MatCalc
Engineering

"ABC"-models for subgrain structure evolution in MatCalc 6

(MatCalc 6.00.0258)

P. Warczok

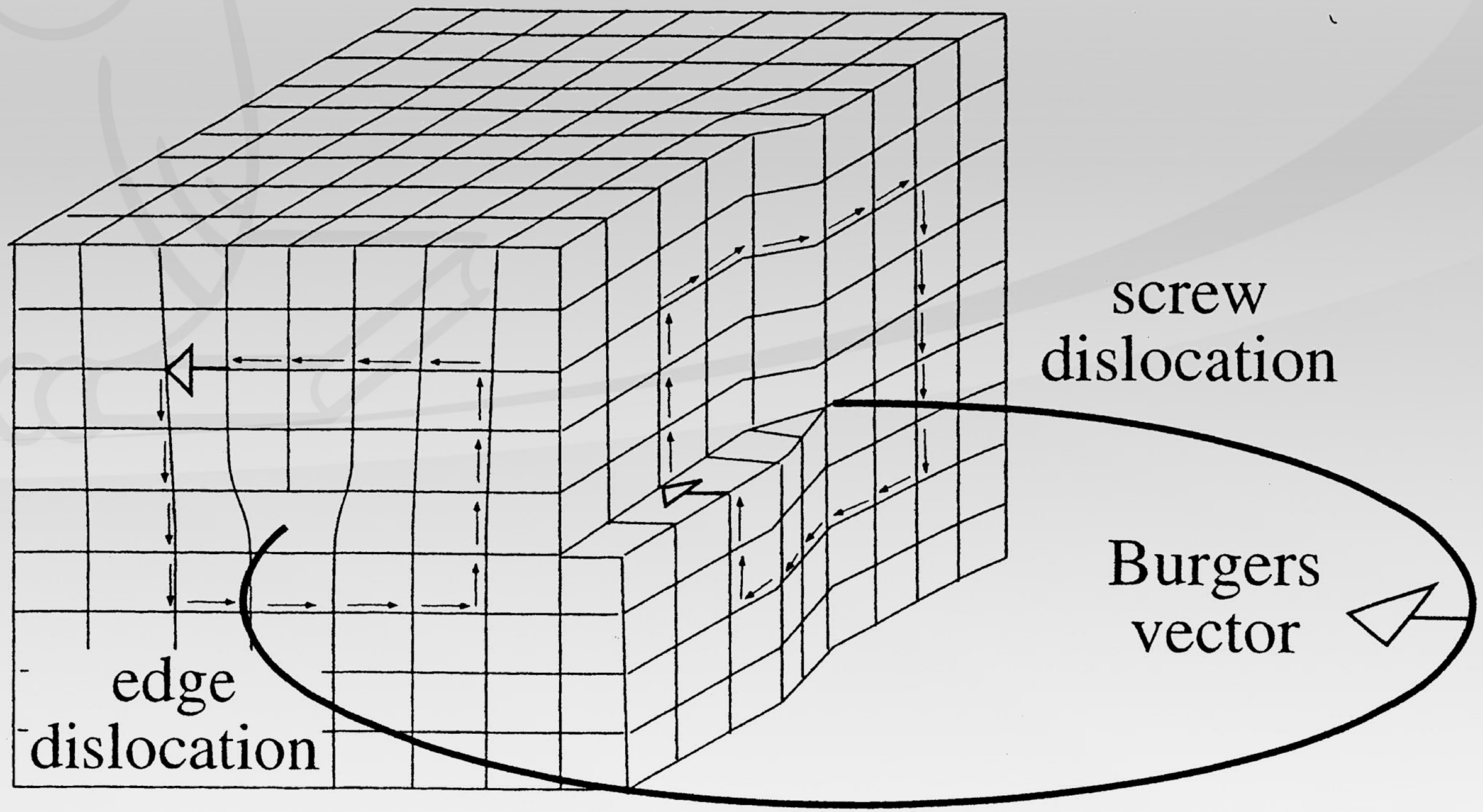
Outlook

- Few words on substructure
- Dislocation density evolution
- Subgrain size evolution
- Model demonstration

