



# Modeling the supercurrent flow in polycrystalline Fe-based superconductors

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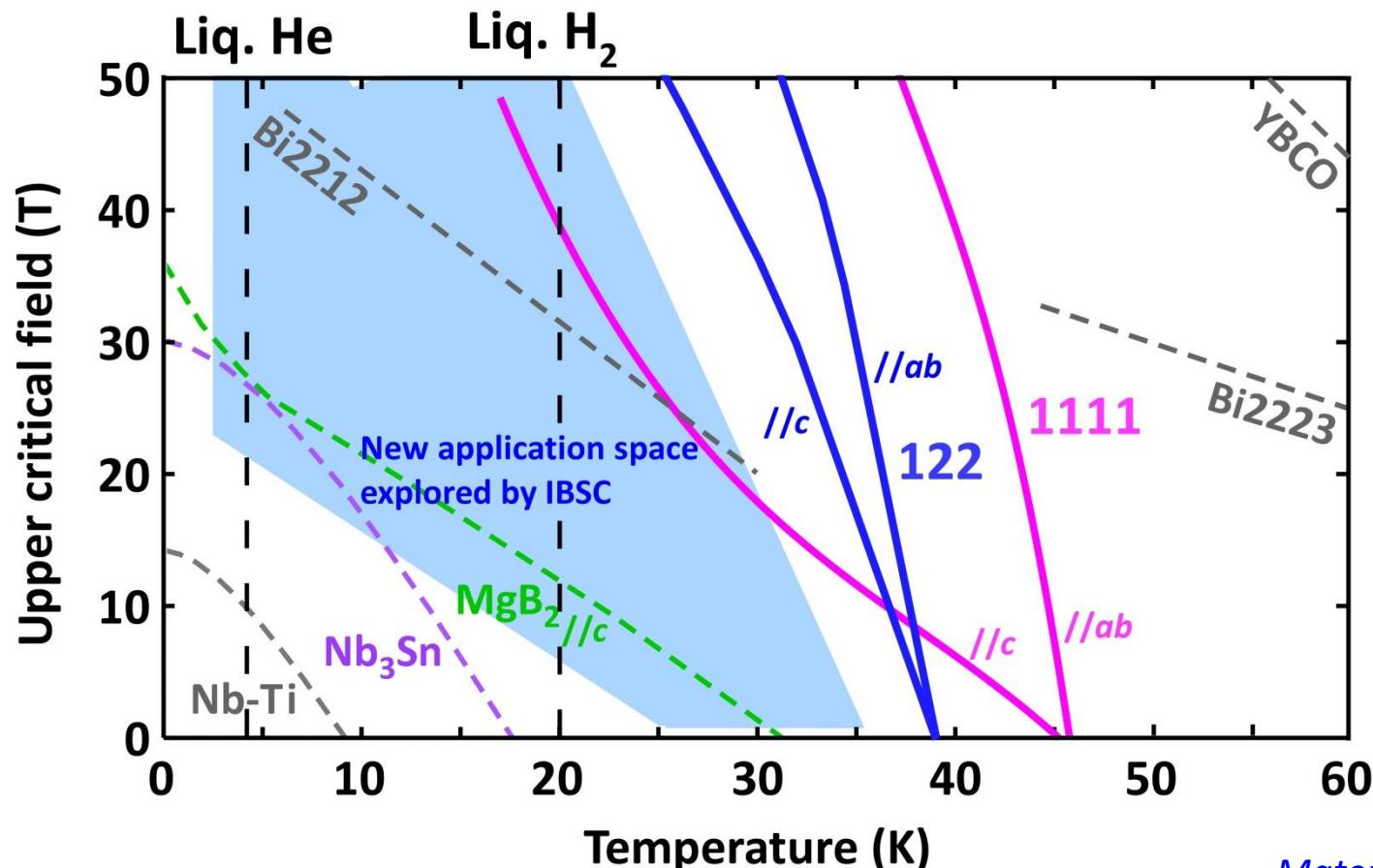
Atominstitut, TU Wien



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Fruitful discussion with Prof. Teruo Matsushita (Kyushu Inst. Technol.)



# Iron-based SCs (IBSC): application point of view



**122**

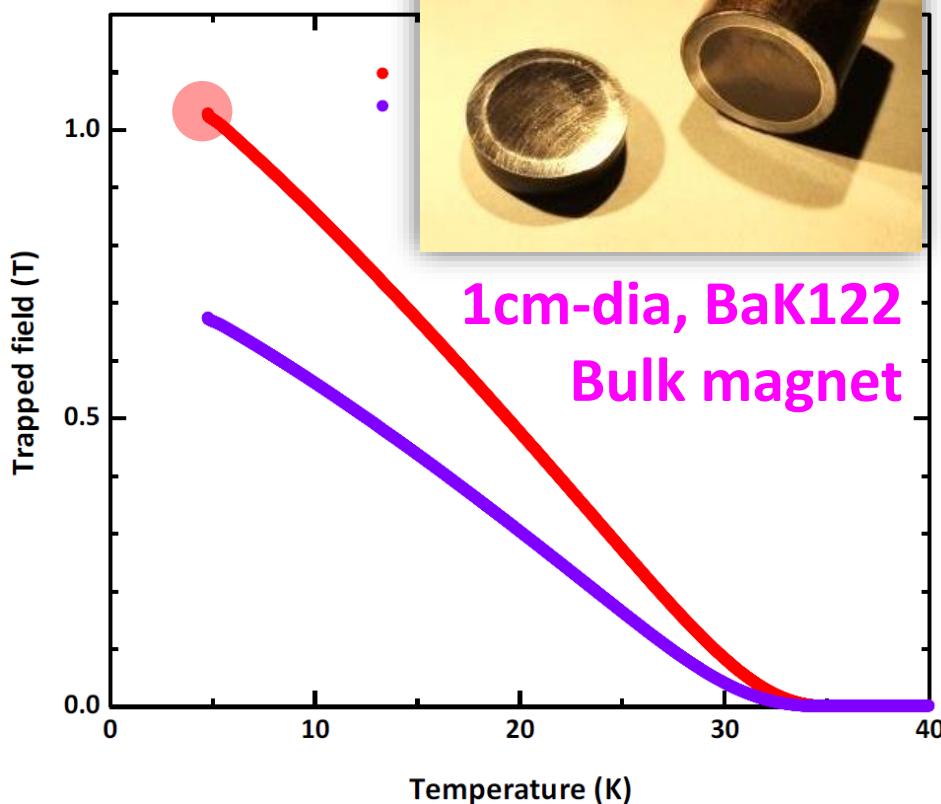
- high  $T_c \sim 38$  K ( $\sim 56$  K in  $1111$ )
- very high  $H_{c2} > 50$  T,
- small anisotropy ( $\gamma < 2$ )
- strong pinning
- $H_{\text{irr}}$  close to  $H_{c2}$

H. Hosono *et al.*,  
Materials Today (2017)

**Properties interesting for magnet applications at 4-30 K**

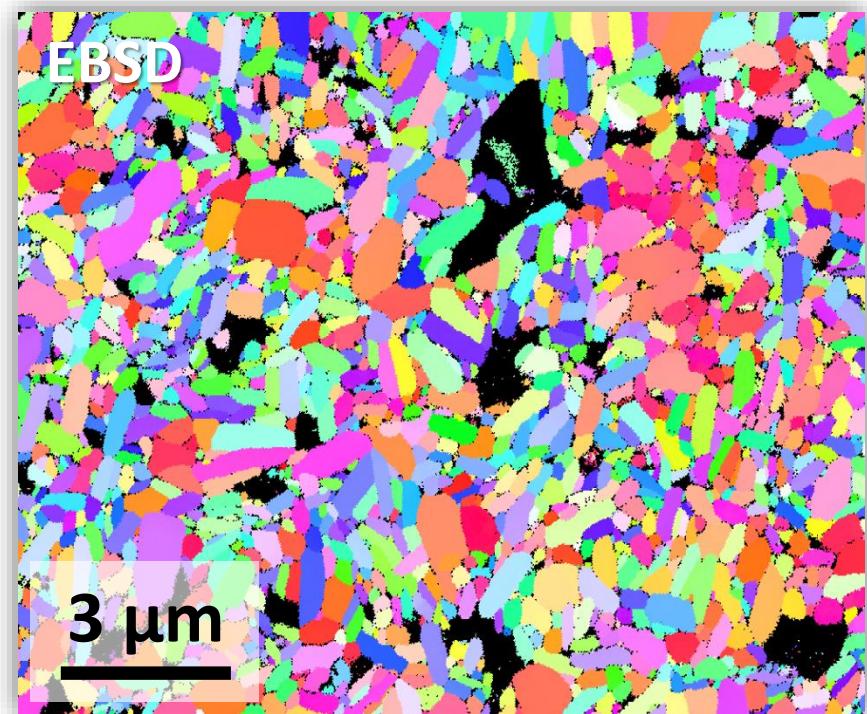
# Large current in untextured, polycrystalline IBSC (bulk trapped field magnet)

