2003. 11.

Thermodynamics

Micro MonteCarlo Simulation

이 병 주

포항공과대학교 신소재공학과

calphad@postech.ac.kr

Micro Monte Carlo Simulation - Literature (from N.M. Hwang)

1. “**Texture Evolution by Grain Growth in the System of Anisotropic Grain Boundary Energy**”
   N.M. Hwang, B.-J. Lee and C.H. Han, Scripta Materialia 37, 1761-1767 (1997).

2. “**Grain Growth Behavior in the System of Anisotropic Grain Boundary Mobility**”
   Nong Moon Hwang, Scripta Materialia 37, 1637-1642 (1997).

3. “**Formation of Island and Peninsular Grains during Secondary Recrystallization of Fe-3%Si Alloy**”
   S.B. Lee, N.M. Hwang C.H. Hahn, D.Y. Yoon, Scripta Mater. 39, 825-829 (1998).

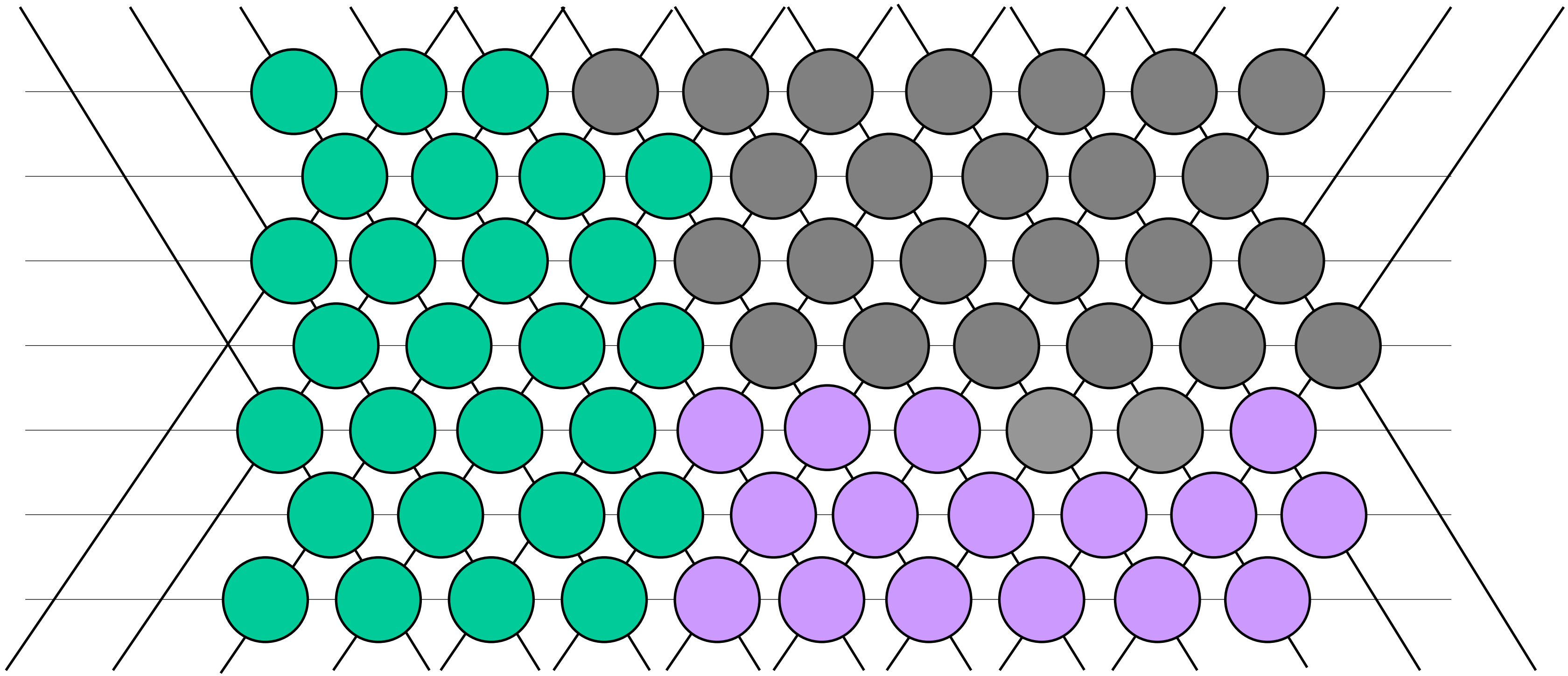
4. “**Simulation of Effect of Anisotropic Grain Boundary Mobility and Energy on Abnormal Grain Growth**”, N.M. Hwang, J. Mater. Sci. vol. 33, 5625-5629 (1998).

