERFORMING ORGANIZATION REPORT NUMBER
AFRL-RX-WP-TP-2010-4140

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, OH 45433-7750
Air Force Materiel Command
United States Air Force

10. SPONSORING/MONITORING AGENCY ACRONYM(S)
AFRL/RXLMP

11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S)
AFRL-RX-WP-TP-2010-4140

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES
Conference paper submitted for publication in the Proceedings of the 7th Pacific Rim International Conference on Advanced Materials & Processing; conference to be held 1 - 5 August 2010 in Cairns, Australia. PAO Case Number: 88ABW-2010-0923; Clearance Date: 02 Mar 2010. The U.S. Government is joint author of this work and has the right to use, modify, reproduce, release, perform, display, or disclose the work. Paper contains color.

14. ABSTRACT

The recrystallization behavior of cold-rolled, commercial-purity titanium was studied experimentally and with Monte-Carlo (MC) modeling. Utilization of EBSD-OIM as input for MC modeling resulted in realistic predictions of recrystallization kinetics, microstructure and texture, which were in good agreement with experimental results. MC modeling of recrystallization kinetics predicted that non-uniform stored energy distribution, heterogeneous nucleation of recrystallization and recovery in combination leads to a negative deviation from linear JMAK kinetics. It was found that concurrent recovery that takes place during recrystallization is an important process that controls both the overall recrystallization kinetics and the deviation of linear JMAK kinetics. On the other hand, non-uniformly distributed stored energy itself has little effect on the negative deviation from JMAK kinetics but intensifies the deviation when heterogeneous nucleation is combined. Modeling results also revealed that heterogeneous nucleation of recrystallized grains and their early impingement in local areas of high deformation are essential for producing a log- normal distribution of grain size and a typical recrystallization texture in rolled titanium.

15. SUBJECT TERMS

Monte-Carlo modeling, electron backscatter diffraction, titanium, recrystallization, Johnson-Mehl-Avrami-Kolmogorov model

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT:	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON (Monitor)
a. REPORT	b. ABSTRACT	c. THIS PAGE			Sheldon L. Semiatin
Unclassified	Unclassified	Unclassified	SAR	12	19b. TELEPHONE NUMBER *(Include Area Code)* N/A

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39-18

Monte-Carlo Modeling of Recrystallization Kinetics of Cold-Rolled Titanium

Y. B. Chun[1,a], S. L. Semiatin[2,b] and S. K. Hwang[3,c]

[1]ARC Centre of Excellence for Design in Light Metals, Department of Materials Engineering, Monash University, Clayton, Victoria 3800, Australia

[2]Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/RXLM, Wright-Patterson Air Force Base, OH 45433, USA

[3]School of Materials Science and Engineering, Inha University, 253 Yonghyun-dong, Nam-gu, 402-751, Incheon, South Korea

[a]borobang@gmail.com, [b]Lee.Semiatin@wpafb.af.mill, [c]skhwang2@gmail.com

Keywords: Monte-Carlo modeling; electron backscatter diffraction; titanium; recrystallization; Johnson-Mehl-Avrami-Kolmogorov model

Abstract. The recrystallization behavior of cold-rolled, commercial-purity titanium was studied experimentally and with Monte-Carlo (MC) modeling. Utilization of EBSD-OIM as input for MC modeling resulted in realistic predictions of recrystallization kinetics, microstructure and texture, which were in good agreement with experimental results. MC modeling of recrystallization kinetics predicted that non-uniform stored energy distribution, heterogeneous nucleation of recrystallization and recovery in combination leads to a negative deviation from linear JMAK kinetics. It was found that concurrent recovery that takes place during recrystallization is an important process that controls both the overall recrystallization kinetics and the deviation of linear JMAK kinetics. On the other hand, non-uniformly distributed stored energy itself has little effect on the negative deviation from JMAK kinetics but intensifies the deviation when heterogeneous nucleation is combined. Modeling results also revealed that heterogeneous nucleation of recrystallized grains and their early impingement in local areas of high deformation are essential for producing a log-normal distribution of grain size and a typical recrystallization texture in rolled titanium.