1.02 T @ 5 K



1cm-dia, BaK122  
Bulk magnet

Untextured polycrystal



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

Jeremy Weiss, AY *et al.*, *Supercond. Sci. Technol.* FTC **28**, 112001 (2015).

# Objective

- **Modeling macroscopic current transport ( $I/I_0$ ) in polycrystalline IBSC**
- Predicting the ultimate performance of the optimized IBSC conductors
- Simulating the influences of anisotropy, local defects, texturing, processing...

Future works

## General approach

- Simulation using site/bond percolation model
- Consider **current** only

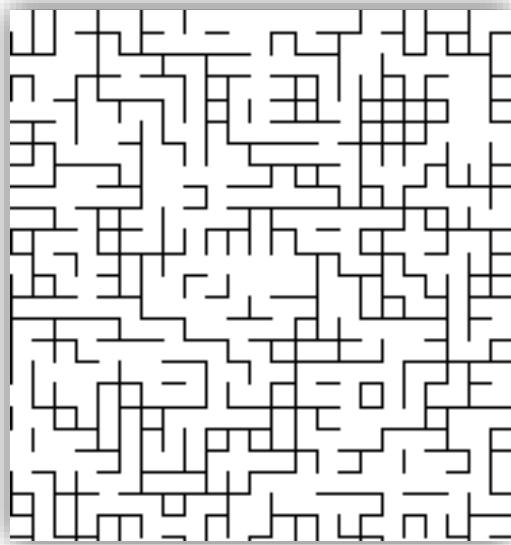
# Model: 3D hybrid site/bond percolation system

(Demerit: valid only for  $z = 6$ )

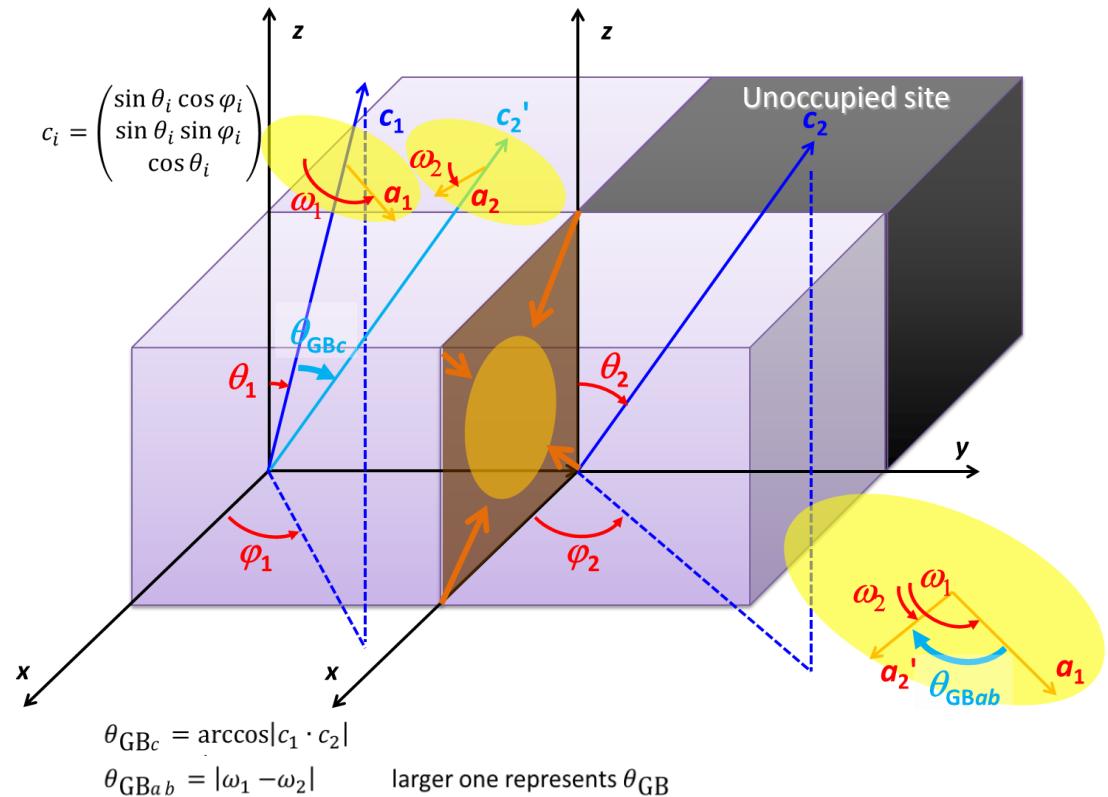
**Site = Material :** Cristal grain (*orientation, porosity(occupied/un-occupied)*)

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

Random resistor network (bond)



$$\text{Kirchhoff's law} \quad \sum_z i = 0$$



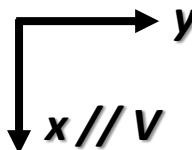
**Calculation :** calculating local site/bond current according to Kirchhoff's law, convergence judgement.

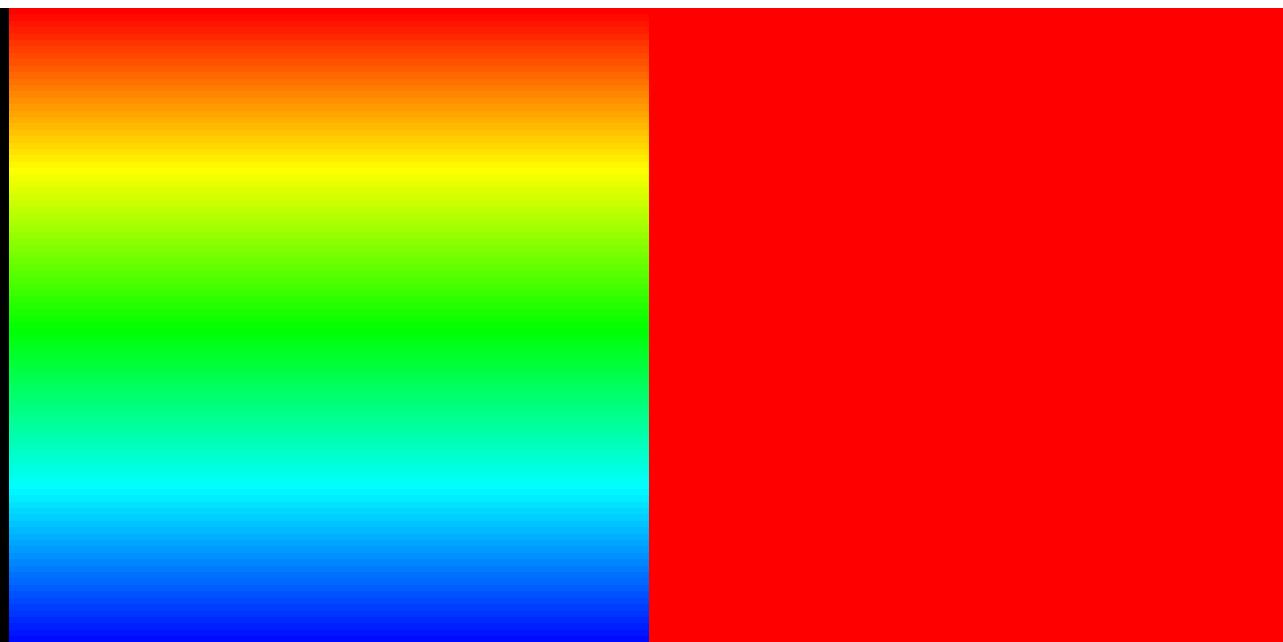
**Bond current :** normal current  $\Rightarrow$  Ohm's law  $v = r \times i$     super current  $\Rightarrow$  maximum flow problem

(Ford–Fulkerson algorithm was applied.)

