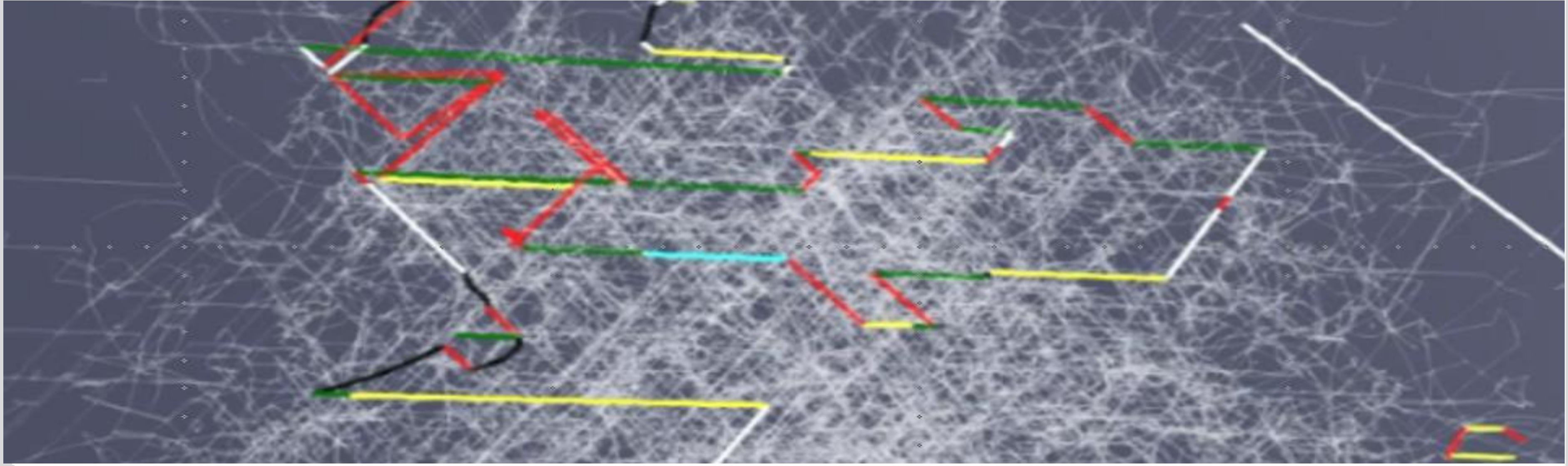
Exploring dislocation networks for continuum modelling

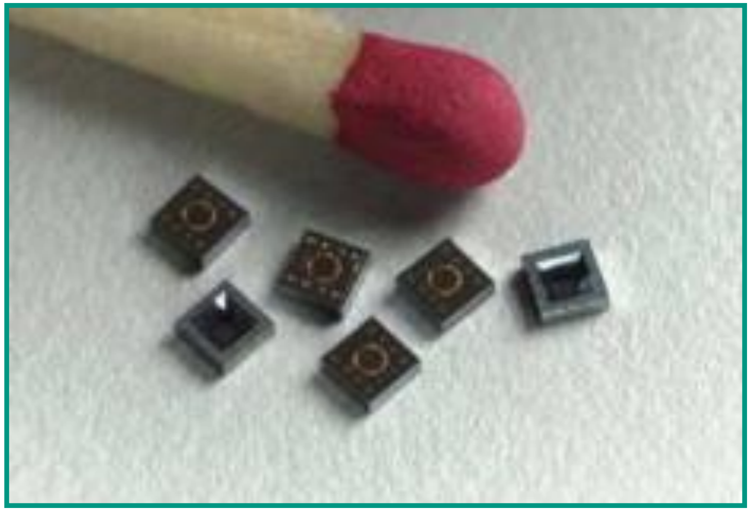
Katrin Schulz

Institute for Applied Materials – Reliability and Microstructure (IAM-ZM), KIT, Karlsruhe



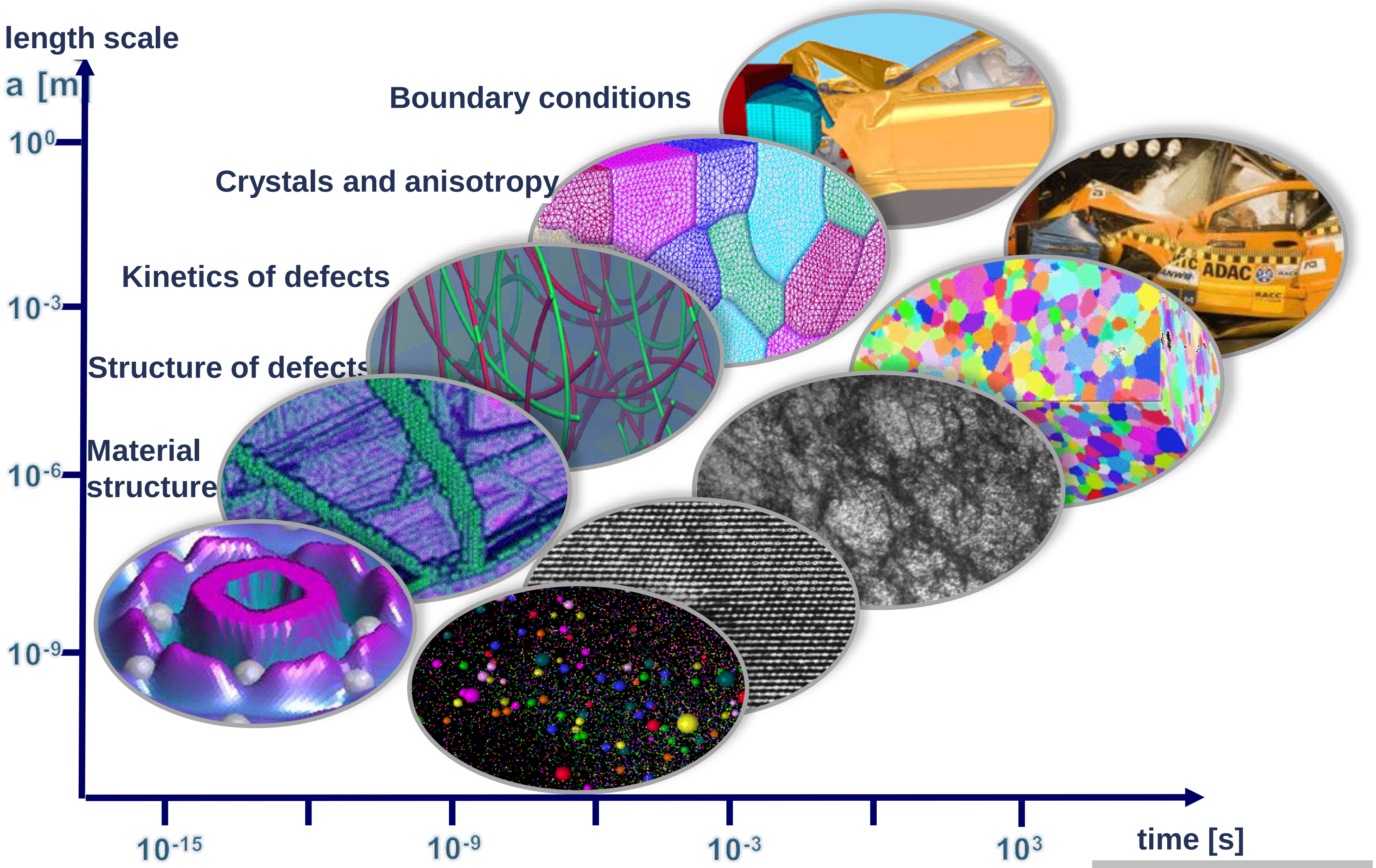
Challenge in material modelling

Is COPPER = copper ?



- ✓ centimeter-sized specimen can be used to predict meter-sized components
- ϟ materials' behavior in small dimensions is not scale-invariant anymore