5. “**Abnormal Grain Growth by Solid-State Wetting along Grain Boundary or Triple Junction**”
   N.M. Hwang, S.B. Lee and D.Y. Kim, Scripta Mater. 44, 1153-1160 (2001).

Micro Monte Carlo Simulation - General Scheme (Potts Model)

$$E = J\sum_{nn}(1-\delta_{S_iS_j})$$

$$E = \begin{cases} J_1\sum_{nn}(1-\delta_{S_iS_j}) & S_i \le C \text{ and } S_j \le C \quad \text{Type I – Type I} \\ J_2\sum_{nn}(1-\delta_{S_iS_j}) & \begin{cases} S_i > C \text{ and } S_j > C & \text{Type II – Type II} \\ S_i \le C \text{ and } S_j > C & \text{Type I – Type II} \\ S_i > C \text{ and } S_j \le C & \text{Type II – Type I} \end{cases} \end{cases}$$



Effect of Anisotropy of Grain Boundary Energy on Texture Evolution

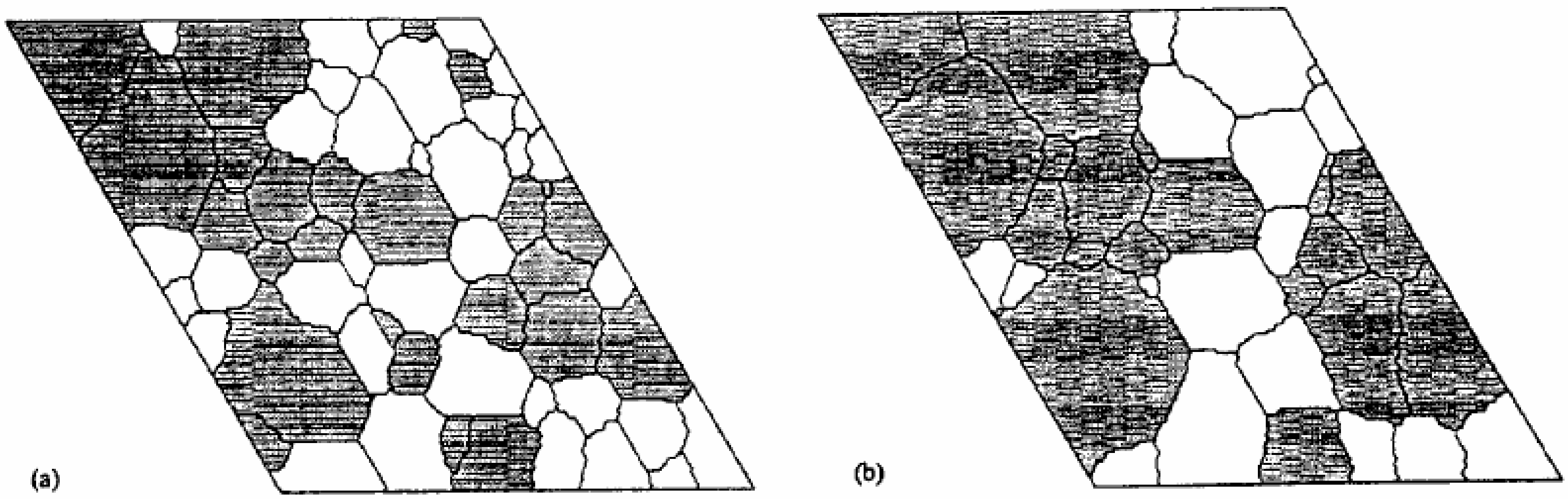


Figure 2. Microstructural evolution after (a) 500 MCS and (b) 1000 MCS with the condition that the grain boundary between the type II (white) grains has an energy 3 times that between the type I (shaded) grains. The fraction of the shaded grains increased from an initial 20% to (a) 54% and (b) 63%.