# Normal-state current

# 2D Normal current

  $x \parallel v$  **P = 100%**



Occupied site distribution

Voltage distribution

Current distribution

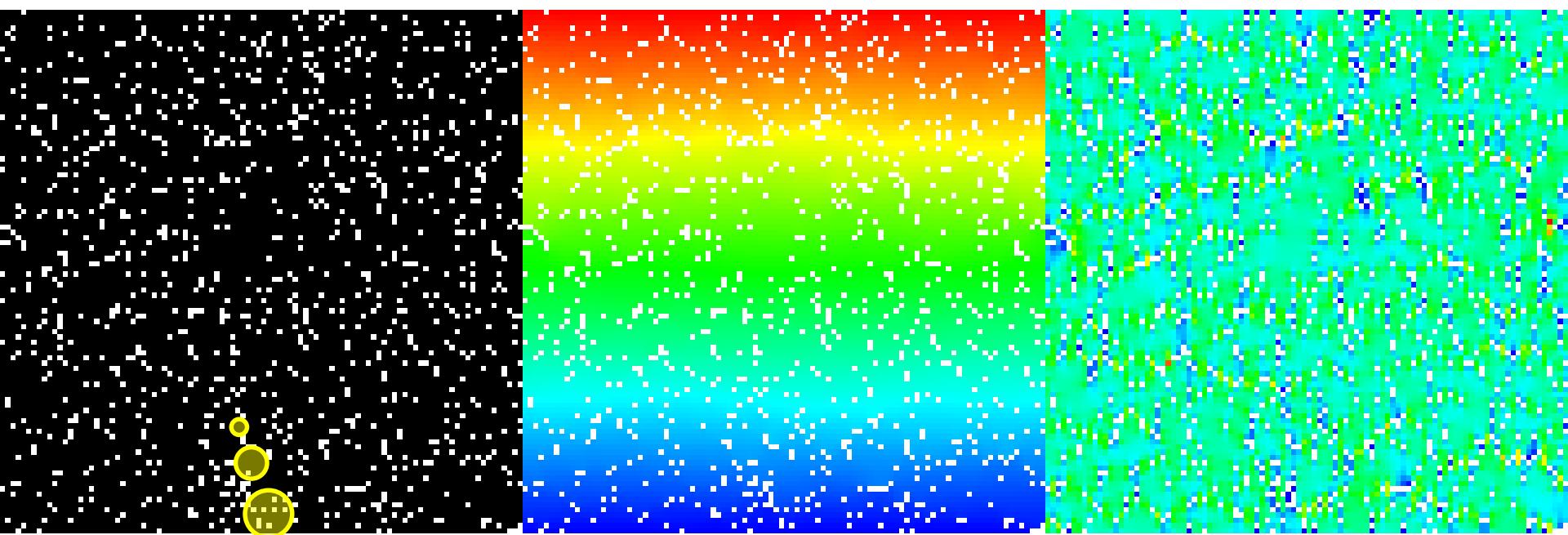


Connectivity: 100%

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

# 2D Normal current

$x \parallel v$   $P = 90\%$

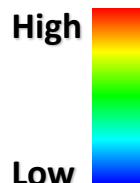


Occupied site distribution  
Introducing  
defects  
(porosity)

Voltage distribution

Connectivity: 70.3%

Current distribution

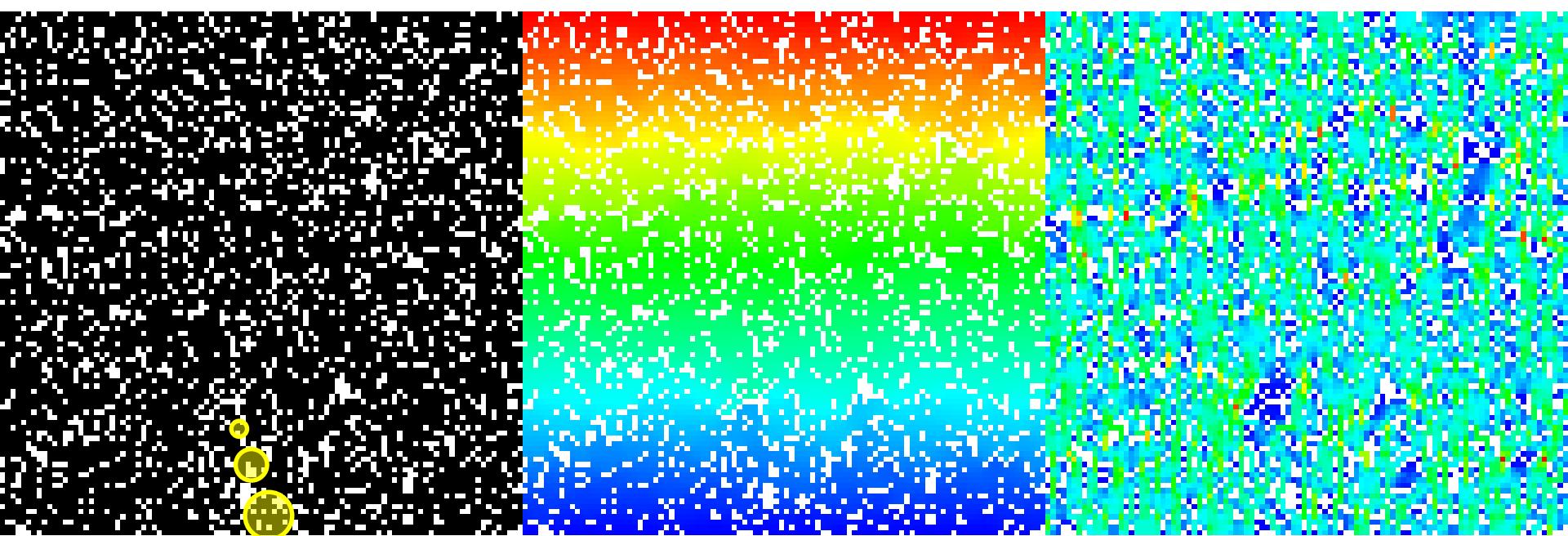


$P = 90\%, 100 \times 100 \times 1$  matrix,  $b=1$

# 2D Normal current

$x \parallel v$

$P = 80\%$



Occupied site distribution  
Introducing more defects (porosity)