Introduction

Recrystallization is of considerable theoretical interest and practical importance and thus various approaches, such as analytical, cellular-automaton, Avrami, and Monte-Carlo (MC) techniques [1-4], have been developed and utilized to describe recrystallization phenomena. Among those methods, the MC approach is very attractive because it can describe a number of different aspects of recrystallization, including the overall kinetics and the evolution of microstructure and texture. However, detailed quantitative information, including initial grain morphology, crystal orientation, and the distribution of stored energy, is needed for MC modeling. Unfortunately, unrealistic assumptions, for example, a random distribution of the nuclei, homogeneous distribution of stored energy, or random starting texture, have been employed. Therefore, predictions of recrystallization phenomena based on such unrealistic assumptions may lead to marked deviations from experimental observations.

To overcome these limitations, we have developed a methodology to treat recrystallization phenomena using electron backscatter diffraction (EBSD) measurements and two-dimensional MC simulation [5], and applied these techniques to model the recrystallization of cold-rolled commercial-purity titanium. Since the modeling of the recrystallization kinetics of work hardened materials has important industrial applications both for fabrication and for the prediction of in service performance, particular attention was focused on the effects of microstructural parameters on recrystallization kinetics.

Experimental procedures

Commercial-purity titanium (cp-Ti with chemical composition of 600 O, 200 Fe, 15 H, 50 C, 100 N, balance titanium in wppm) was chosen as the program material for this investigation. The as-received material was cold rolled at room temperature to 60% total thickness reduction and then recrystallization heat treated at 600°C for various times.

Microstructure evolution during heat treatment was established using EBSD analysis and micro-Vickers hardness measurements were conducted to determine recrystallization kinetics. For EBSD analysis, samples were mechanically polished and then electro-polished in a solution consisting of 5 ml perchloric acid and 95 ml methanol at 30V and -40°C. For EBSD measurement, a Hitachi 3400SE field-emission-gun scanning-electron microscope (FEG-SEM) and TSL-OIM^{TM} software were used.

Monte-Carlo modeling of recrystallization

The details of MC framework and recrystallization model employed in the present work were fully described in previous work [5], and thus only a brief description is provided in the following.

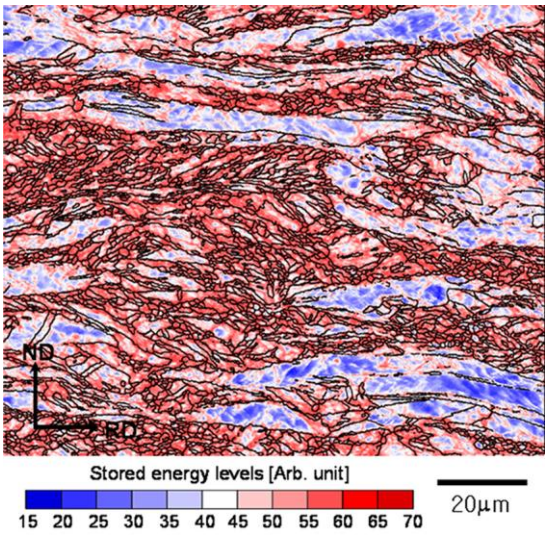

Figure 1. The stored-energy map comprising a 924×665 triangular lattice, which was used as an initial input for MC modeling of recrystallization. The microstructure was produced by mapping the EBSD microstructure of 60% cold-rolled cp-Ti onto an MC grid. The step size of the EBSD scan was 0.15 μm; black lines represent high-angle boundaries. The microstructure contains 2,167 grains with an average grain size of 30 μm. Note that the fine grains show higher stored energy, compared to the coarse grains.

Construction of input microstructure. The initial microstructure used for MC modeling was generated by mapping the EBSD microstructure of 60% cold-rolled cp-Ti onto the MC simulation grid (Fig. 1). Each lattice site in the MC grid thus generated contains information on the orientation in terms of Euler angles and image quality (IQ) value, at a measurement point specified by the coordinate pair (x, y) from an area measuring 120 μm × 100 μm. The IQ value is used as a measure of the stored energy in the present work, and the stored energy of each lattice site is calculated as follows:

$$H_i = k(1 - \frac{IQ_i}{f \cdot IQ_{max}}) \qquad (1)$$

in which H_i and IQ_i denote the relative stored energy in arbitrary units and the IQ value, respectively, of the MC lattice site i, and IQ_{max} is the maximum value of IQ. The factors k and f are constants which determine the upper and lower bounds for the stored-energy distribution and were set as 70 and 1.3, respectively, in the present modeling.