Introduction to dislocations

Dislocations

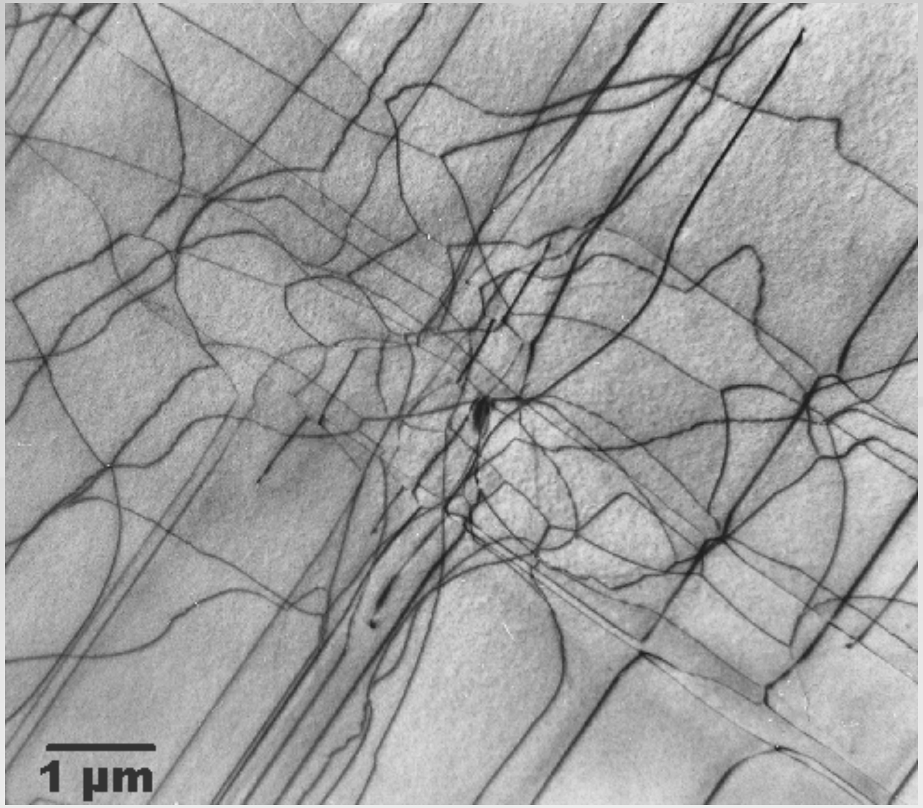
- Two geometries:
  - Edge
  - Screw



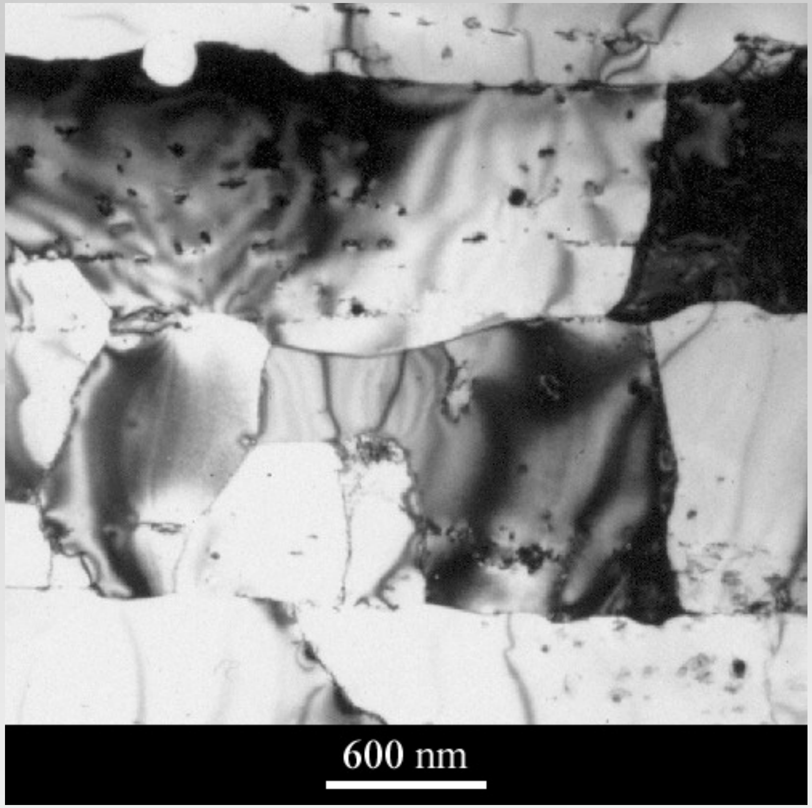
http://www.geology.um.maine.edu/geodynamics/AnalogWebsite/UndergradProjects2010/PatrickRyan/Content/dislocationdiagram.jpg

Dislocations

Intrinsic dislocations



Wall dislocations



Dislocation density

- Impact:
  - Diffusion (pipe-diffusion)
  - Nucleation rate (number of nucleation sites)
  - Subgrain size (through similitude principle)
  - Recrystallization onset
  - Yield strength
    - Directly - work hardening
    - Indirectly – subgrain size, precipitate size