Challenge in material modelling



Boundary conditions

Crystals and anisotropy

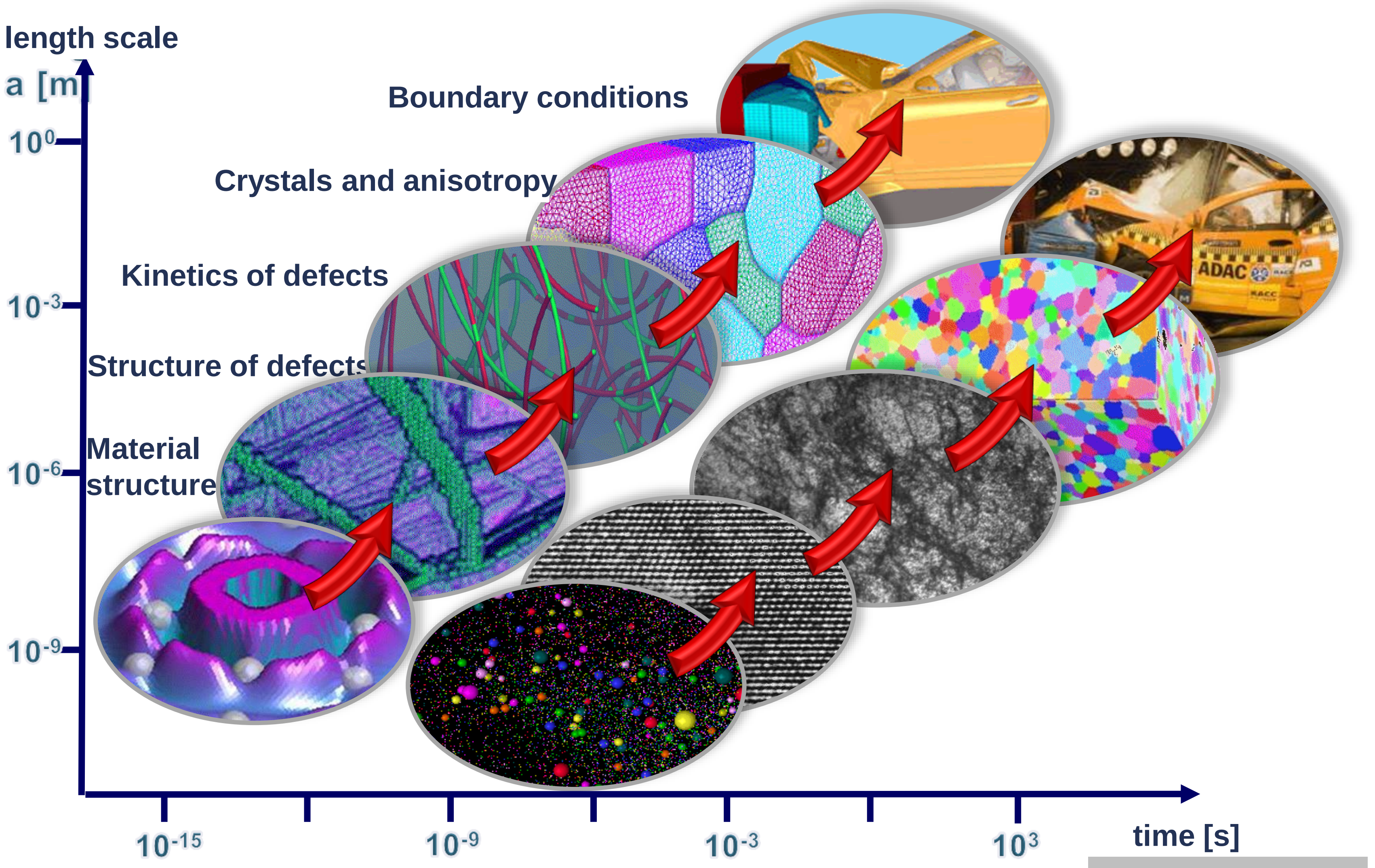
Kinetics of defects

Structure of defects

Material structure

Source of picutres: MPI

Challenge in material modelling



Boundary conditions

Crystals and anisotropy

Kinetics of defects

Structure of defects

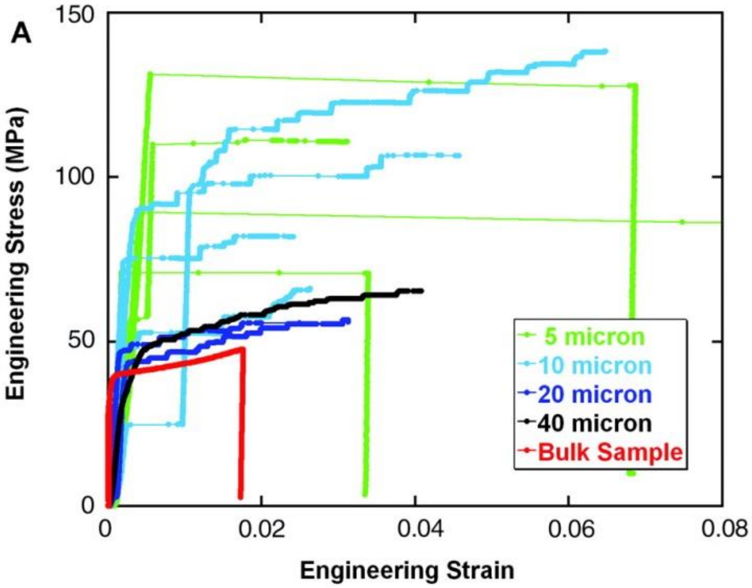
Material structure

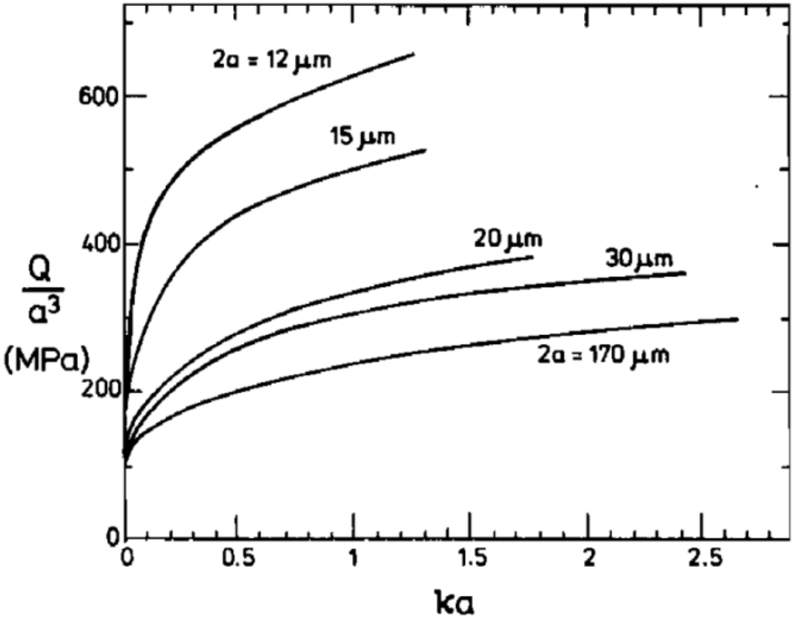
Source of picutres: MPI

Challenge in material modelling

Singel crystalline micro pillar compression test
(Uchic et al. , Science, 2004)

Torsional response of polycrystalline copper wires
(Felck et al. Acta Metall. 42, 1994)