Recrystallization model. During recrystallization, the microstructure evolves through competition between recovery, nucleation of recrystallization, and grain growth: all three stages of the process were taken into account in the present modeling. For nucleation kinetics, site-saturated nucleation was assumed so that all nucleation events take place simultaneously at the beginning of recrystallization. For the spatial distribution of nuclei, two cases were considered: random nucleation

without regard to location in the microstructure and high-stored-energy nucleation (HSEN) in which nuclei form preferentially at high-stored-energy regions such as grain boundaries, triple junctions, and transition bands. The movement of the recrystallization front was treated with the strain-induced boundary migration (SIBM) model [6] and the velocity of the recrystallization front, v_{ij}, is thus expressed as follows:

$$v_{ij} = a \cdot \Delta H_{ij} \cdot M_m [1 - m \cdot exp(-\frac{\theta_{ij}}{10})^3] \quad (2)$$

where a is proportionality constant and m is a parameter which controls degree of anisotropic grain boundary mobility [7]; ΔH_{ij} and θ_{ij} are the difference in stored energy and misorientation angle, respectively, between neighboring sites i and j; M_m is the maximum mobility corresponding to a random high-angle boundary. The velocity of the recrystallization front in Eq. (2) varies from 0 to positive values less than unity, depending on the local variation of the stored energy and the grain-boundary mobility throughout the microstructure. When v_{ij} is greater than a random probability obtained from a random-number generator that produces numbers between 0 and 1, then the recrystallized grain grows at the expense of the deformed site j; as a consequence, the stored energy of site j is reset to zero, and the orientation of site j is changed to that of site i.

The recovery process during recrystallization was simulated such that when a chosen deformed site fails to undergo recrystallization, the stored energy of that lattice site was lowered by a fixed factor, b ($0<b<1$), without changing its crystal orientation. Thus, the stored energy of a given lattice site which underwent recovery, H_{new}, was calculated as follows:

$$H_{new} = (1-b)H_{old} \quad (3)$$

where H_{old} is the stored energy of a lattice site just before recovery takes place. For grain growth, curvature-driven grain growth was assumed [8] as is in a conventional MC modeling.

Results and discussion

Recrystallization kinetics of 60% cold-rolled cp-Ti at 600°C was determined by hardness measurements and EBSD analyses. The kinetic curve exhibited a sigmoidal shape (Fig. 2(a)) which is commonly found in recrystallization of deformed metals.

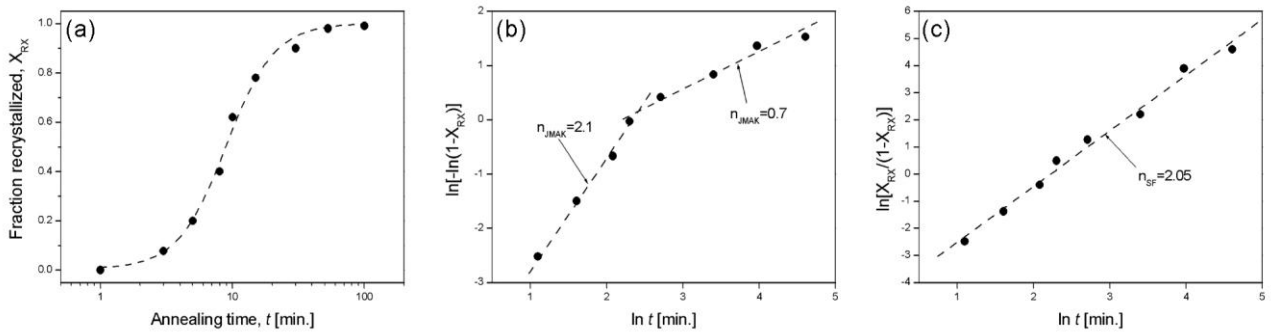

Figure 2. Recrystallization kinetics of 60% cold-rolled cp-Ti during heat treatment at 600°C: (a) plot of fraction recrystallized against logarithm of time, (b) the JMAK plot of (a), and (c) the SF plot of (a). Note that experimentally-determined RX kinetics deviates from linear JMAK kinetics while exhibiting linearity when plotted based on the SF relation.

