Modeling the supercurrent flow in polycrystalline Fe-based superconductors

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Fruitful discussion with Prof. Teruo Matsushita (Kyushu Inst. Technol.)
Iron-based SCs (IBSC): application point of view

- High $T_c \sim 38$ K ($\sim 56$ K in 1111)
- Very high $H_{c2} > 50$ T
- Small anisotropy ($\gamma < 2$)
- Strong pinning
- $H_{irr}$ close to $H_{c2}$

Properties interesting for magnet applications at 4-30 K

Large current in untextured, polycrystalline IBSC (bulk trapped field magnet)

1.02 T @ 5 K


Y. Shimada, S. Hata et al., to be submitted.
Objective

• Modeling macroscopic current transport (I/I₀) in polycrystalline IBSC
• Predicting the ultimate performance of the optimized IBSC conductors
• Simulating the influences of anisotropy, local defects, texturing, processing...

General approach

• Simulation using site/bond percolation model
• Consider current only
Model: 3D hybrid site/bond percolation system

Site = Material: Cristal grain (orientation, porosity (occupied/un-occupied))

Bond = Conduction: Grain boundary (weak-link, structural connection factor)

Random resistor network (bond)

Kirchhoff’s law: $\sum_i a_i = 0$

Calculation: calculating local site/bond current according to Kirchhoff’s law, convergence judgement.

Bond current: normal current ⇒ Ohm’s law $\nu = r \times i$  
super current ⇒ maximum flow problem 
(Ford–Fulkerson algorithm was applied.)
Normal-state current
2D Normal current

\[ x \parallel V \quad P = 100\% \]

<table>
<thead>
<tr>
<th>Occupied site distribution</th>
<th>Voltage distribution</th>
<th>Current distribution</th>
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Connectivity: 100%

\[ P = 100\%, \ 100 \times 100 \times 1 \text{ matrix, } b=1 \]
2D Normal current

\[ x \parallel \nu \quad P = 90\% \]

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Occupied site distribution

Voltage distribution

Current distribution

Connectivity: \( 70.3\% \)

P = 90%, 100x100x1 matrix, b=1

Introducing defects (porosity)
2D Normal current

\[ \mathbf{P} = 80\% \]

Occupied site distribution

Introducing more defects (porosity)

Voltage distribution

Connectivity: 44.1%

Current distribution

\[ \mathbf{P} = 80\%, \ 100 \times 100 \times 1 \text{ matrix, } b=1 \]
2D Normal current

P = 70%

Occupied site distribution
Introducing more defects (porosity)

Connectivity: 18.7%

Voltage distribution

Current distribution

P = 70%, 100x100x1 matrix, b=1
2D Normal current

$P = 60\%$ (close to critical $P_c \sim 59\%$)

Occupied site distribution
Voltage distribution
Current distribution

Connectivity: $3.2\%$

Introducing more defects (porosity)


$P = 60\%, 100\times100\times1$ matrix, $b=1$
3D Normal current

\[ P = 75\% \]

Occupied site distribution

Voltage distribution

Current distribution

Connectivity: 46.3\%

\[ P = 75\%, \ 50 \times 50 \times 50 \ matrix, \ b=1 \]
3D Normal current

$P = 35\%$

Occupied site distribution

Voltage distribution

Current distribution

Connectivity: 0.7%

$P = 35\%, 50\times50\times50$ matrix, b=1

High

Low
Super current
Approach for super current

• Consider current only
• Each bond current: Consider weak-link due to GB tilt angle between neighboring sites
• 1 Assumption!
  \[ \frac{I_c(\theta_{\text{GB}})}{I_0} = \exp \left( -\frac{\theta_{\text{GB}}}{\theta_c} \right) \]
• Conductivity of the system:
  ⇒ Maximum flow problem

Transport super current distribution for randomly oriented sites with weak-link effect

Grain orientation map

Transport supercurrent distribution ($\theta_c = 9$ deg)

Following the EBSD rule

Color map

Current

P = 100%, 30x30x30 matrix, b=1, G=1
Transport super current distribution for randomly oriented sites with weak-link effect

$\theta_c = 9$ deg, 2D plane ($z = 15$)

Grain orientation map

Transport supercurrent distribution

P = 100%, 30x30x30 matrix, b=1, G=1
Transport super current distribution for randomly oriented sites with weak-link effect

Macroscopic conductivity is suppressed to only 0.6% due to weak link with $\theta = 9$deg.
Influence of critical misorientation angle $\theta_c$

$\theta_c = 5-9^\circ$ (FBS122) $J_c/J_d = \sim 10^{-3}$

$\theta_c = \sim 3^\circ$ (YBCO) $J_c/J_d = \sim 10^{-5}-10^{-6}$

$\theta_c = 90^\circ$ (MgB$_2$) $J_c/J_d = \sim 10^{-2}$

percolation threshold: 0.2487

$J_c/J_d$ (A/cm$^2$)

YBCO $10^{2-3}/10^8$
FBS122 $10^5/10^8$
MgB$_2$ $10^6/10^8$
Conclusion

• Simple model could explain large difference of current transport among materials (cuprates, FBS, MgB$_2$)
• More bicrystal film data for other types of GBs would be helpful
• New FBS with +5deg $\theta_c$ could change everything
• The J-$\theta_{GB}$ slope is most important
• Our model could simulate the influences of anisotropy, texturing, structural defects

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