Copper nanoprecipitates in steel studied by atom probe tomography and ab initio based Monte Carlo simulation

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Thanks to: DFG
Overview

- Motivation: Electromobility
- Fe-3%Si-1% (2%) Cu model system
- Fe-3%Si-Cu engineering alloy
- Simulations (DFT + kMC, model system)
- Conclusions and challenges
Avoid use of permanent magnets and use instead electrical magnets in synchronous electrical engines

High strength soft magnetic steels in car engines reduce CO₂ emission
Electrical steels for electrical cars
Electrical steels

Standard soft magnetic steel: based on Fe–3 wt. % Si ⇒ ferritic phase, coarse grains ⇒ soft-magnetic properties

Improvement of the mechanical strength!
precipitation hardening: 1-2 wt. % Cu, aging at 450°C
Nano-precipitates in soft magnetic Fe-3%Si steels

nanoparticles too small for Bloch-wall interaction but effective as dislocation obstacles

mechanically very strong soft magnets for motors
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Precipitation hardened electrical steels:
nucleation of copper precipitates in iron-silicon matrix

I. Fe II. Fe
Si 3 wt. % Si 3 wt. %
Cu 1 wt. % Cu 2 wt.%

• solute annealing 950°C-1150°C for 1h
• water quenching
• age hardening at 400-450°C for 10 min - 100 h
Precipitation hardened electrical steels

Atom probe tomography

450°C

1 wt. % Cu

2 wt. % Cu

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LEAP (Local Electrode Atom Probe) 3000X HR

initiated evaporation

or by

high voltage

~ 10 kV

3-dimensional reconstructed model of specimen
(about 100 Millions of atoms)

~100 nm

Time of flight \Rightarrow mass / charge state

mass spectrum

48Ti$^{+2}$
55Mn$^{+2}$
56Fe$^{+2}$
58Ni$^{+2}$
54Fe$^{+2}$
60Ni$^{+2}$

200 nm

24 26 28 30

24 26 28 30
APT results: 3D atomic maps (Laser mode at 60K, 0.4 nJ)

Cu 1 wt.% ⇒

120 min

Isocencentration surfaces at Cu 11 at.%
APT results: 3D atomic maps (Laser mode at 60K, 0.4 nJ)

Cu 1 wt.% ⇒

120 min

6000 min

Cu 2 wt.% ⇒

120 min

6000 min

Iso-concentration surfaces at Cu 11 at.%

450°C aging

Fe-Si-Cu, LEAP 3000X HR

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## APT results: quantification

<table>
<thead>
<tr>
<th></th>
<th>Cu 1 wt.% ⇒</th>
<th></th>
<th>Cu 2 wt.% ⇒</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>120 min</td>
<td>6000 min</td>
<td>120 min</td>
</tr>
<tr>
<td></td>
<td>3.2 nm ± 0.8 nm</td>
<td>5.0 nm ± 0.8 nm</td>
<td>4.3 nm ± 0.8 nm</td>
</tr>
<tr>
<td><strong>Cluster:</strong></td>
<td>Fe 62.9 at%</td>
<td>Fe 60.7 at%</td>
<td>Fe 71 at%</td>
</tr>
<tr>
<td></td>
<td>Cu 32.1 at%</td>
<td>Cu 35.2 at%</td>
<td>Cu 24 at%</td>
</tr>
<tr>
<td></td>
<td>Si 5.0 at%</td>
<td>Si 4.1 at%</td>
<td>Si 5 at%</td>
</tr>
<tr>
<td></td>
<td><strong>Matrix (without clusters):</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Cu 0.2 at%</td>
<td>Cu 0.1 at%</td>
<td>Cu 0.2 at%</td>
</tr>
<tr>
<td><strong>“Enrichment factor”:</strong></td>
<td>content in cluster / content in alloy</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Fe 0.68</td>
<td>Fe 0.65</td>
<td>Fe 0.77</td>
</tr>
<tr>
<td></td>
<td>Cu 40.1</td>
<td>Cu 44.0</td>
<td>Cu 17</td>
</tr>
<tr>
<td></td>
<td>Si 0.75</td>
<td>Si 0.68</td>
<td>Si 0.78</td>
</tr>
<tr>
<td></td>
<td><strong>clusters number density, ( m^{-3} )</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( 6.1 \cdot 10^{23} )</td>
<td>( 0.9 \cdot 10^{23} )</td>
<td>( 6.4 \cdot 10^{23} )</td>
</tr>
<tr>
<td></td>
<td><strong>volume fraction of clusters</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>~ 2%</td>
<td>~ 2%</td>
<td>~ 5%</td>
</tr>
</tbody>
</table>
APT results: Proximity histogram

Cu 2 wt.%; 450°C/6000 min

Cluster size
- 5 nm
- 8 nm

Cluster size
- bigger cluster
- smaller cluster

Matrix → Cluster center

Cu concentration, at. %

- kinetic reasons?
  (different stages of particle growth)
- slow diffusion; misfit?
  → residual Fe-content
  → diffuse interface
Motivation: Electromobility

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Fe-3%Si-Cu engineering alloy

Simulations (DFT + kMC, model system)

Conclusions and challenges
Overall content in the analysis volume:

Fe 92.1 at.%
Cu 1.49 at.%
Al 0.56 at.%
Si 5.83 at. %
3D-concentration profiles

Iso-concentration-Surfaces at Cu 6 at.%
d = 5.0 ± 1.0 nm
(density corrected: d = 6.0 ± 1.4 nm)
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Modeling: ab-initio, DFT / GGA, binding energies

Fe-Si steel with Cu nano-precipitates
Modeling: ab-initio, DFT / GGA, binding energies

Fe-Si steel with Cu nano-precipitates
Modeling: ab-initio, DFT / GGA, binding energies

Fe-Si steel with Cu nano-precipitates
Modeling: ab-initio, DFT / GGA, binding energies
Ab-initio, binding energies: Cu-Cu in Fe matrix

CuCu System 3x3x3

Total Energy in eV vs. Distance in Angstrom
Ab-initio, binding energies: Si-Si in Fe matrix

SiSi System 4x4x4

Total Energy in eV

Distance in Angstrom
For neighbor interaction energy take difference (in eV)

\[ E_{SiSi}^{\text{bin}} \] (repulsive) = 0.390

\[ E_{SiCu}^{\text{bin}} \] (attractive) = -0.124

\[ E_{CuCu}^{\text{bin}} \] (attractive) = -0.245
Ab-initio, use binding energies in kinetic Monte Carlo model

<table>
<thead>
<tr>
<th>Cu 1 wt.%</th>
<th>Cu 5 wt.%</th>
</tr>
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<tbody>
<tr>
<td>T = 250 °C</td>
<td>T = 450 °C</td>
</tr>
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<td>T = 250 °C</td>
<td>T = 450 °C</td>
</tr>
</tbody>
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1 nm
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Conclusions and challenges

- Soft magnetic steels for electromobility
- Increase mechanical strength without losing good soft magnetic properties
- Use nanoprecipitates with size below Bloch wall thickness
- APT suited to provide statistics and composition of nanoparticles
- Ab-initio thermodynamics in system Fe-Si-Cu
- Kinetics: QM – kMC
- Coupling DFT/kMC with atomic-scale experiments