The experimental data were re-plotted in Fig. 2(b), based on Johnson-Mehl-Avrami-Kolmogorov (JMAK) model [9] in which the fraction recrystallized, X_{RX}, depends time, t, as follows:

$$X_{RX} = 1 - exp(-Bt^{n}) \quad (4)$$

in which B is a parameter that depends on nucleation and growth characteristics and n_{JMAK} is the JMAK exponent. The JMAK kinetics (Fig. 2(b)) exhibited two different JMAK exponents, 2.1 and 0.7, at the initial and later stages of recrystallization, respectively, indicating a deviation of recrystallization behavior of the present material from the JMAK model. On the other hand, the experimental data were linear when plotted based on the empirical Speich-Fisher (SF) parabolic relation [10]:

$$X_{RX}/(1-X_{RX}) = Kt^{n_{SF}} \quad (5)$$

in which K is a constant for isothermal reaction and n_{SF} is the SF exponent. Linearity with n_{SF} of 2.05 was found in the SF kinetics (Fig. 2(c)), thus suggesting that the recrystallization kinetics of the current material can be well explained by the SF relation and that the growth rate, G, of new grain decreases with time, i.e., G is proportional to 1/t.

In order to investigate the effects of microstructural factors on recrystallization kinetics, MC modeling was conducted assuming various conditions in which distribution type and the number of nuclei, stored energy distribution, recovery rate and grain boundary characteristics were varied; the MC-predicted recrystallization kinetics are plotted based on the JMAK relation in Fig. 3..