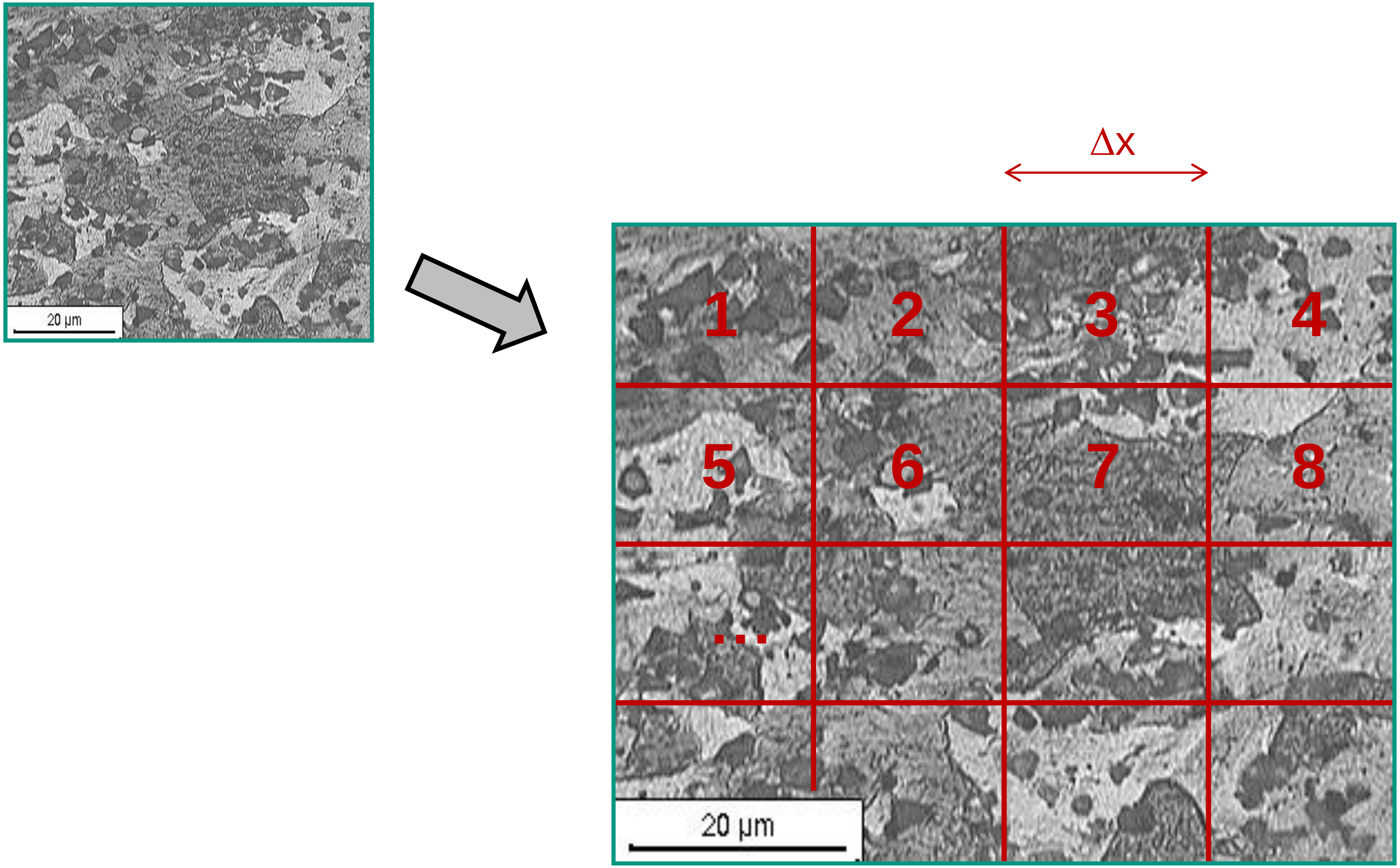




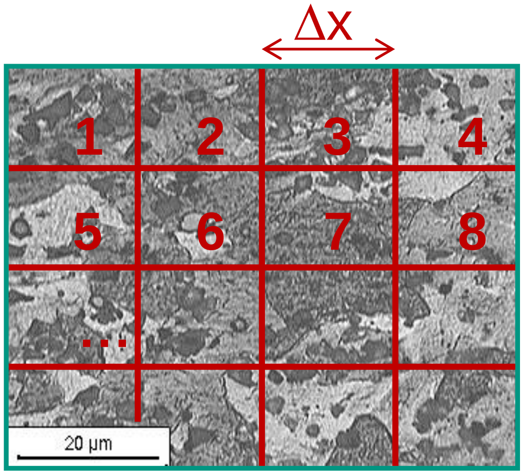
Size effect „Smaller is Stronger“

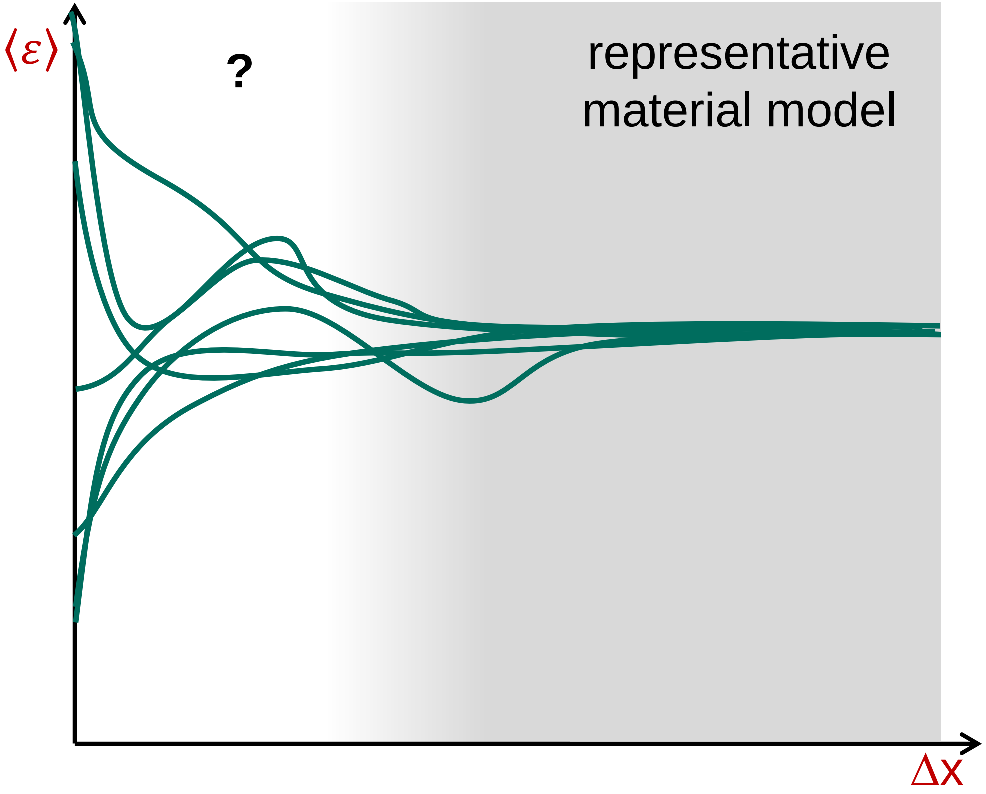
Hall-Petch effect

Challenge in material modelling



Challenge in material modelling



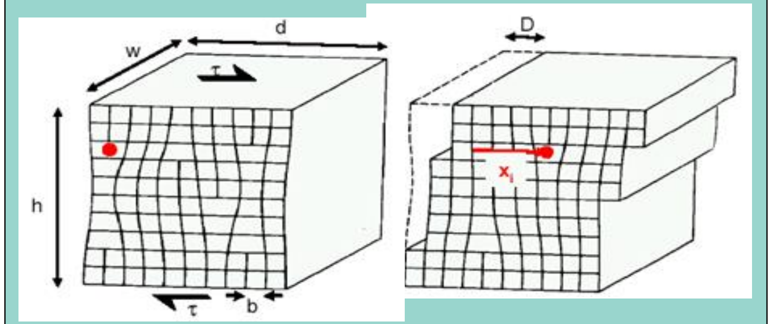


⇨ Is a material model able to represent the underlying microstructure of a material?
Where is transition between length scales?
What are the parameters for a material model on a certain scale?

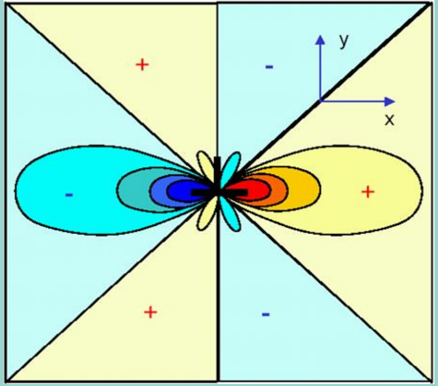
Dislocation Microstructures

Physics

Dislocations cause plasticity

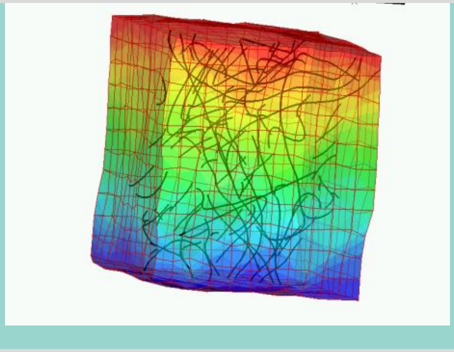


Dislocation stress field

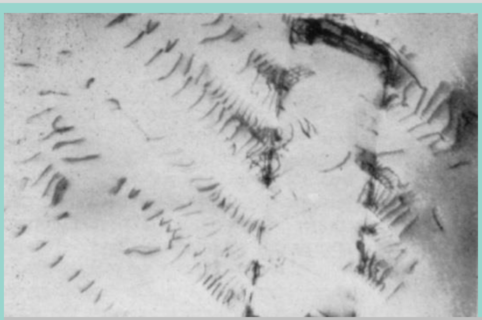


Microstructural behaviour

Dislocations interaction dictates constitutive behaviour



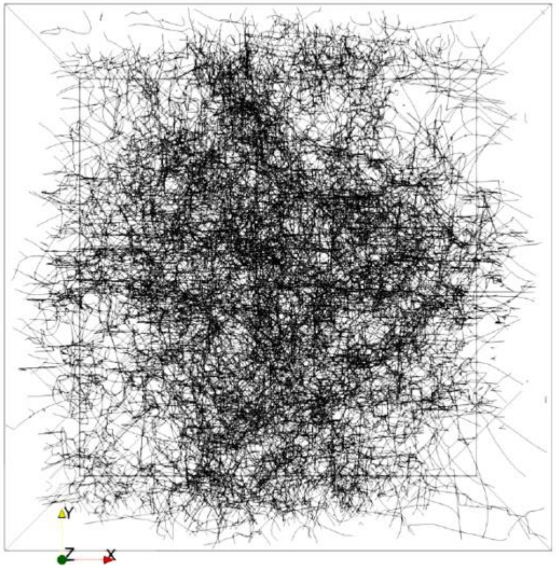
Dislocation pile-up in copper-4.5% aluminium alloy



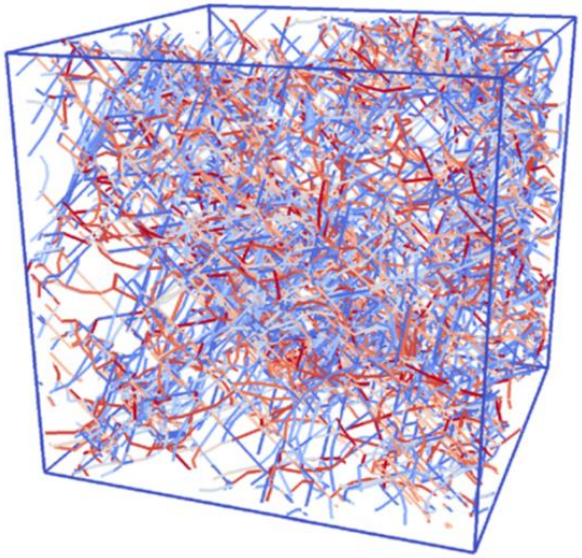
Swann et al., *Journal of the Institute of Metals*, 90(4) (1961).

Dislocation Network Structures

TEM (Zhang et al., Phil.Mag. 2003)



DDD (Stricker et al., JMPS, 2018)



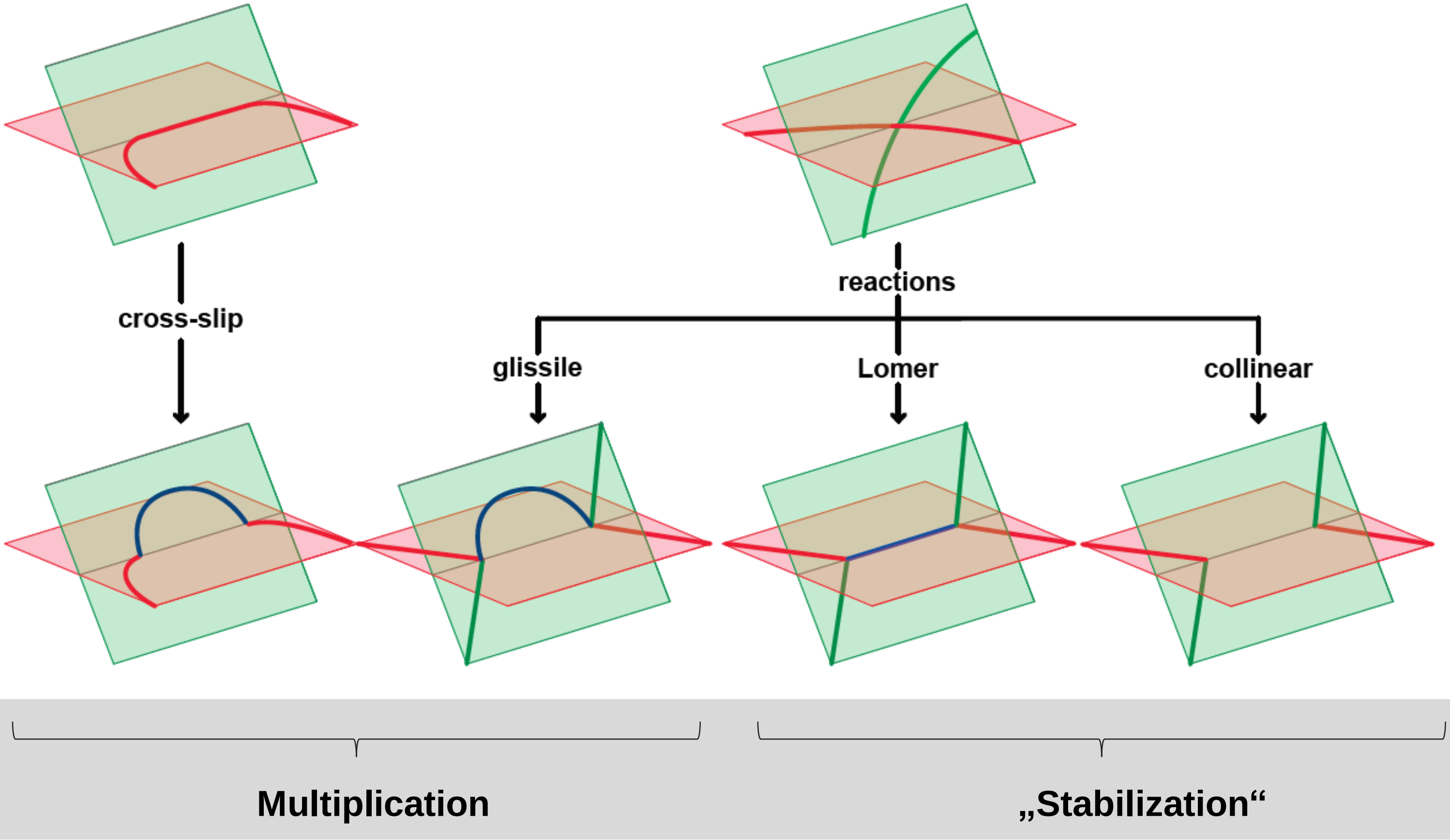
DDD (Sills et al., Phys. Rev. lett., 2018)

Competing mechanisms:

i. Generation of new dislocations (line length), which allow for further plasticity
ii. Limitation of the dislocation mobility, which limit the plasticity generated by dislocation motion