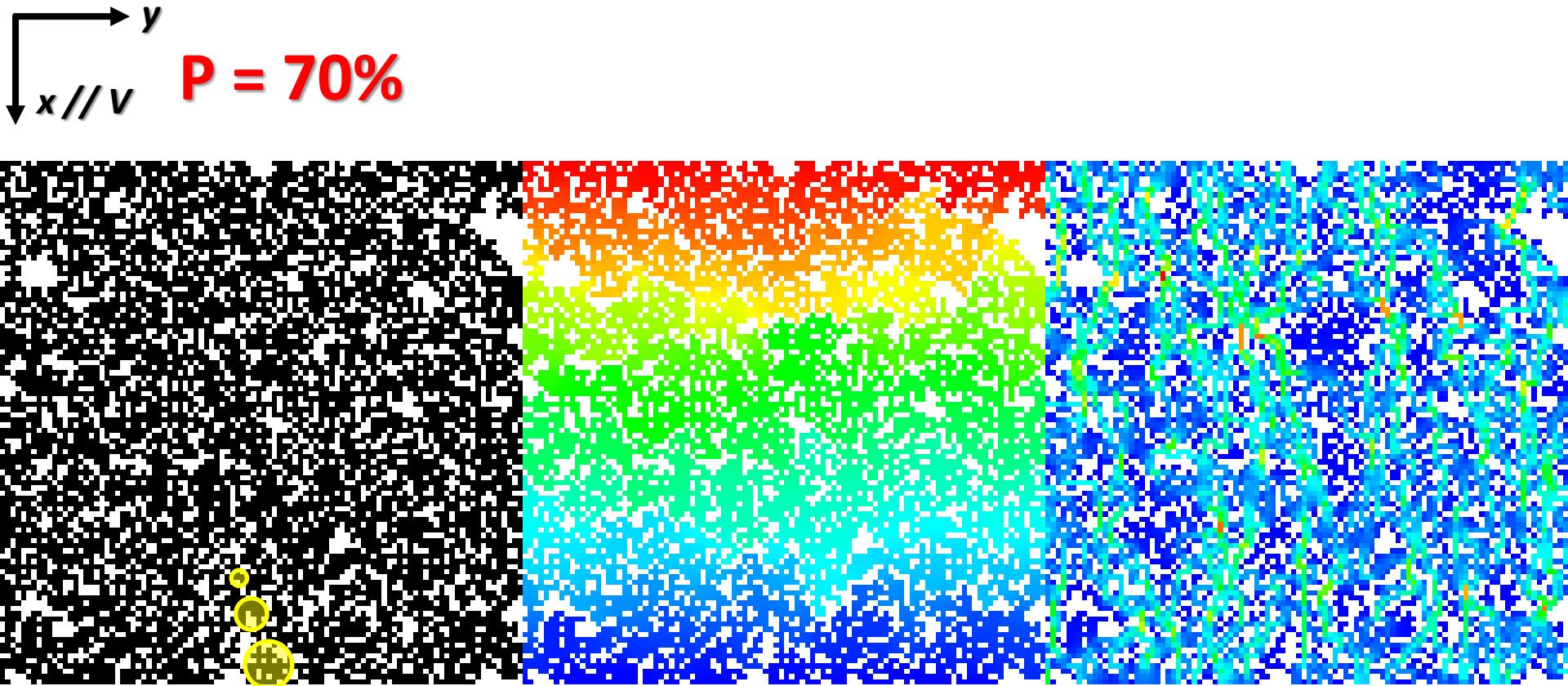
Voltage distribution  
Connectivity: 44.1%

Current distribution

High  
Low

$P = 80\%, 100 \times 100 \times 1$  matrix,  $b=1$

# 2D Normal current



Occupied site distribution

Introducing  
more defects  
(porosity)

Voltage distribution

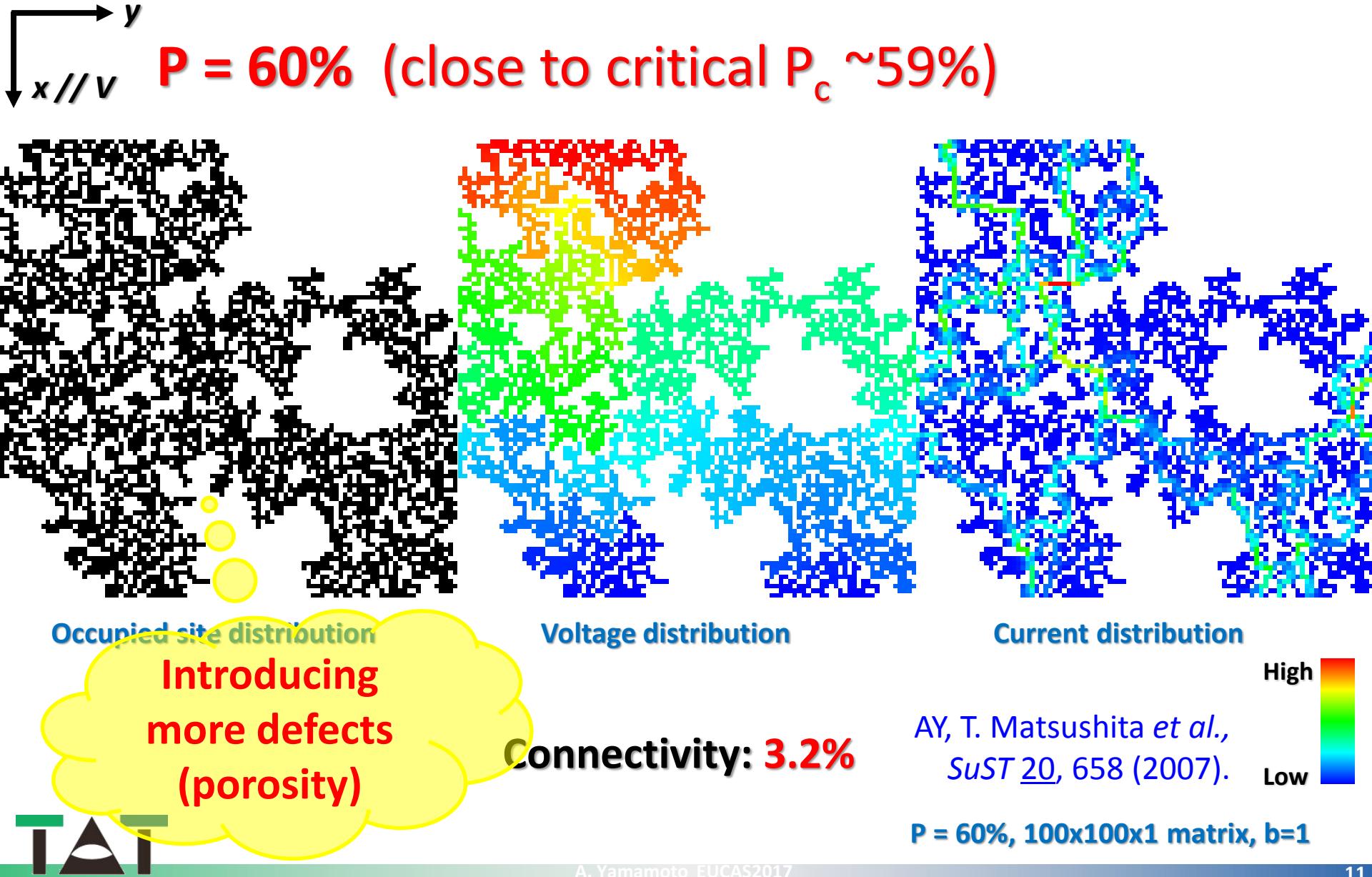
Connectivity: 18.7%

Current distribution

High  
Low

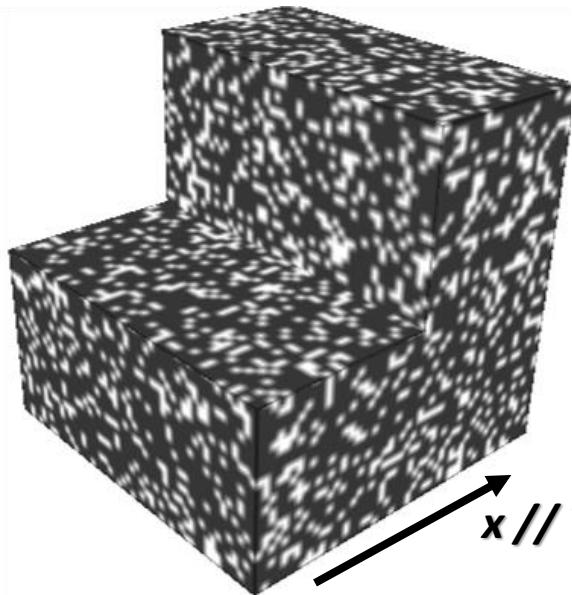
$P = 70\%$ ,  $100 \times 100 \times 1$  matrix,  $b=1$