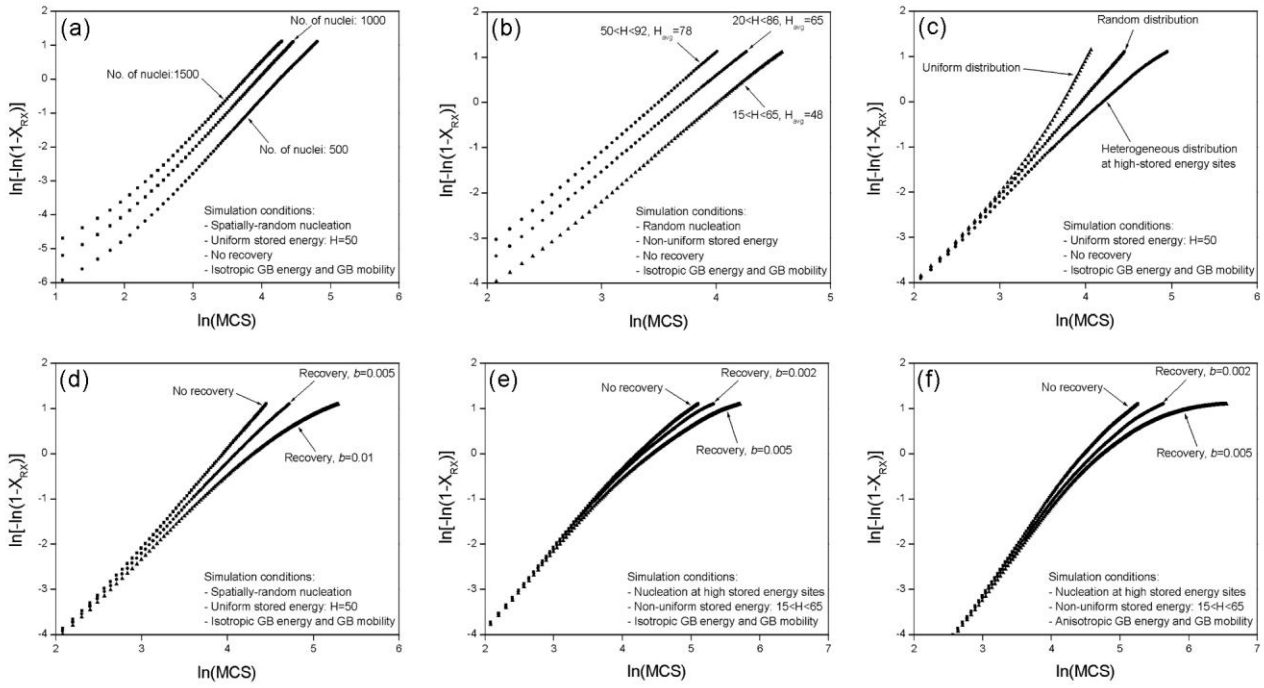

Figure 3. MC-modeling results showing the effect on recrystallization kinetics of: (a) the number of nuclei, (b) average stored energy, (c) the spatial distribution of nuclei, and concurrent recovery under (d) random nucleation and isotropic grain boundary motion, (e) HSEN and isotropic grain boundary motion and (f) HSEN and anisotropic grain boundary motion.

It was found from the modeling that increasing the number of nuclei accelerates the overall recrystallization kinetics but has little influence on the slope of the JMAK plot (Fig. 3(a)). The increase in the average stored-energy under the non-uniform-distribution of stored-energy condition also showed similar effects to the number of nuclei on recrystallization kinetics (Fig. 3(b)). A variation of the distribution pattern of nuclei, on the other hand, was found to have a considerable effect on the JMAK kinetics: random distribution of nuclei resulted in a linear JMAK kinetics while

uniform and heterogeneous distributions of nuclei led to positive and negative deviations, respectively, from the theoretical JMAK kinetics (Fig. 3(c)). Concurrent recovery with recrystallization also affected the JMAK kinetics such that an increase in recovery rate (i.e., increase in the parameter 'b') led to a more pronounced deviation from a linear JMAK kinetics (Fig. 3(d)). It was also revealed that a combination of recovery with microstructural inhomogeneities, such as heterogeneous distribution of nuclei, non-uniform distribution of stored-energy, and anisotropic grain boundary mobility, led to a significant deviation from the theoretical JMAK kinetics (Figs. 3(e) and (f)).

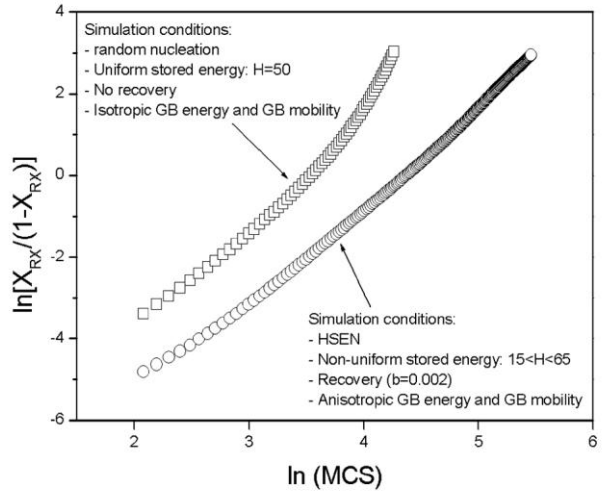

Figure 4. Recrystallization kinetics predicted by MC modeling under two extreme conditions: one satisfying assumptions in the JMAK model and the other including the effects of heterogeneous distribution of nuclei, non-uniform stored-energy, recovery and anisotropic energy and mobility of grain boundaries. The predicted recrystallization kinetics is plotted based on the SF relation (Eq. (5)).

Shown in Fig. 4 are the SF plots of recrystallization kinetics which were predicted by MC modeling under two extreme conditions: one for the assumptions in the classical JMAK model and the other including various microstructural effects of heterogeneous distribution nuclei, non-uniform stored-energy, recovery and anisotropic energy and mobility of grain boundary. Recrystallization kinetics under the former assumptions exhibited a positive deviation from linearity, reflecting a constant growth rate of new grains in the JMAK model. On the other hand, recrystallization kinetics predicted using the latter assumptions showed near-linearity, which is in good agreement with experimental observation (Fig. 2(c)).

The effect of such microstructural parameters on the grain-size distribution was also predicted by MC modeling, as shown in Fig. 5. The experimental results showed near log-normal distributions, which were unaffected by the extent of recrystallization (Fig. 5(a)). When effects from either non-uniform stored-energy, recovery or heterogeneous distribution of nuclei were included in the JMAK assumptions (Fig. 5(b)), MC modeling showed that the former two effects have little influence on the distribution of grain size, leading to a narrow distribution skewed toward smaller grain sizes. On the other hand, a broader and less skewed distribution was predicted when heterogeneous distribution of nuclei was included in the JMAK assumptions, suggesting a critical role of the distribution pattern of nuclei in developing a log-normal type distribution. When all of the aforementioned microstructural effects were included, MC modeling predicted a near log-normal distribution and an insensitivity of the distribution pattern to X_{RX} (Fig. 5(d)), both of which are in good agreement with the experimental observations.