Dislocation Network Structures

Modeling dislocation reactions and cross-slip



Modelling Dislocation Network Structures

- All reactions considered with the same formulation

$$\partial_t \rho_{\mathrm{react}} = C_{\mathrm{react}} \left(\rho^{\xi}_{\mathrm{M}} |v^{\xi}| \sqrt{\rho^{\zeta}_{\mathrm{M}} + \rho^{\zeta}_{\mathrm{S}}} + \rho^{\zeta}_{\mathrm{M}} |v^{\zeta}| \sqrt{\rho^{\xi}_{\mathrm{M}} + \rho^{\xi}_{\mathrm{S}}} \right) \qquad \text{with } \xi, \zeta = r', r'' \text{ and } \xi \neq \zeta$$

- Resulting full set of evolution equations:

$$\partial_t \rho^{\xi}_{\mathrm{M}} = -\nabla \cdot \left(v^{\xi} \, \boldsymbol{\kappa}^{\xi}_{\perp} \right) + v^{\xi} q^{\xi} + \partial_t \bar{\rho}^{\xi}_{\mathrm{M}} + \partial_t \hat{\rho}^{\xi}_{\mathrm{M}} + \partial_t \bar{\rho}^{\xi}_{\mathrm{M,Lomer}} + \partial_t \rho^{\xi}_{\mathrm{M,react}} + \partial_t \rho^{\xi}_{\mathrm{M,cross}}$$

$$\partial_t \boldsymbol{\kappa}^{\xi} = \nabla \times \left(\rho^{\xi}_{\mathrm{M}} v^{\xi} \mathbf{m}^{\xi} \right) + \partial_t \bar{\boldsymbol{\kappa}}^{\xi}_{\mathrm{cross}}$$

$$\partial_t \rho^{\xi}_{\mathrm{net}} = 0.5 \partial_t \rho^{\xi}_{\mathrm{Lomer}} - \partial_t \bar{\rho}^{\xi}_{\mathrm{M,Lomer}} + \partial_t \hat{\rho}^{\xi}_{\mathrm{net}} + \partial_t \rho^{\xi}_{\mathrm{S,react}}$$

$$\partial_t q^{\xi} = -\nabla \cdot \left(\frac{q^{\xi}}{\rho^{\xi}_{\mathrm{M}}} \boldsymbol{\kappa}^{\xi}_{\perp} v^{\xi} + \mathbf{A}^{\xi} \nabla v^{\xi} \right) + \partial_t \bar{q}^{\xi} + \partial_t q^{\xi}_{\mathrm{react}} + \partial_t q^{\xi}_{\mathrm{cross}}$$

🟥 Decrease of ρ^{ξ}

🟩 Increase of ρ^{ξ}

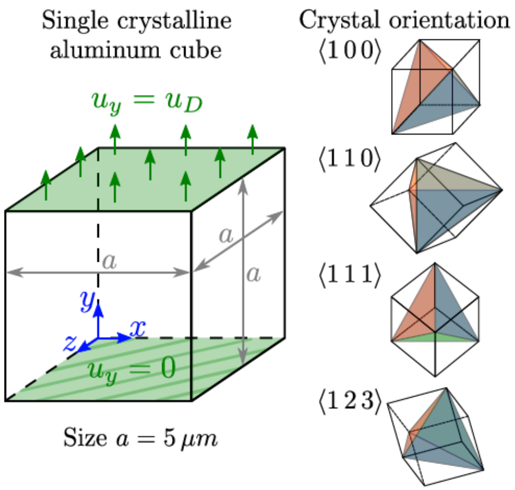
- Mobility law

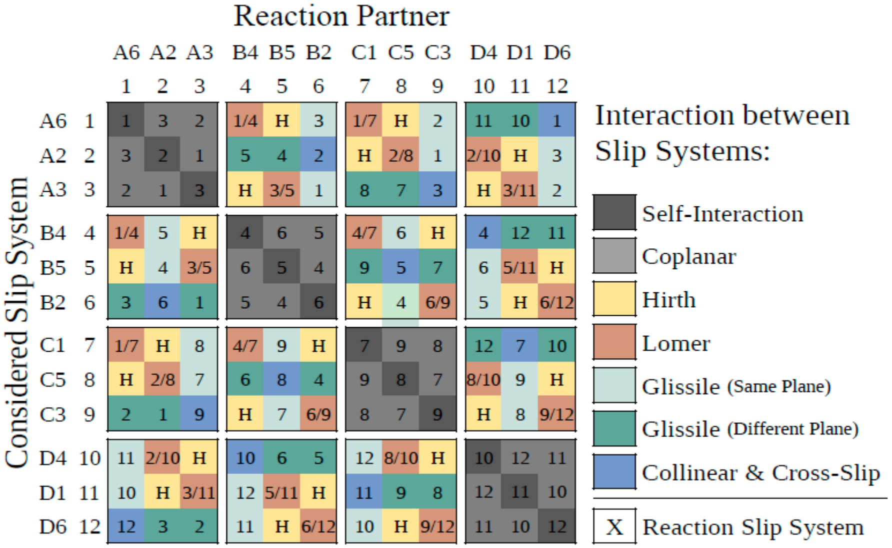
$$\tau^{\xi}_{\mathrm{fl,mat}} = Gb \sqrt{ \sum_{\zeta} \left(a^{\xi\zeta} \left(\rho^{\zeta}_{\mathrm{M}} + \rho^{\zeta}_{\mathrm{S}} \right) + \bar{a}_{\mathrm{Lomer}} \rho^{\zeta}_{\mathrm{Lomer}} \right) }$$

↳

$$v^{\xi} = \begin{cases} \frac{b}{B} \left(|\tau^{\xi}| - \tau^{\xi}_{\mathrm{fl,mat}} \right) \, \mathrm{sign} \left(\tau^{\xi} \right) & \text{if } |\tau^{\xi}| > \tau^{\xi}_{\mathrm{fl,mat}} \\ 0 & \text{if } |\tau^{\xi}| \leq \tau^{\xi}_{\mathrm{fl,mat}} \end{cases}$$

Modelling Dislocation Network Structures





Reaction Partner

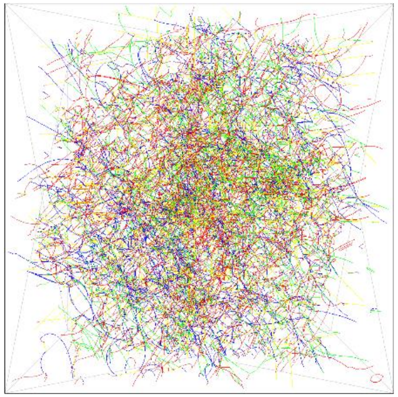
Considered Slip System

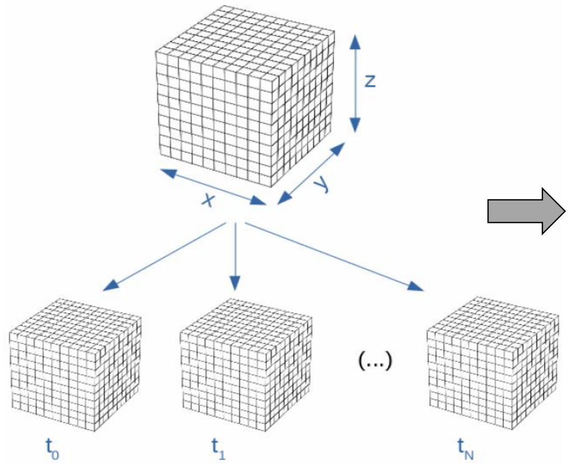
		A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
		1	2	3	4	5	6	7	8	9	10	11	12
A6	1	1	3	2	1/4	H	3	1/7	H	2	11	10	1
A2	2	3	2	1	5	4	2	H	2/8	1	2/10	H	3
A3	3	2	1	3	H	3/5	1	8	7	3	H	3/11	2
B4	4	1/4	5	H	4	6	5	4/7	6	H	4	12	11
B5	5	H	4	3/5	6	5	4	9	5	7	6	5/11	H
B2	6	3	6	1	5	4	6	H	4	6/9	5	H	6/12
C1	7	1/7	H	8	4/7	9	H	7	9	8	12	7	10
C5	8	H	2/8	7	6	8	4	9	8	7	8/10	9	H
C3	9	2	1	9	H	7	6/9	8	7	9	H	8	9/12
D4	10	11	2/10	H	10	6	5	12	8/10	H	10	12	11
D1	11	10	H	3/11	12	5/11	H	11	9	8	12	11	10
D6	12	12	3	2	11	H	6/12	10	H	9/12	11	10	12

Interaction between Slip Systems:

■ Self-Interaction
■ Coplanar
■ Hirth
■ Lomer
■ Glissile (Same Plane)
■ Glissile (Different Plane)
■ Collinear & Cross-Slip

X Reaction Slip System

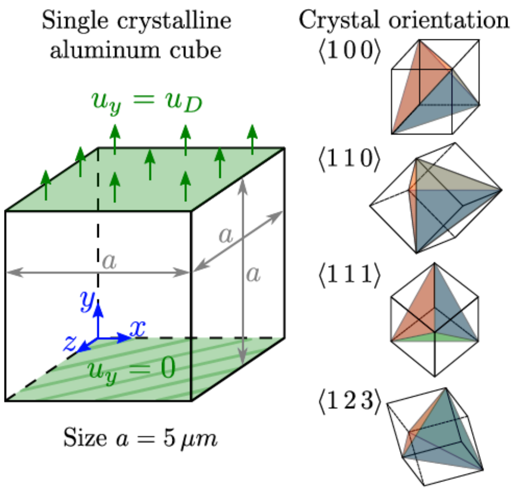


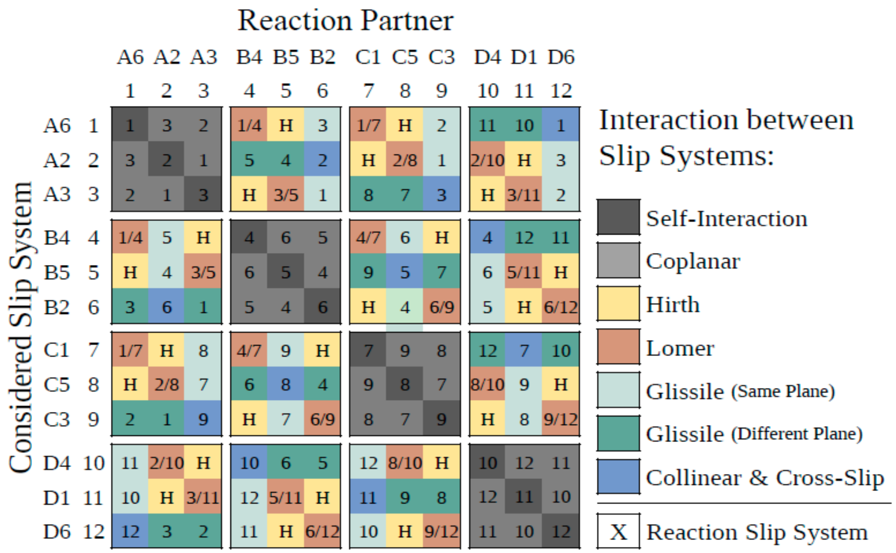


→ Data driven approach

- Observation of dislocation networks by a voxel-wise approach
- Measuring dislocation densities and reaction densities