Effect of Anisotropy of Grain Boundary Energy on Texture Evolution

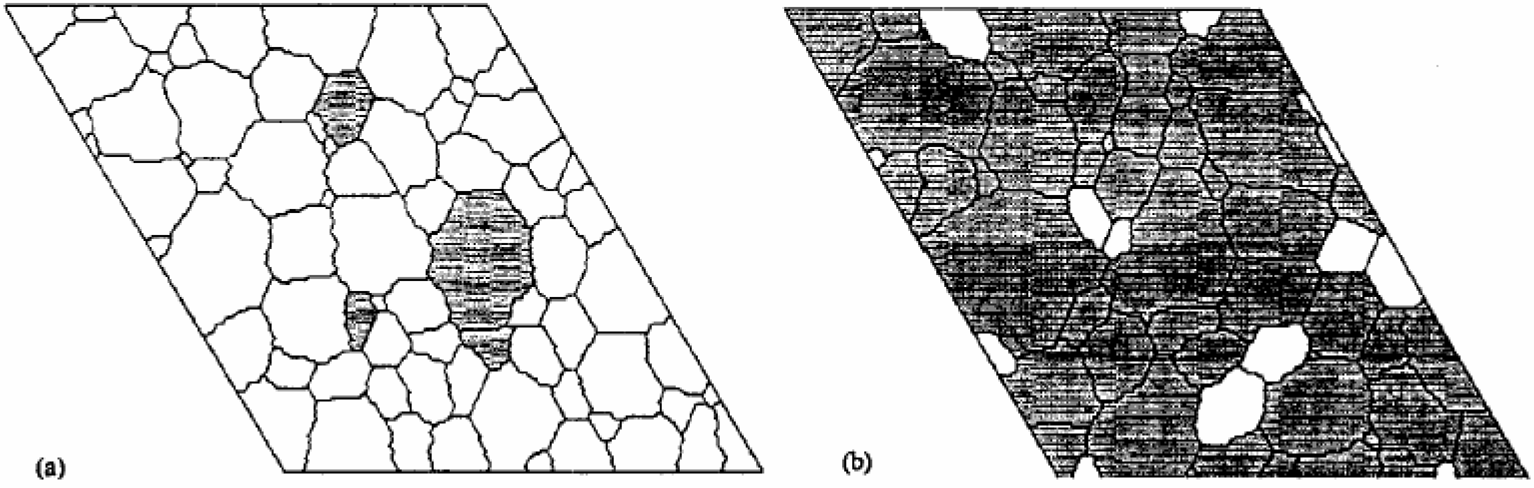


Figure 3. Microstructural evolution after 500 MCS with the initial fraction of the shaded grains (a) 10% and (b) 30%. The grain boundaries between the white grains have an energy 3 times that between the shaded grains. The fractions of the shaded grain are 8% and 90%, respectively.

Effect of Anisotropy of Grain Boundary Energy on Texture Evolution

$$E = \begin{cases} J_1 \sum_{nn} (1 - \delta_{S_i S_j}) & S_i \le C \quad \text{and} \quad S_j \le C \quad \text{Type I – Type I} \\ J_2 \sum_{nn} (1 - \delta_{S_i S_j}) & S_i > C \quad \text{and} \quad S_j > C \quad \text{Type II – Type II} \\ J_3 \sum_{nn} (1 - \delta_{S_i S_j}) & \begin{cases} S_i \le C \quad \text{and} \quad S_j > C \quad \text{Type I – Type II} \\ S_i > C \quad \text{and} \quad S_j \le C \quad \text{Type II – Type I} \end{cases} \end{cases}$$