# 2D Normal current

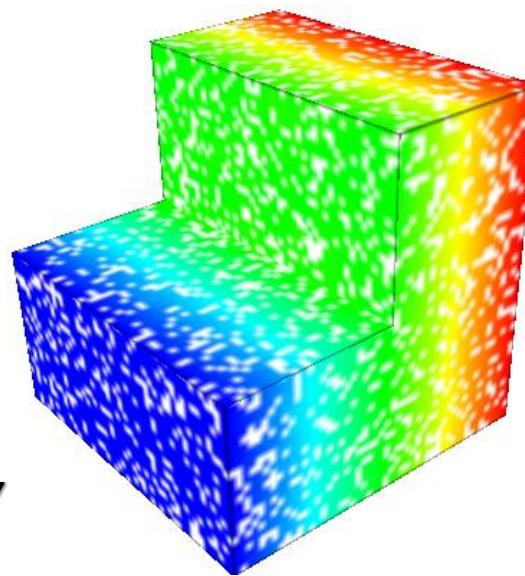


# 3D Normal current

P = 75%

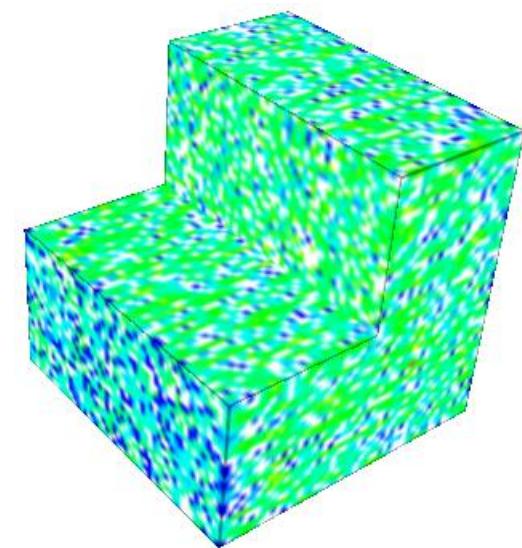


Occupied site distribution

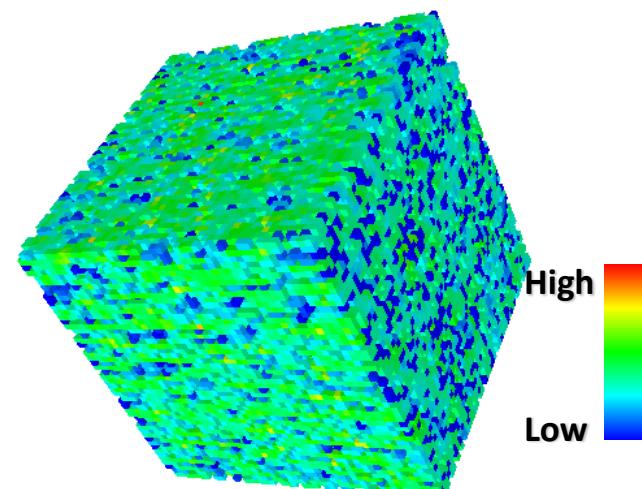
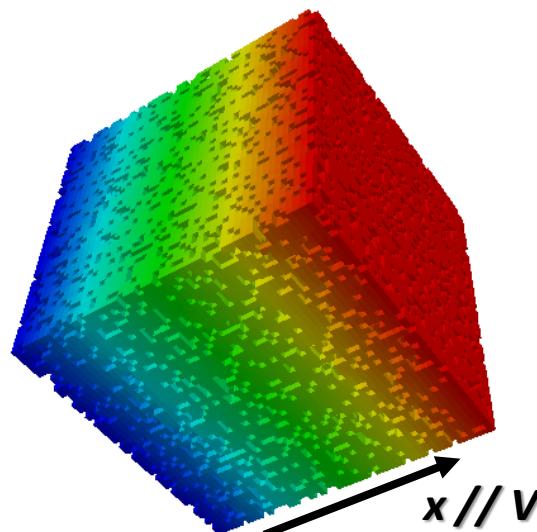
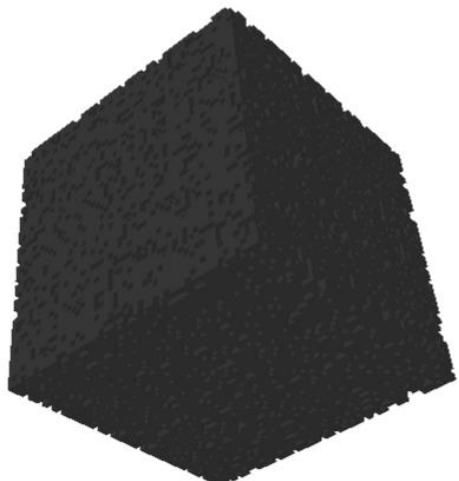


Voltage distribution

Connectivity: 46.3%



Current distribution

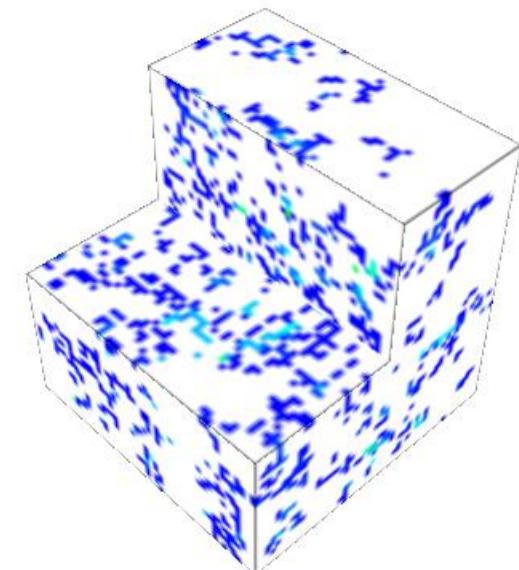
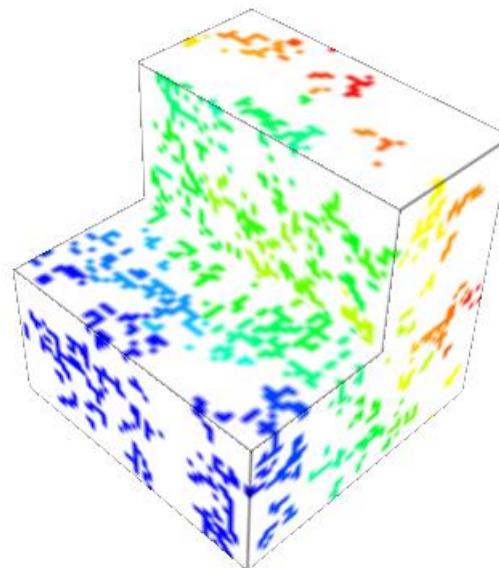
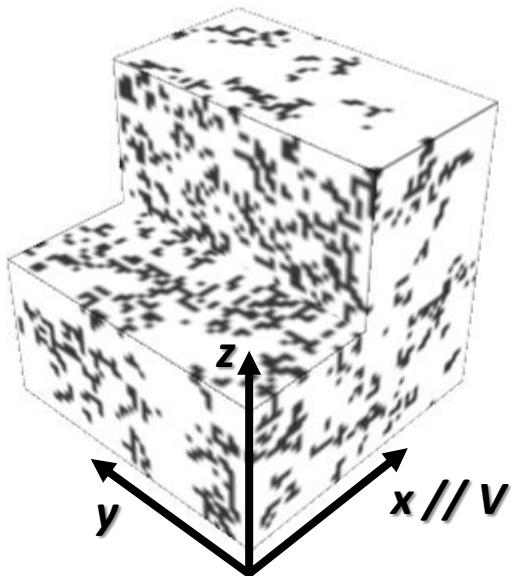