Modelling Dislocation Network Structures





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A2	2	3	2	1	5	4	2	H	2/8	1	2/10	H	3
A3	3	2	1	3	H	3/5	1	8	7	3	H	3/11	2
B4	4	1/4	5	H	4	6	5	4/7	6	H	4	12	11
B5	5	H	4	3/5	6	5	4	9	5	7	6	5/11	H
B2	6	3	6	1	5	4	6	H	4	6/9	5	H	6/12
C1	7	1/7	H	8	4/7	9	H	7	9	8	12	7	10
C5	8	H	2/8	7	6	8	4	9	8	7	8/10	9	H
C3	9	2	1	9	H	7	6/9	8	7	9	H	8	9/12
D4	10	11	2/10	H	10	6	5	12	8/10	H	10	12	11
D1	11	10	H	3/11	12	5/11	H	11	9	8	12	11	10
D6	12	12	3	2	11	H	6/12	10	H	9/12	11	10	12

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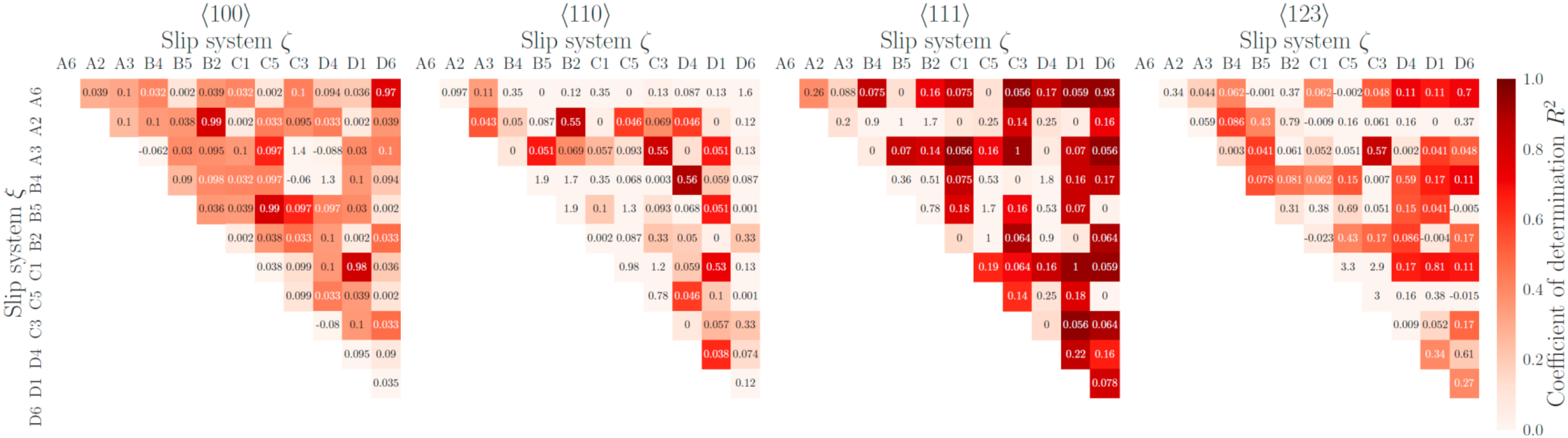
X Reaction Slip System



⟨100⟩ Slip system ζ

	A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
A6		0.039	0.1	0.032	0.002	0.039	0.032	0.002	0.1	0.094	0.036	0.97
A2			0.1	0.1	0.038	0.99	0.002	0.033	0.095	0.033	0.002	0.039
A3				-0.062	0.03	0.095	0.1	0.097	1.4	-0.088	0.03	0.1
B4					0.09	0.098	0.032	0.097	-0.06	1.3	0.1	0.094
B5						0.036	0.039	0.99	0.097	0.097	0.03	0.002
B2							0.002	0.038	0.033	0.1	0.002	0.033
C1								0.038	0.099	0.1	0.98	0.036
C5									0.099	0.033	0.039	0.002
C3										-0.08	0.1	0.033
D4											0.095	0.09
D1												0.035
D6												

⟨110⟩ Slip system ζ

	A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
A6		0.097	0.11	0.35	0	0.12	0.35	0	0.13	0.087	0.13	1.6
A2			0.043	0.05	0.087	0.55	0	0.046	0.069	0.046	0	0.12
A3				0	0.051	0.069	0.057	0.093	0.55	0	0.051	0.13
B4					1.9	1.7	0.35	0.068	0.003	0.56	0.059	0.087
B5						1.9	0.1	1.3	0.093	0.068	0.051	0.001
B2							0.002	0.087	0.33	0.05	0	0.33
C1								0.98	1.2	0.059	0.53	0.13
C5									0.78	0.046	0.1	0.001
C3										0	0.057	0.33
D4											0.038	0.074
D1												0.12
D6												

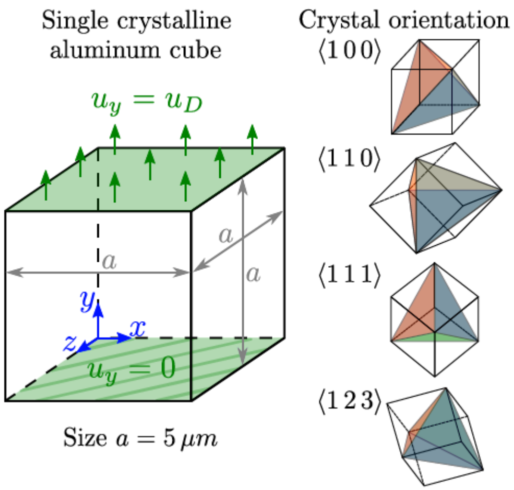
⟨111⟩ Slip system ζ

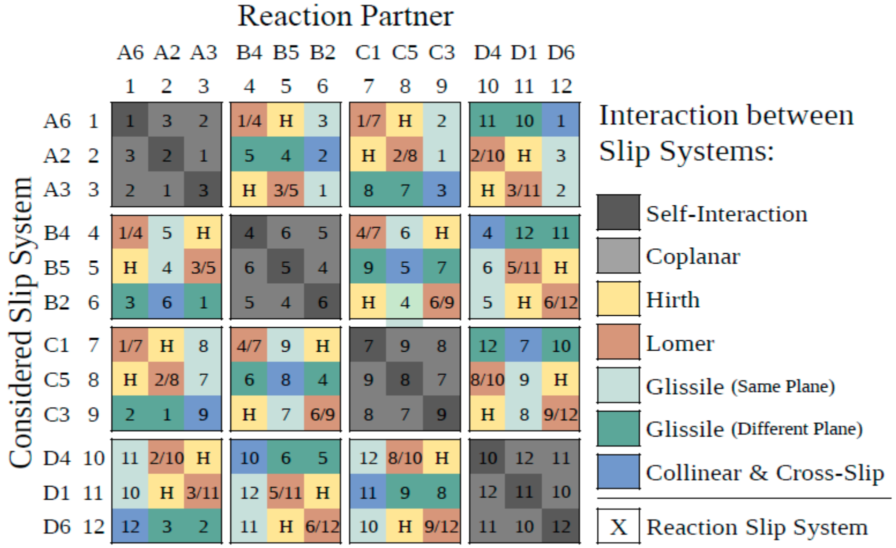
	A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
A6		0.26	0.088	0.075	0	0.16	0.075	0	0.056	0.17	0.059	0.93
A2			0.2	0.9	1	1.7	0	0.25	0.14	0.25	0	0.16
A3				0	0.07	0.14	0.056	0.16	1	0	0.07	0.056
B4					0.36	0.51	0.075	0.53	0	1.8	0.16	0.17
B5						0.78	0.18	1.7	0.16	0.53	0.07	0
B2							0	1	0.064	0.9	0	0.064
C1								0.19	0.064	0.16	1	0.059
C5									0.14	0.25	0.18	0
C3										0	0.056	0.064
D4											0.22	0.16
D1												0.078
D6												

⟨123⟩ Slip system ζ

	A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
A6		0.34	0.044	0.062	-0.001	0.37	0.062	-0.002	0.048	0.11	0.11	0.7
A2			0.059	0.086	0.43	0.79	-0.009	0.16	0.061	0.16	0	0.37
A3				0.003	0.041	0.061	0.052	0.051	0.57	0.002	0.041	0.048
B4					0.078	0.081	0.062	0.15	0.007	0.59	0.17	0.11
B5						0.31	0.38	0.69	0.051	0.15	0.041	-0.005
B2							-0.023	0.43	0.17	0.086	-0.004	0.17
C1								3.3	2.9	0.17	0.81	0.11
C5									3	0.16	0.38	-0.015
C3										0.009	0.052	0.17
D4											0.34	0.61
D1												0.27
D6												

Modelling Dislocation Network Structures





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A6	1	1	3	2	1/4	H	3	1/7	H	2	11	10	1
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B4	4	1/4	5	H	4	6	5	4/7	6	H	4	12	11
B5	5	H	4	3/5	6	5	4	9	5	7	6	5/11	H
B2	6	3	6	1	5	4	6	H	4	6/9	5	H	6/12
C1	7	1/7	H	8	4/7	9	H	7	9	8	12	7	10
C5	8	H	2/8	7	6	8	4	9	8	7	8/10	9	H
C3	9	2	1	9	H	7	6/9	8	7	9	H	8	9/12
D4	10	11	2/10	H	10	6	5	12	8/10	H	10	12	11
D1	11	10	H	3/11	12	5/11	H	11	9	8	12	11	10
D6	12	12	3	2	11	H	6/12	10	H	9/12	11	10	12