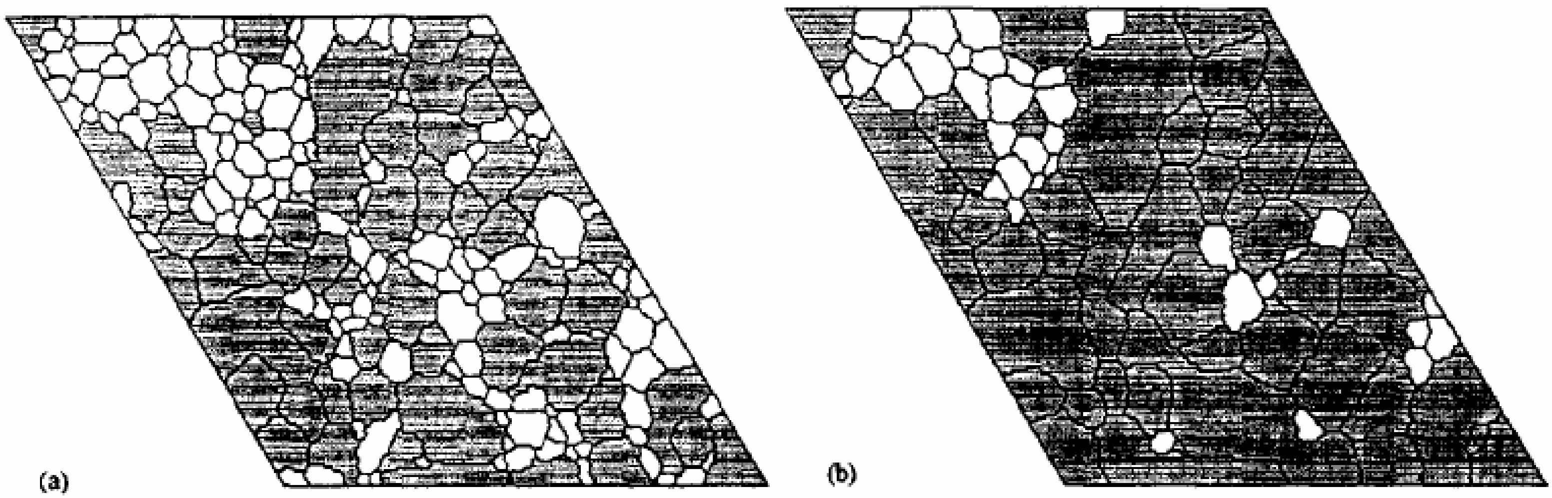


Figure 4. Microstructural evolution (a) after 100 MCS and (b) after 200 MCS with the condition that the grain boundaries between the white grains and between the white and the shaded grains have an energy, respectively, 1.5 times and 1.3 times that between the shaded grains. The fractions of the shaded grains are 62% and 85%, respectively.