P = 75%, 50x50x50 matrix, b=1

# 3D Normal current

P = 35%

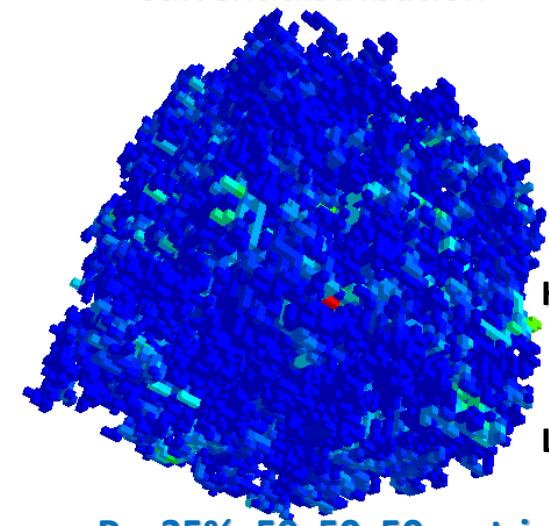
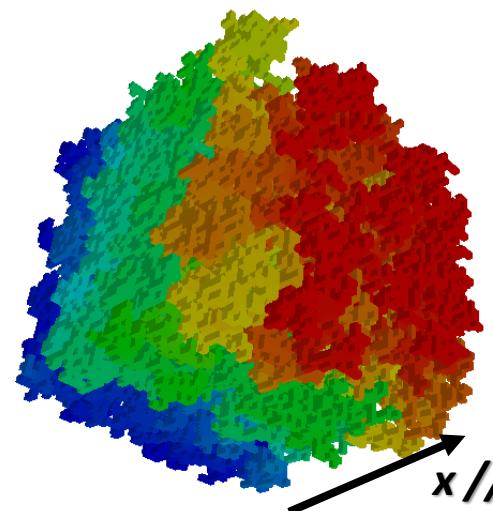
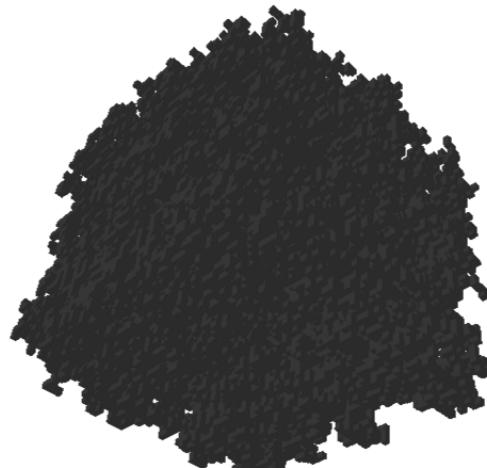
Connectivity: 0.7%



Occupied site distribution

Voltage distribution

Current distribution



High  
Low

P = 35%, 50x50x50 matrix, b=1

# Super current

# Approach for super current

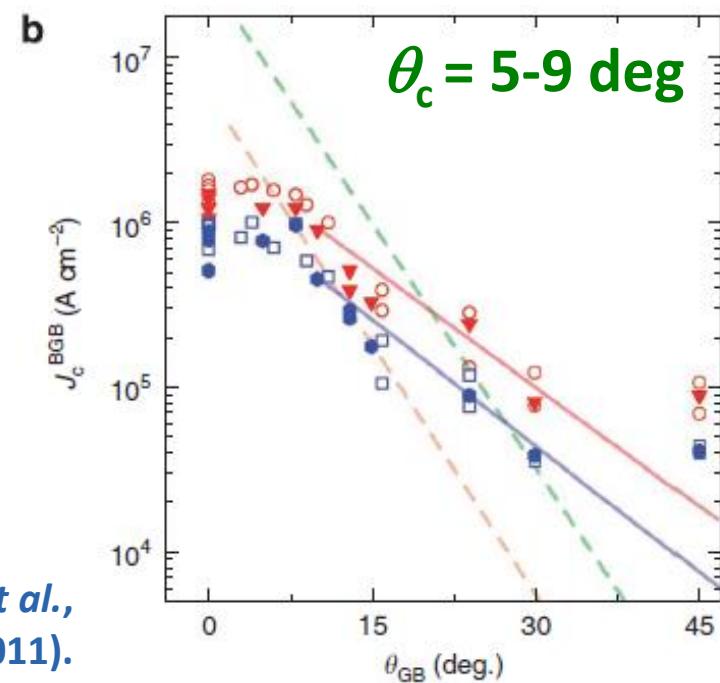
- Consider **current** only
- Each bond current: Consider **weak-link** due to GB tilt angle between neighboring sites

- 1 Assumption!

$$\frac{I_c(\theta_{GB})}{I_0} = \exp\left(-\frac{\theta_{GB}}{\theta_c}\right)$$

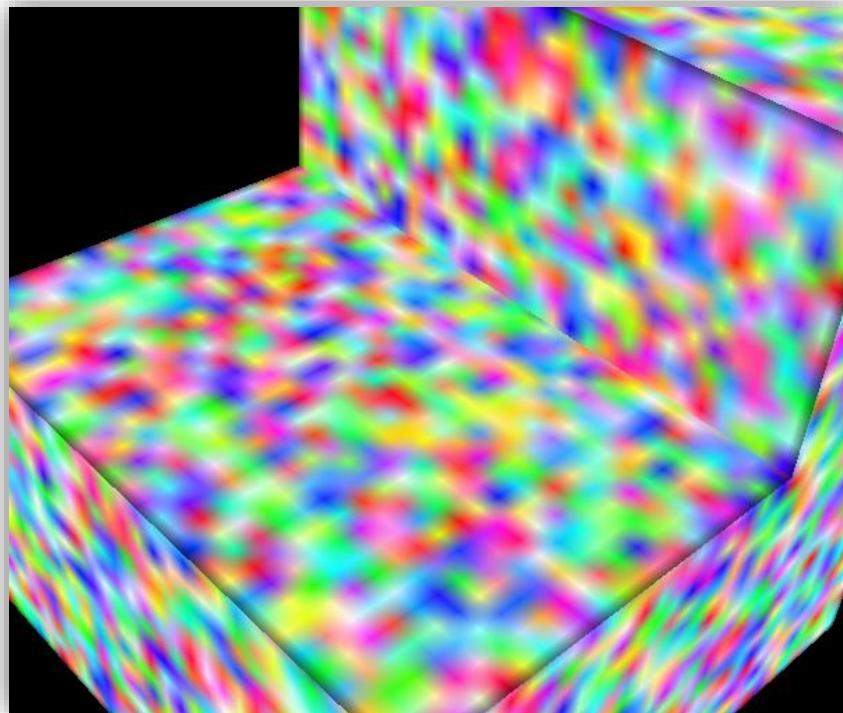
- Conductivity of the system:  
⇒ Maximum flow problem