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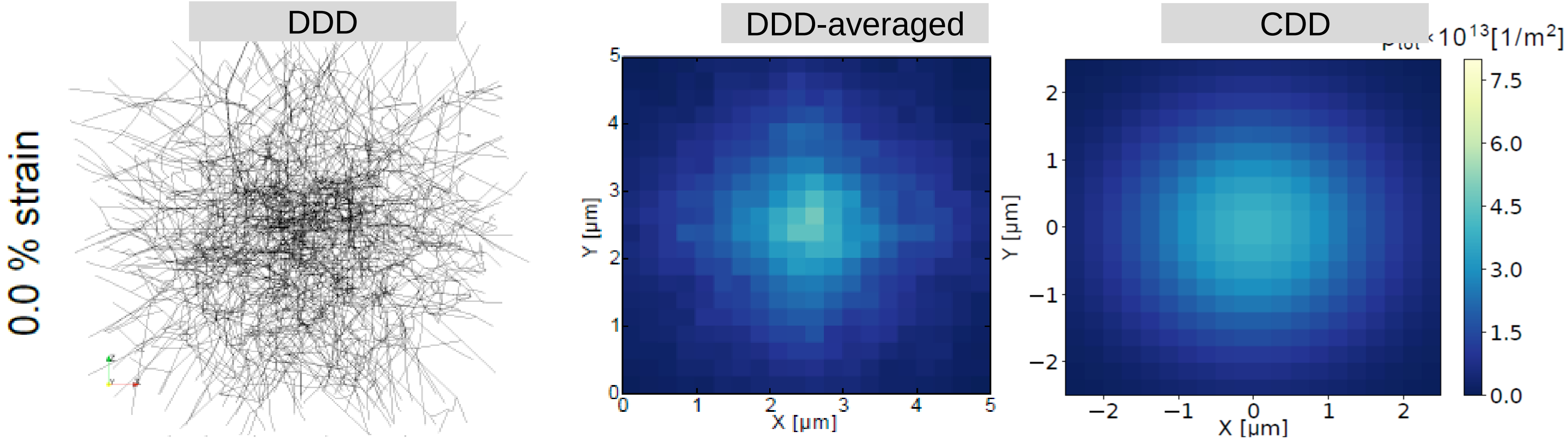
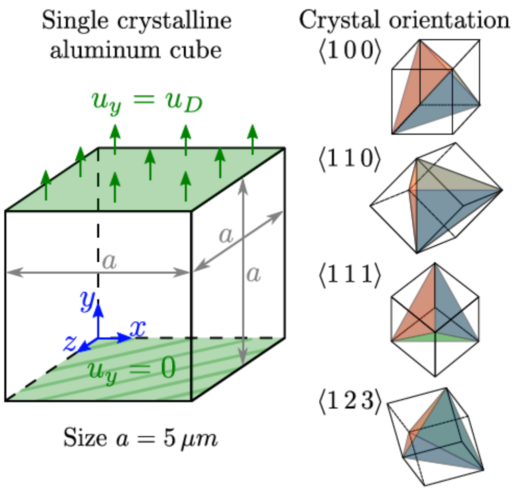
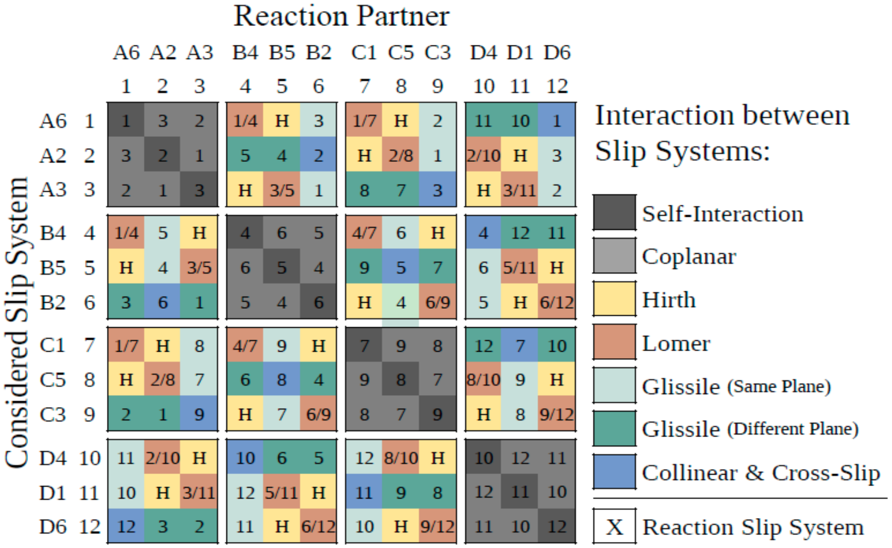
X Reaction Slip System



Modelling Dislocation Network Structures





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A3	3	2	1	3	H	3/5	1	8	7	3	H	3/11	2
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B5	5	H	4	3/5	6	5	4	9	5	7	6	5/11	H
B2	6	3	6	1	5	4	6	H	4	6/9	5	H	6/12
C1	7	1/7	H	8	4/7	9	H	7	9	8	12	7	10
C5	8	H	2/8	7	6	8	4	9	8	7	8/10	9	H
C3	9	2	1	9	H	7	6/9	8	7	9	H	8	9/12
D4	10	11	2/10	H	10	6	5	12	8/10	H	10	12	11
D1	11	10	H	3/11	12	5/11	H	11	9	8	12	11	10
D6	12	12	3	2	11	H	6/12	10	H	9/12	11	10	12

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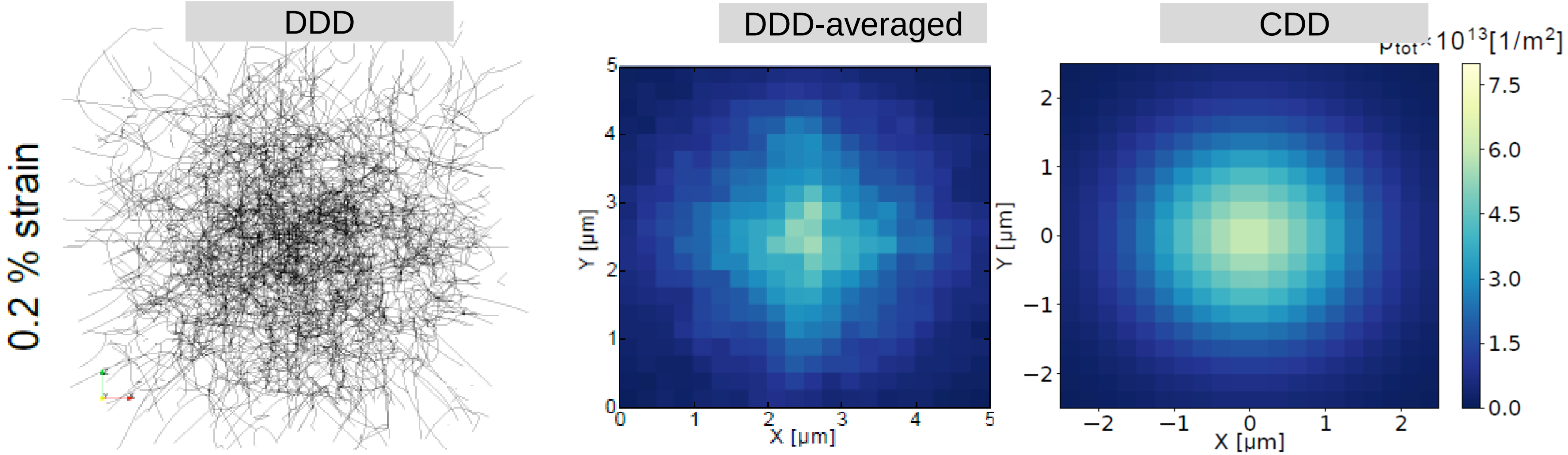
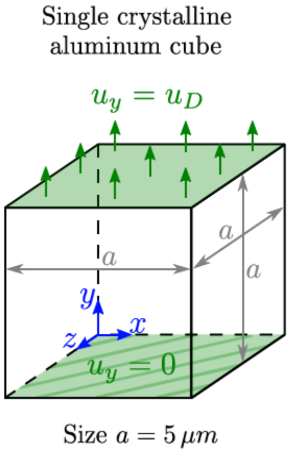
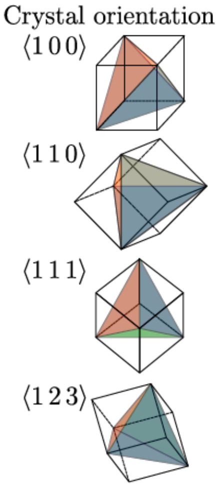
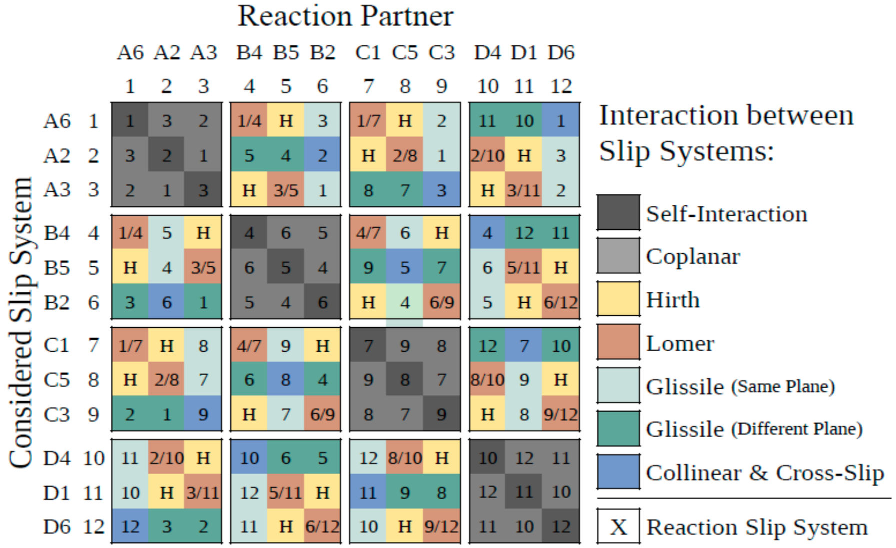


Modelling Dislocation Network Structures







Reaction Partner

Considered Slip System

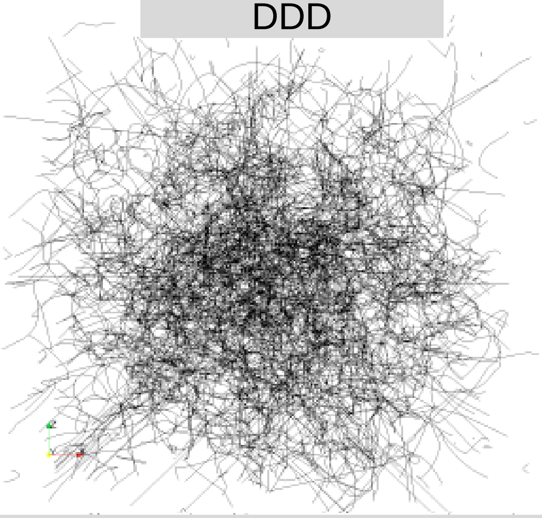
		A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
		1	2	3	4	5	6	7	8	9	10	11	12
A6	1	1	3	2	1/4	H	3	1/7	H	2	11	10	1
A2	2	3	2	1	5	4	2	H	2/8	1	2/10	H	3
A3	3	2	1	3	H	3/5	1	8	7	3	H	3/11	2
B4	4	1/4	5	H	4	6	5	4/7	6	H	4	12	11
B5	5	H	4	3/5	6	5	4	9	5	7	6	5/11	H
B2	6	3	6	1	5	4	6	H	4	6/9	5	H	6/12
C1	7	1/7	H	8	4/7	9	H	7	9	8	12	7	10
C5	8	H	2/8	7	6	8	4	9	8	7	8/10	9	H
C3	9	2	1	9	H	7	6/9	8	7	9	H	8	9/12
D4	10	11	2/10	H	10	6	5	12	8/10	H	10	12	11
D1	11	10	H	3/11	12	5/11	H	11	9	8	12	11	10
D6	12	12	3	2	11	H	6/12	10	H	9/12	11	10	12