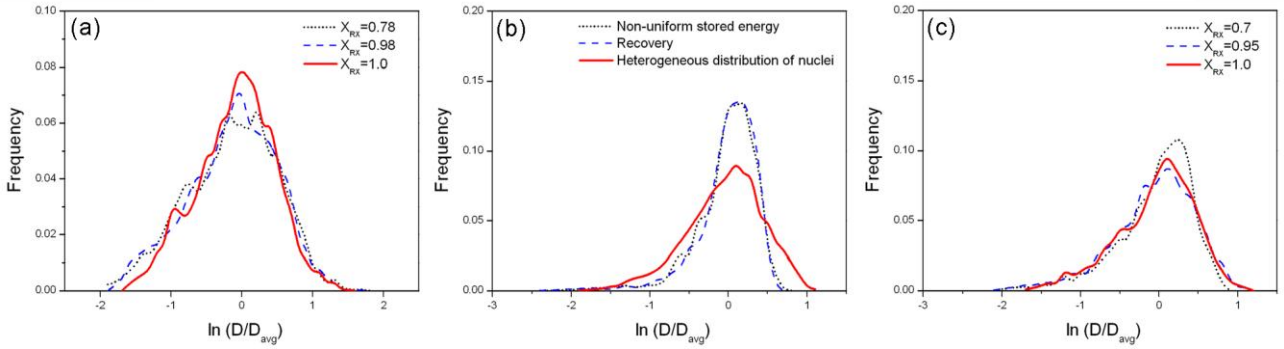

Figure 5. Size distributions of new grains: (a) experimental results, and the distributions predicted by MC modeling under conditions (b) that include an effect from either of non-uniform stored-energy, recovery or heterogeneous distribution of nuclei in the JMAK assumptions and (c) that include all of the effects in (b).

Conclusions

Both experimental observations and MC modeling of recrystallization of cold-rolled cp-Ti reveal that the assumptions in the classical JMAK model result in a failure to accurately predict recrystallization kinetics while the SF relation provides a better description. MC modeling suggests that the inclusion of a heterogeneous distribution of nuclei is an essential prerequisite for more realistic predictions of recrystallization kinetics and grain-size distributions.

Acknowledgement

The present work was performed under the auspices of the Air Force Office of Scientific Research and its Asian Office of Aerospace Research and Development. It was also partially supported by the KOSEF 2008-0058854 program of the Korea Ministry of Science and Technology.

References

[1] V. Erukhimovitch and J. Baram: Mater. Sci. Eng. A Vol. 214 (1996), p. 78

[2] R.L. Goetz, and V. Seetharaman: Metall. Mater. Trans. A Vol. 29 (1998), p. 2307

[3] T. Furu, K. Marthinsen and E. Nes: Mater. Sci. Technol. Vol. 6 (1990), p. 1093

[4] A.D. Rollett, D.J. Srolovitz, R.D. Doherty, M.P. Anderson: Acta Metall. Vol. 37 (1989), p. 627

[5] Y.B. Chun, S.L. Semiatin and S.K. Hwang: Acta Mater. Vol. 54 (2006), 3673

[6] P.A. Beck and P.R. Sperry: J. Appl. Phys Vol. 21 (1950), p. 150

[7] A.D. Rollett and E. Holm, in: *Recrystallization and related phenomena*, edited by T.R. McNelley, Monterey, USA (1997), p. 31

[8] H.N. Lee, H.S. Ryoo and S.K. Hwang: Mater. Sci. Eng. A Vol. 281 (2000), p. 176

[9] M. Avrami: J. Chem. Phys. Vol. 8 (1940), p. 212

[10] G.R. Speich, R.M. Fisher, in: *Recrystallization, Grain Growth and Textures*, edited by H. Margolin, ASM, Metals Park (1966), p. 563