T. Katase, H. Hosono *et al.*,  
*Nature Commun.* **2**, 409 (2011).

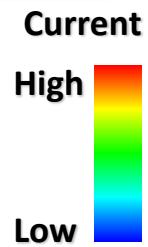
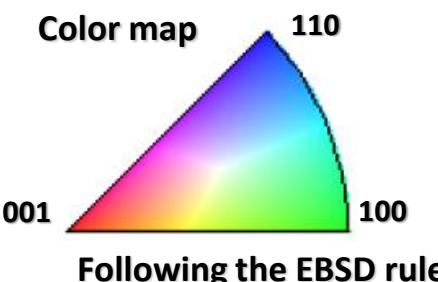
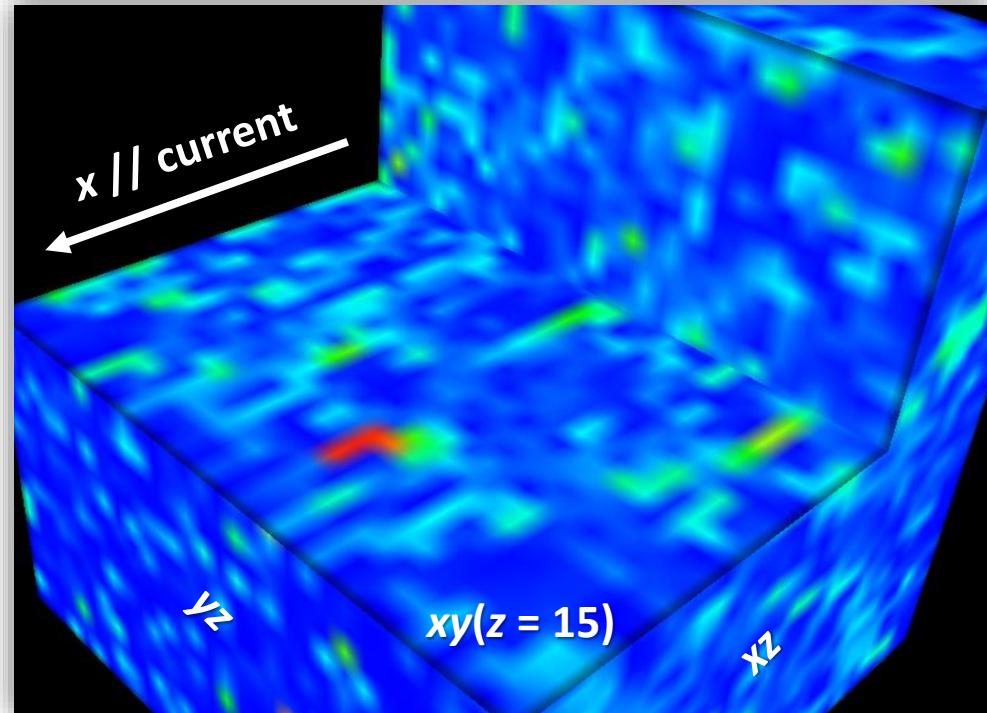


# Transport super current distribution for randomly oriented sites with weak-link effect

Grain orientation map



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

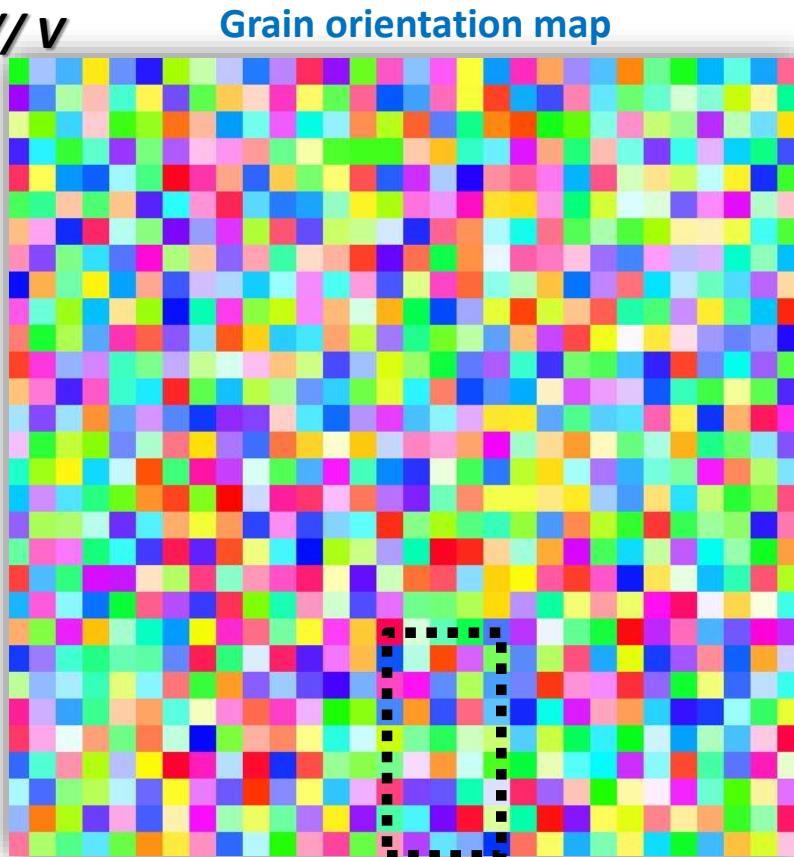


P = 100%, 30x30x30 matrix, b=1, G=1

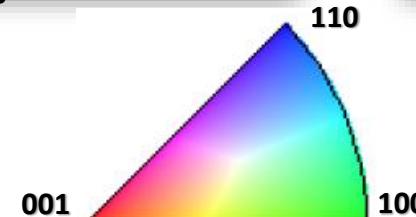
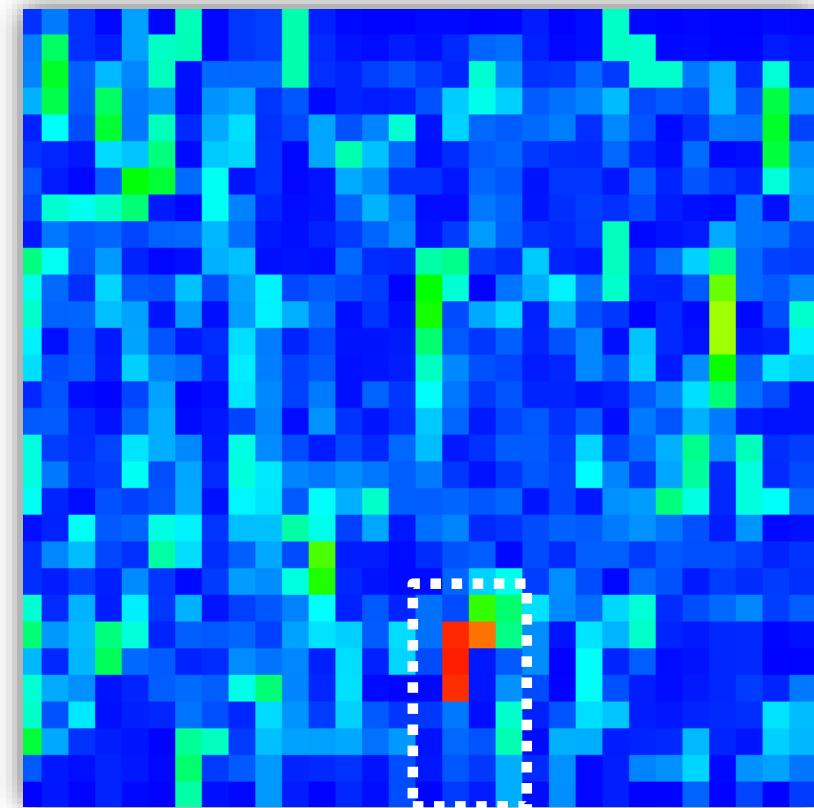
# Transport super current distribution for randomly oriented sites with weak-link effect

$y$   $\theta_c = 9 \text{ deg}$ , 2D plane ( $z = 15$ )