Interaction between Slip Systems:

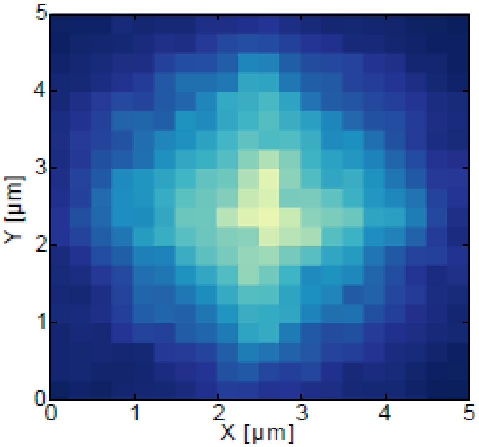
- ■ Self-Interaction
- ■ Coplanar
- 🟨 Hirth
- 🟧 Lomer
- ■ Glissile (Same Plane)
- 🟩 Glissile (Different Plane)
- 🟦 Collinear & Cross-Slip
- X Reaction Slip System

0.4 % strain

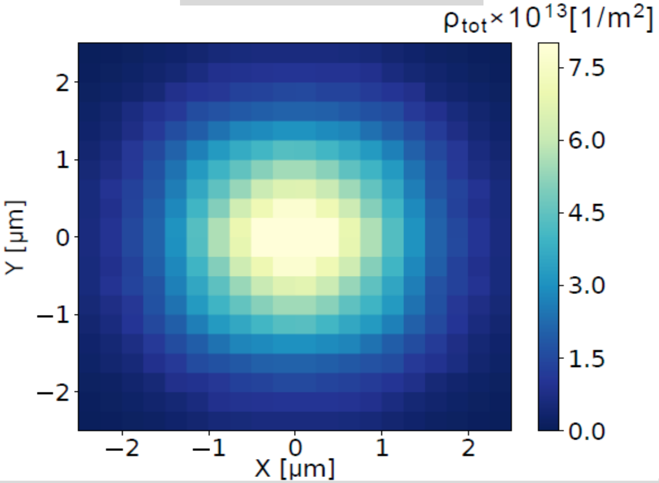
DDD



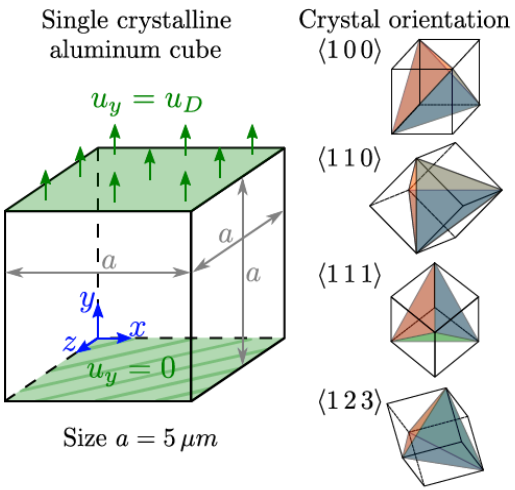
DDD-averaged

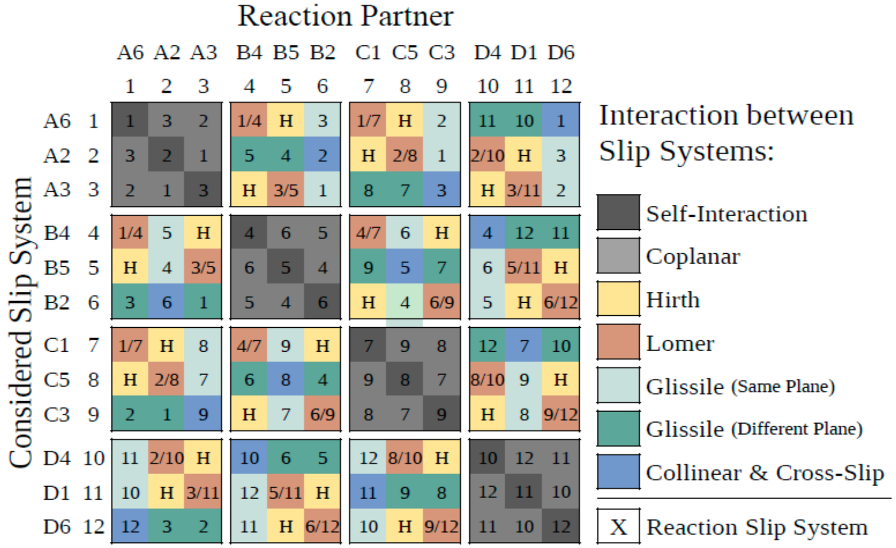


CDD



Modelling Dislocation Network Structures





Reaction Partner

Considered Slip System

		A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
		1	2	3	4	5	6	7	8	9	10	11	12
A6	1	1	3	2	1/4	H	3	1/7	H	2	11	10	1
A2	2	3	2	1	5	4	2	H	2/8	1	2/10	H	3
A3	3	2	1	3	H	3/5	1	8	7	3	H	3/11	2
B4	4	1/4	5	H	4	6	5	4/7	6	H	4	12	11
B5	5	H	4	3/5	6	5	4	9	5	7	6	5/11	H
B2	6	3	6	1	5	4	6	H	4	6/9	5	H	6/12
C1	7	1/7	H	8	4/7	9	H	7	9	8	12	7	10
C5	8	H	2/8	7	6	8	4	9	8	7	8/10	9	H
C3	9	2	1	9	H	7	6/9	8	7	9	H	8	9/12
D4	10	11	2/10	H	10	6	5	12	8/10	H	10	12	11
D1	11	10	H	3/11	12	5/11	H	11	9	8	12	11	10
D6	12	12	3	2	11	H	6/12	10	H	9/12	11	10	12

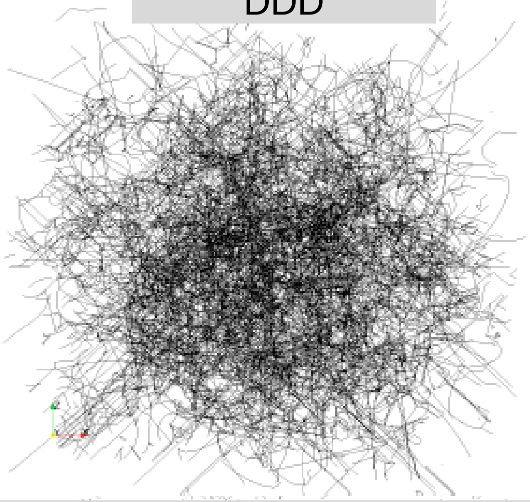
Interaction between Slip Systems:

⬛ Self-Interaction
◼ Coplanar
🟨 Hirth
🟧 Lomer
⬜ Glissile (Same Plane)
🟩 Glissile (Different Plane)
🟦 Collinear & Cross-Slip