Effect of Anisotropy of Grain Boundary Mobility on Abnormal GG

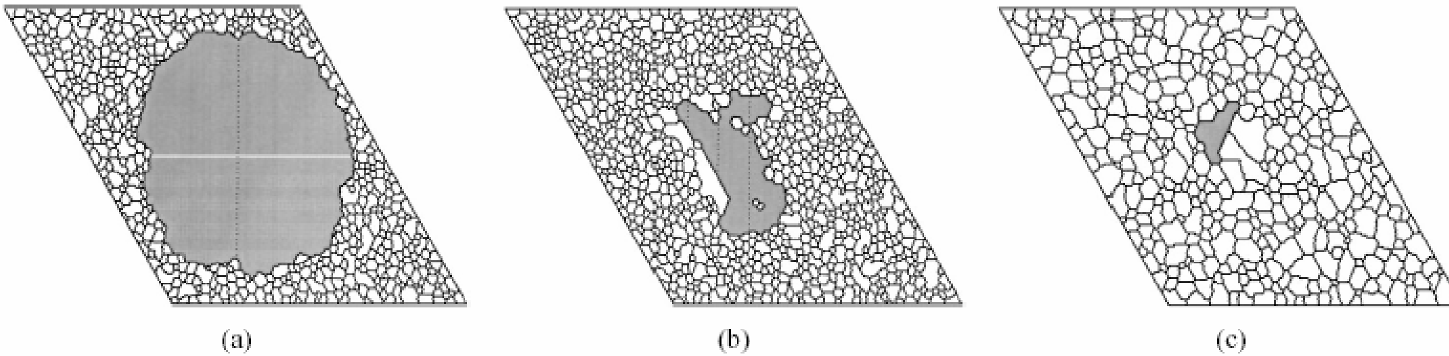


Figure 1 Microstructure evolution after (a) 500 MCS, (b) 500 MCS and (c) 3000 MCS with the percentages of type II grains, (a) 100%, (b) 90% and (c) 80%. The grain boundary between AGG and type II grains has mobility 100 times higher than that between AGG and type I grains or between type I and type II grains.

Effect of Anisotropy of Grain Boundary Energy on Abnormal GG

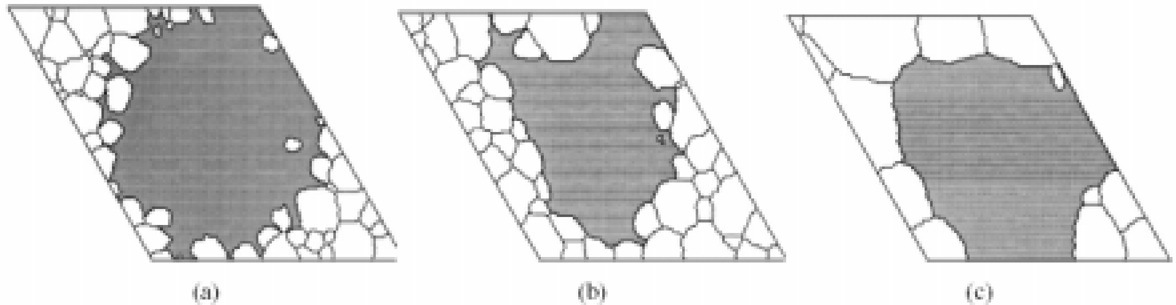


Figure 2 Microstructure evolution after (a) 500 MCS, (b) 500 MCS and (c) 2000 MCS with the percentages of type II grains, (a) 100%, (b) 70% and (c) 40%. The grain boundary between AGG and type I grains has energy 3 times that between AGG and type II grains or between type I and type II grains.

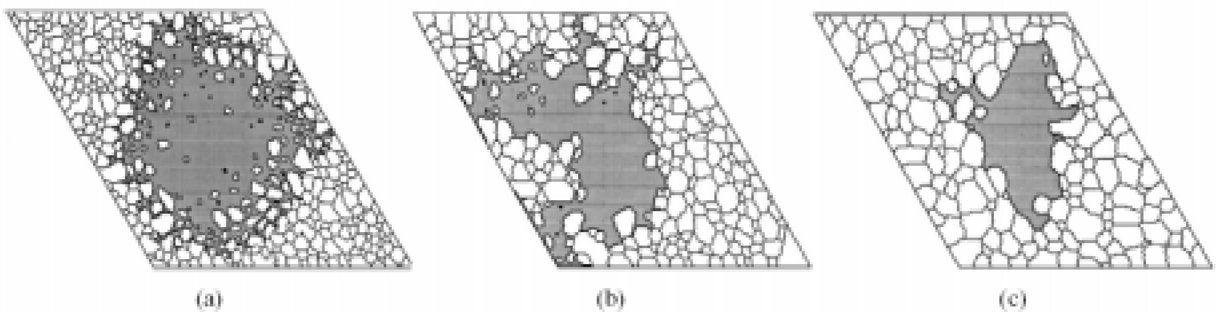


Figure 3 Microstructure evolution after (a) 500 MCS, (b) 500 MCS and (c) 1000 MCS with percentages of type II grains, (a) 100%, (b) 80% and (c) 60%. The overall mobility except at the triple junction is reduced by 10 times. Conditions for anisotropy in grain boundary energy are the same as Fig. 2.