Influence of grain boundary mobility on microstructure evolution during recrystallization

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Investigation whether there is any influence of low angle grain boundaries on the microstructure and texture evolution during recrystallization.

- Recrystallization: change of microstructure as well as of the properties of crystalline materials.
- Experimental evidence for influence of low angle grain boundaries, but they are usually not taken into account.
- Recrystallization models discriminate between three different types of grain boundaries.
- Only few simulations investigated the effect of different grain boundary mobilities on the recrystallization behavior, but without taken into account a non-zero low angle grain boundary mobility.
• Attribute of each cell: orientation, dislocation density
• State: „recrystallized“ or „non-recrystallized“
• Switching rule: probabilistic formulation of the Turnbull equation

• Turnbull equation:
  \[ v = m_p = m_0 \exp(-Q/kT) \rho \]

• New formulation with two contributions: \[ v = v_0 w \]

Deterministic part:

\[ v_0 = \frac{kTm_0}{b^3} \]

Probabilistic part:

\[ w = \frac{pb^3}{kT} \cdot \exp\left(-\frac{Q}{kT}\right) \]
– simulation box 100x100x100 cells with 1x1x1µm³ cell size
– Al single crystal with Cube orientation
– nucleation takes place site saturated and randomly at t = 0
– driving force results only from difference in stored energy
– constant dislocation density

**Case 1:**

HAGB: $\Delta H = 1.6\text{eV}$ and $m_0 = 1.45 \times 10^{12} \text{µm/sMPa}$

LAGB: $m = 0$

**Case 2:**

HAGB: $\Delta H = 1.6\text{eV}$ and $m_0 = 1.45 \times 10^{12} \text{µm/sMPa}$

LAGB: $\Delta H = 1.3\text{eV}$ and $m_0 = 2.65 \times 10^{10} \text{µm/sMPa}$

**Case 3:**

HAGB: $\Delta H = 1.0\text{eV}$ and $m_0 = 7.78 \times 10^{8} \text{µm/sMPa}$

LAGB: $\Delta H = 1.3\text{eV}$ and $m_0 = 2.65 \times 10^{10} \text{µm/sMPa}$
Nucleus distribution very similar for case 1, case 2 and case 3

Initial fraction of LAGB in nucleus distribution: ~4.9%
Influence of mobility for constant dislocation density $\rho=10^{14}\text{m}^{-2}$, number of nuclei $w=0.05\%$ and temperature $T=573\text{K}$. 

**Results – Kinetics: influence mobility**

- HAGB ($\Delta H_{\text{HAGB}}=1.6\text{eV}$)
- LAGB+HAGB ($\Delta H_{\text{HAGB}}=1.6\text{eV}$)
- HAGB ($\Delta H_{\text{HAGB}}=1.0\text{eV}$)
- LAGB+HAGB ($\Delta H_{\text{HAGB}}=1.0\text{eV}$)
Results – Kinetics: influence number of nuclei

Influence of number of nuclei for constant dislocation density $\rho=10^{14}$m$^{-2}$ and temperature $T=573$K.
Influence of temperature for constant dislocation density $\rho=10^{14} \text{m}^{-2}$ and number of nuclei $w=0.05\%$. 
Influence of dislocation density for constant number of nuclei $w=0.05\%$ and temperature $T=573K$. 
Determination of Avrami exponent $q$ from Avrami plot based on:

$$\ln(-\ln(1-X)) = q \cdot \ln(t) + \ln k_0$$
Obviously, recrystallization in LAGB case is much faster than recrystallization in HAGB case.

\[ q_{\text{theo}} > 3 \text{ site saturated nucleation but different growing rates} \]

\[ \sim q_{\text{theo}} = 3 \text{ site saturated nucleation and constant growing rate} \]