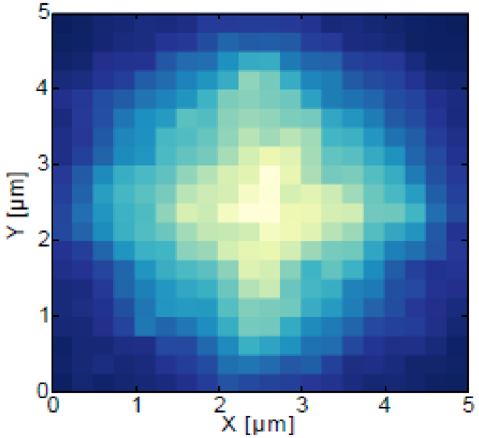
X Reaction Slip System

0.6 % strain

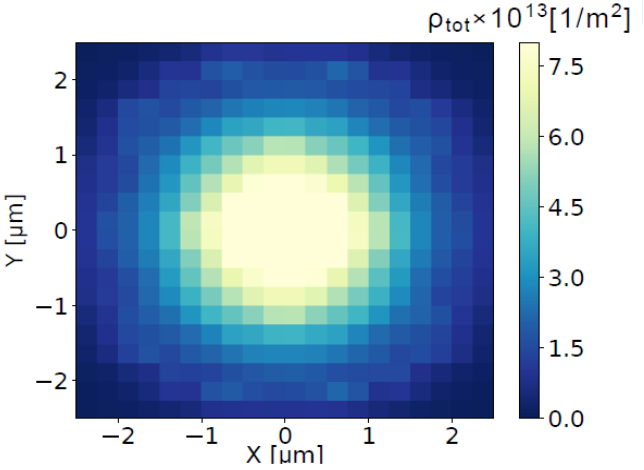
DDD



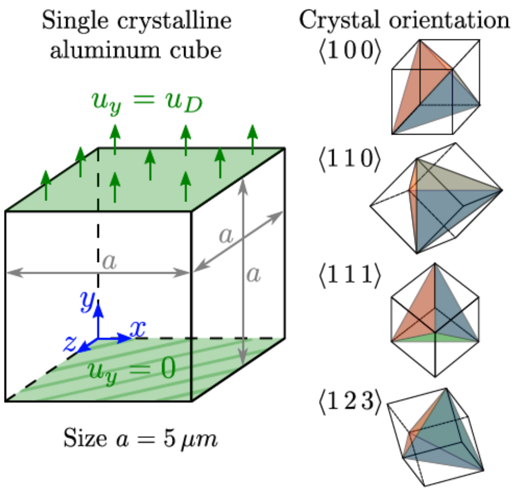
DDD-averaged

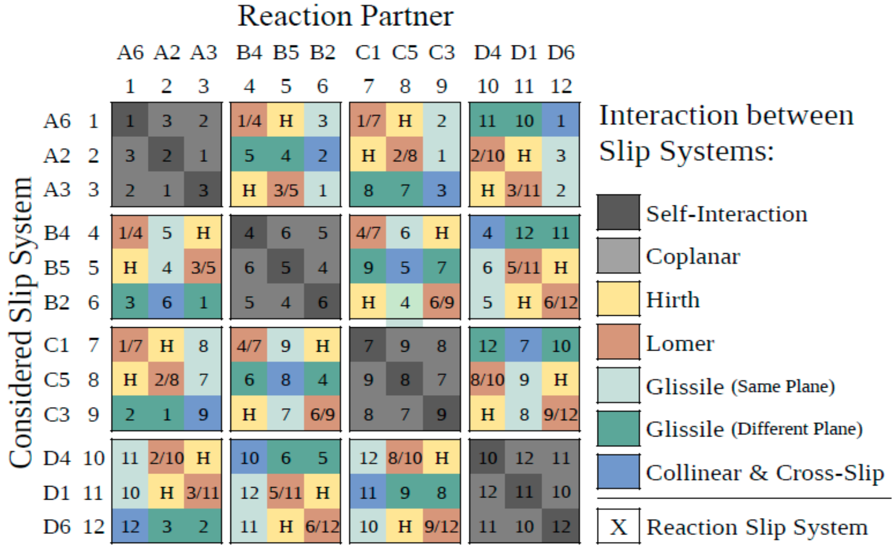


CDD



Modelling Dislocation Network Structures





Reaction Partner

Considered Slip System

		A6	A2	A3	B4	B5	B2	C1	C5	C3	D4	D1	D6
		1	2	3	4	5	6	7	8	9	10	11	12
A6	1	1	3	2	1/4	H	3	1/7	H	2	11	10	1
A2	2	3	2	1	5	4	2	H	2/8	1	2/10	H	3
A3	3	2	1	3	H	3/5	1	8	7	3	H	3/11	2
B4	4	1/4	5	H	4	6	5	4/7	6	H	4	12	11
B5	5	H	4	3/5	6	5	4	9	5	7	6	5/11	H
B2	6	3	6	1	5	4	6	H	4	6/9	5	H	6/12
C1	7	1/7	H	8	4/7	9	H	7	9	8	12	7	10
C5	8	H	2/8	7	6	8	4	9	8	7	8/10	9	H
C3	9	2	1	9	H	7	6/9	8	7	9	H	8	9/12
D4	10	11	2/10	H	10	6	5	12	8/10	H	10	12	11
D1	11	10	H	3/11	12	5/11	H	11	9	8	12	11	10
D6	12	12	3	2	11	H	6/12	10	H	9/12	11	10	12

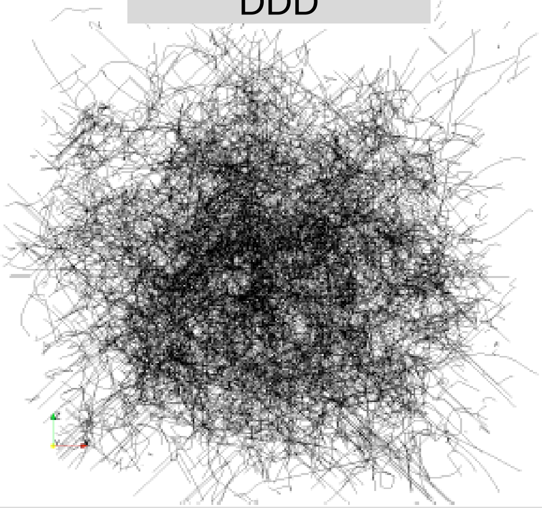
Interaction between Slip Systems:

- Self-Interaction
- Coplanar
- Hirth
- Lomer
- Glissile (Same Plane)
- Glissile (Different Plane)
- Collinear & Cross-Slip

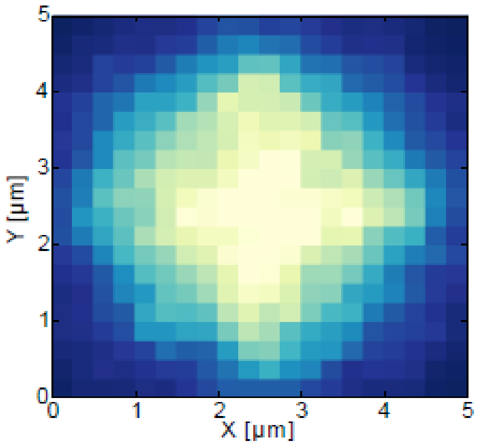
X Reaction Slip System

0.8 % strain

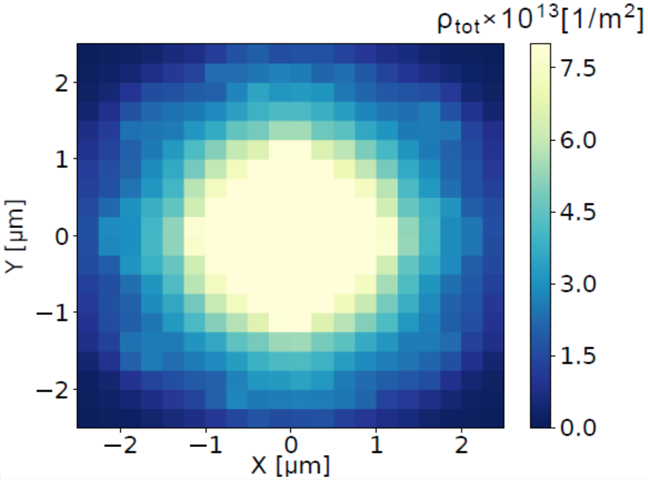
DDD



DDD-averaged



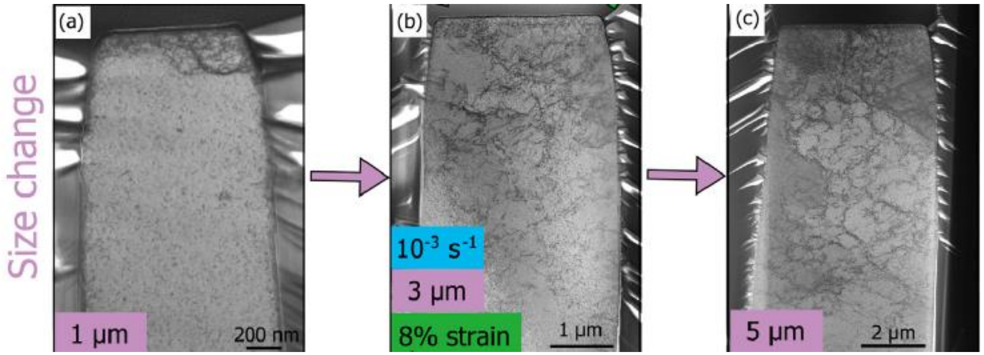
CDD



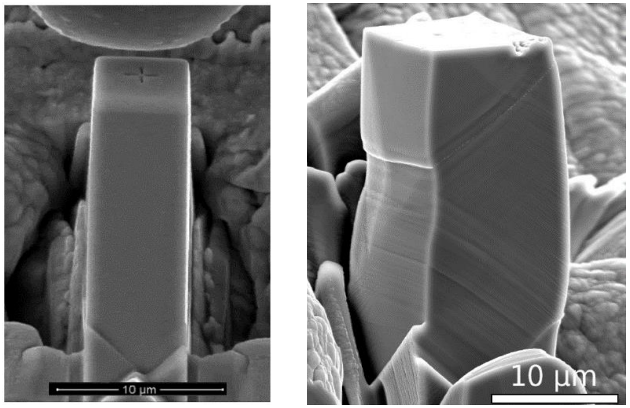
Exploring Dislocation Network Structures

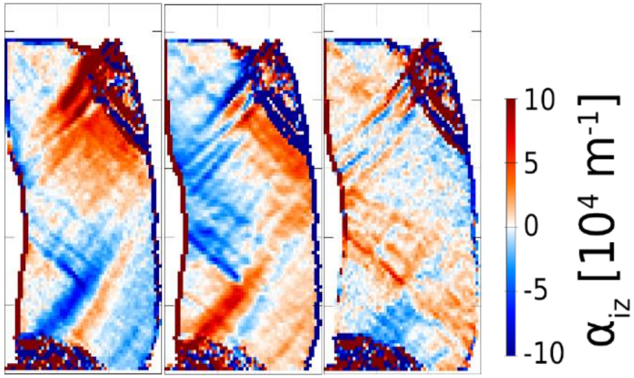
- Varying micropillar sizes (1 to 10 μm → dislocation storage regime)

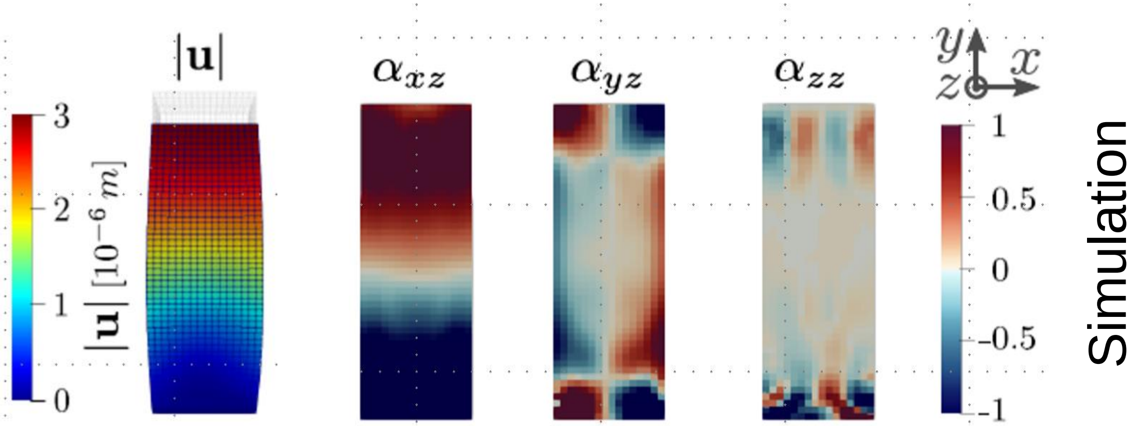
Dislocation structures (post mortem STEM)



Zhao, X.X., Wu, J., Chiu, Y.L., Jones, I.P., Gu, R. and Ngan, A.H.W., 2019. Critical dimension for the dislocation structure in deformed copper micropillars. Scripta Materialia, 163, pp.137-141.







- ➢ Explain (and predict) complex material behavior

Zoller, K.; Kalácska, P.; Ispánovity, P.; Schulz, K.: Comptes Rendus Physique, 2021, pp. 1-27.

Exploring dislocation networks for continuum modeling

Katrin Schulz

Institute for Applied Materials – Reliability and Microstructure (IAM-ZM), KIT, Karlsruhe