$x // v$

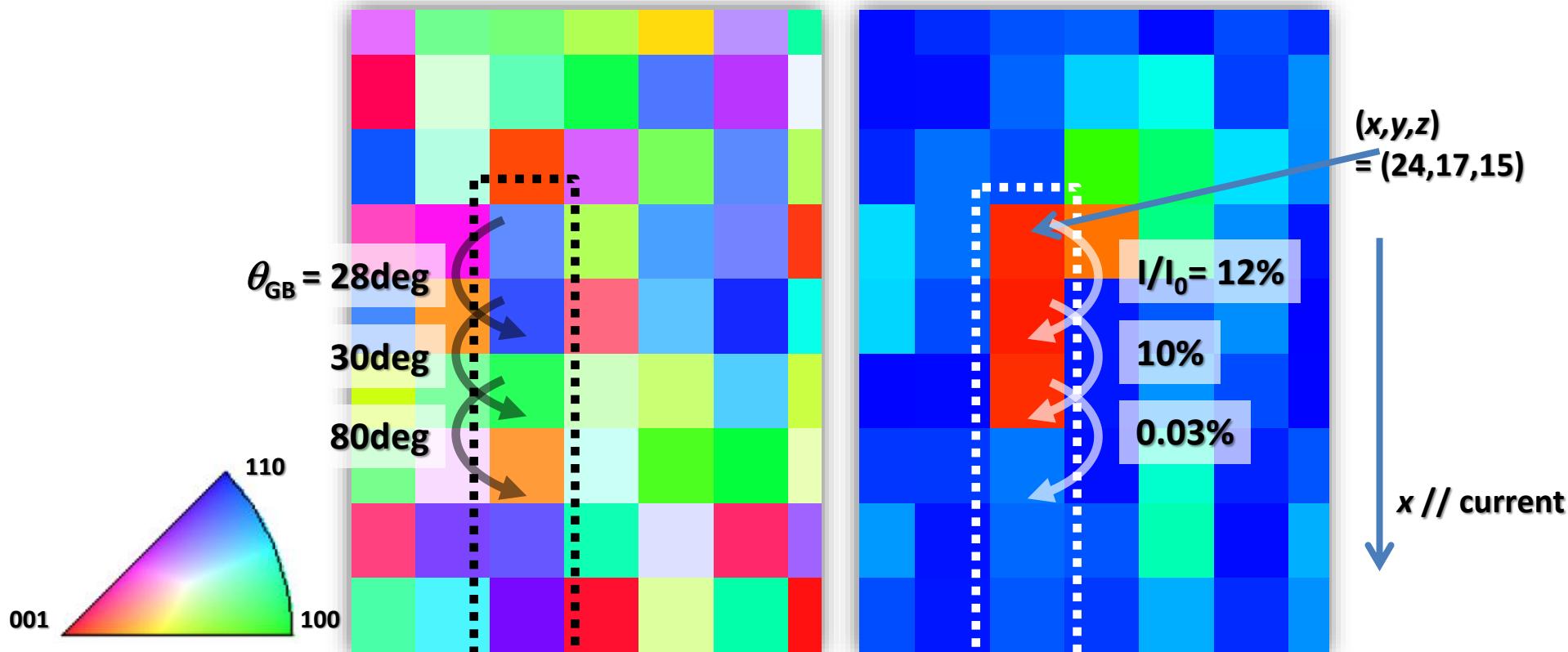


Transport supercurrent distribution



$P = 100\%$ ,  $30 \times 30 \times 30$  matrix,  $b=1$ ,  $G=1$

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

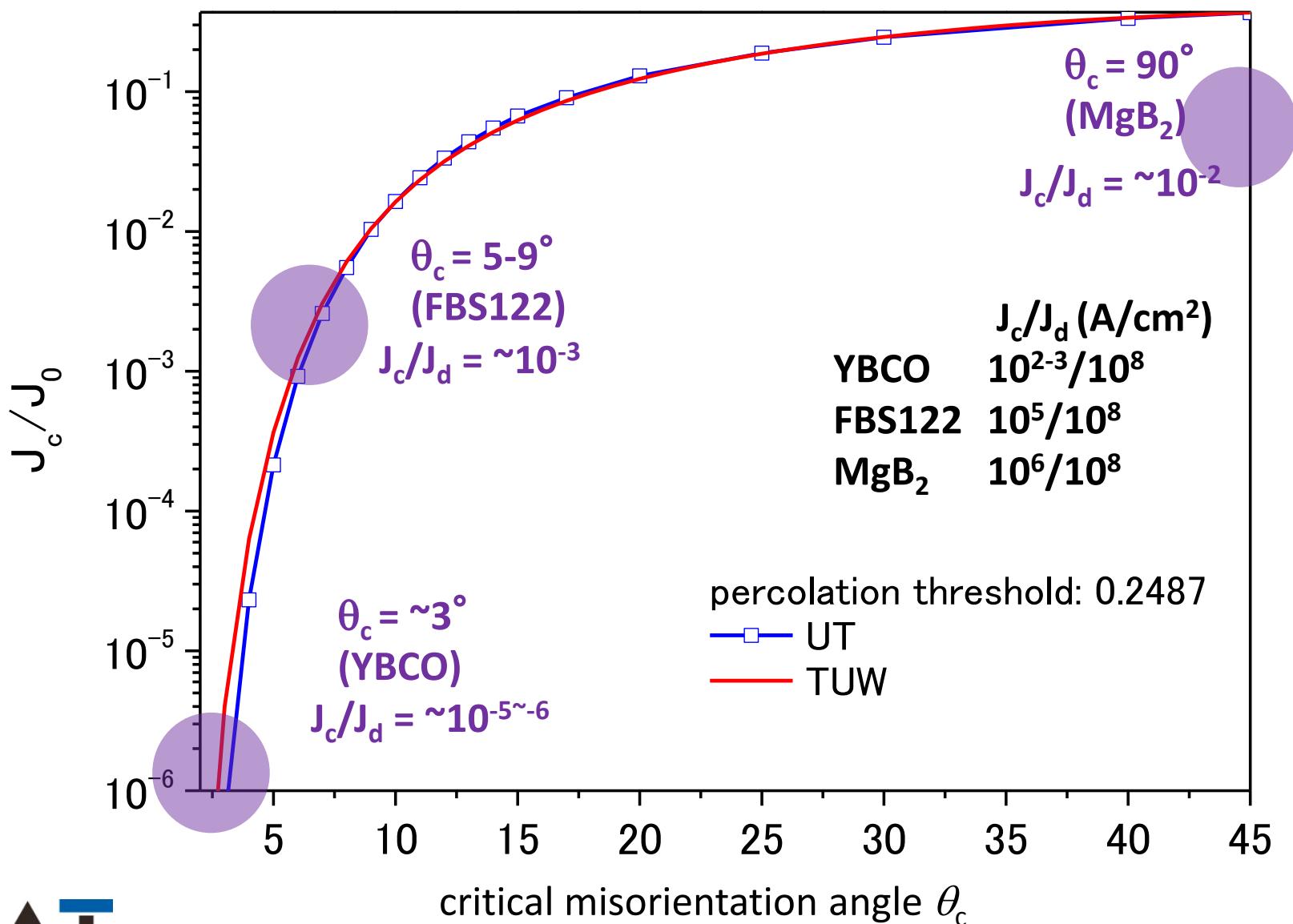


ID <sub>site</sub>	x(30)	y(30)	z(30)	alpha	beta	gamma	current
13103	24	17	15	1.298306	0.180705	0.592797	0.097872
13104	25	17	15	0.240939	0.210582	0.551627	0.098810
13105	26	17	15	0.12379	0.014316	0.123401	0.097164
13106	27	17	15	1.972353	0.454205	0.847588	0.011864
13107	28	17	15	0.836958	0.292742	0.390473	0.010337
13108	29	17	15	1.486906	0.246054	0.618583	0.008584
13109	30	17	15	0.158202	0.362056	0.400881	0.005680

Macroscopic conductivity is suppressed to only 0.6% due to weak-link with  $\theta_c = 9\text{deg}$ .

ID <sub>bond</sub>	site_ID0	site_ID1	thetaGBab	thetaGBC	thetaGB	Maximum current
39803	13103	13104	5.377839	27.93095	27.93095	0.122036
39806	13104	13105	20.98219	7.32811	29.98219	0.097164
39809	13105	13106	16.16561	80.84391	80.84391	0.000341
39812	13106	13107	29.06341	47.57837	47.57837	0.013753
39815	13107	13108	8.403766	59.01759	59.01759	0.003858
39818	13108	13109	20.88033	55.53676	55.53676	0.005680

# Influence of critical misorientation angle $\theta_c$



# Conclusion

- Simple model could explain large difference of current transport among materials (cuprates, FBS, MgB<sub>2</sub>)
- 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

Supported by MEXT Elements Strategy Initiative to Form Core Research Center and by JSPS KAKENHI Grant No. JP15H05519, JST-PRESTO & FP7-EU #283204 “SUPER-IRON”  
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