<table>
<thead>
<tr>
<th>Mobile LAGB and HAGB</th>
<th>Only mobile HAGB</th>
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<tr>
<td>( \rho=10^{14}\text{m}^{-2}, T=573\text{K}, w=0.01%; \ q=3.30 )</td>
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<td>( \rho=10^{14}\text{m}^{-2}, T=573\text{K}, w=0.5%; \ q=2.72 )</td>
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<td>( \rho=10^{14}\text{m}^{-2}, T=673\text{K}, w=0.05%; \ q=2.82 )</td>
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<td>( \rho=10^{14}\text{m}^{-2}, T=773\text{K}, w=0.05%; \ q=3.09 )</td>
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<td>( \rho=10^{12}\text{m}^{-2}, T=573\text{K}, w=0.05%; \ q=3.28 )</td>
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<td>( \rho=10^{15}\text{m}^{-2}, T=573\text{K}, w=0.05%; \ q=3.21 )</td>
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Results – Fractions of grain boundaries

LAGB+HAGB
($\Delta H_{\text{HAGB}}=1.6\text{eV}$)

HAGB
($\Delta H_{\text{HAGB}}=1.6\text{eV}$)

Initial dislocation density for these simulations: $\rho=10^{14}\text{m}^{-2}$, number of nuclei $w=0.05\%$ and $T=573\text{K}$.

The Mackenzie distribution is plotted as solid line and gives the distribution for a completely random distribution.
Results – Microstructure evolution

(a) $m_{LAGB}>0$ and $m_{HAGB}>0$ at 573 K. (b) $m_{LAGB}>0$ and $m_{HAGB}>0$ at 673 K. (c) $m_{LAGB}>0$ and $m_{HAGB}>0$ at 773 K.

(d) $m_{LAGB}=0$ and $m_{HAGB}>0$ at 573 K. (e) $m_{LAGB}=0$ and $m_{HAGB}>0$ at 673 K. (f) $m_{LAGB}=0$ and $m_{HAGB}>0$ at 773 K.

At $T=573$ K: (g) $\Delta H_{LAGB}/\Delta H_{HAGB}=1.3\text{eV}/1.0\text{eV}$. (h) $m_{LAGB}=0$ and $\Delta H_{HAGB}=1.0\text{eV}$. 

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Pole figures for fully recrystallized Al single crystals with initial Cube orientation and $w=2\%$.

Upper row: Predicted textures at different temperatures for the case of mobile low and high angle grain boundaries:
Bottom row: Predicted textures at different temperatures for the case with only mobile high angle grain boundaries.
Initial dislocation density: $\rho=10^{14}\text{m}^{-2}$. 
Results – Texture evolution: influence mobility

Upper row: Predicted textures for the cases of mobile low and high angle grain boundaries: Left side: $\Delta H_{\text{LAGB}}/\Delta H_{\text{HAGB}}=1.3\text{eV}/1.6\text{eV}$; right side: $\Delta H_{\text{LAGB}}/\Delta H_{\text{HAGB}}=1.3\text{eV}/1.0\text{eV}$.

Bottom row: Predicted textures for the cases with only mobile high angle grain boundaries. Left side: $m_{\text{LAGB}}=0$ and $\Delta H_{\text{HAGB}}=1.6\text{eV}$; right side: $m_{\text{LAGB}}=0$ and $\Delta H_{\text{HAGB}}=1.0\text{eV}$.

Initial dislocation density for these simulations: $\rho=10^{14}\text{m}^{-2}$, number of nuclei $w=0.05\%$ and $T=573\text{K}$.
Results of 3D cellular automaton simulations were shown. Three cases were compared in order to study the influence of mobile low angle grain boundaries on the recrystallization behavior.

The texture evolution shows an increasing randomization for the HAGB simulations. For LAGB simulations the texture remains stable up to 100% recrystallized fraction.

The kinetics of recrystallization is faster for the LAGB simulations than for the HAGB simulations.

The fraction of low angle grain boundaries is remarkably larger in the LAGB simulation case.

The presented simulation results show that there is obviously an influence of low angle grain boundaries on the texture evolution during recrystallization.

Further simulations are needed in order to get data which can be compared with experimental results.
The Düsseldorf Max-Planck Team

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