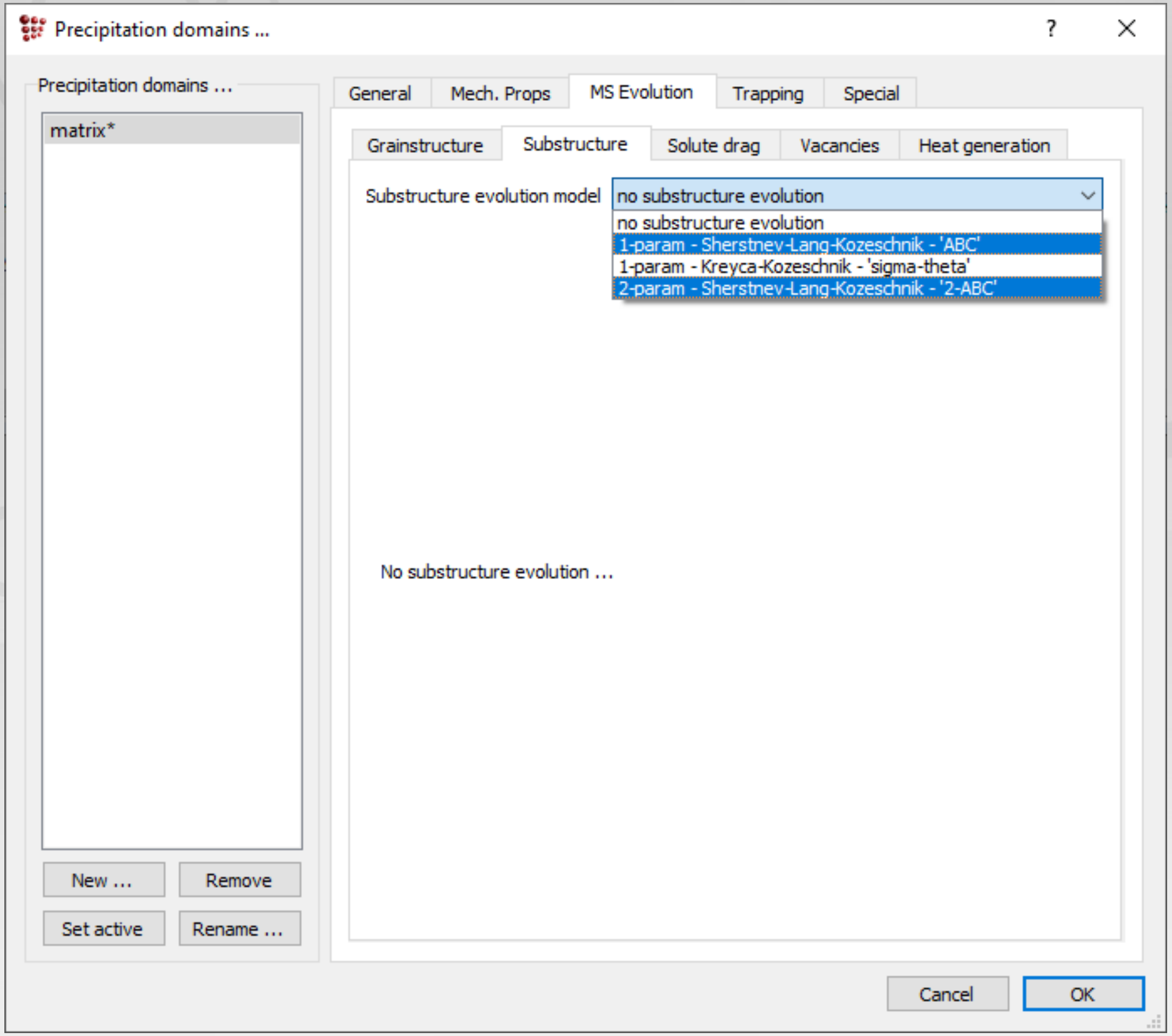
Dislocation density evolution

Dislocation density evolution

- MatCalc models
  - Sherstnev-Lang-Kozeschnik (SLK) models
    - 1 parameter model (a.k.a. „1ABC“)
    - 2 parameters model (a.k.a. „2ABC“)

  - 1 parameter model: global dislocation density evolution
  - 2 parameters model: separate dynamics for intrinsic and wall dislocations

Dislocation density evolution



Dislocation density evolution

$$\dot{\rho} = \dot{\rho}_1 - \dot{\rho}_2 - \dot{\rho}_3$$

- Dislocation generation
  - Deformation → $\dot{\rho}_1$
- Dislocation annihilation
  - Dynamic recovery (dislocations with antiparallel Burgers vectors hit each other) →$\dot{\rho}_2$
  - Static recovery (dislocation climb) → $\dot{\rho}_3$

Dislocation generation (deformation)

$$\dot{\rho}_1 = \frac{M\dot{\varepsilon}}{bA}\sqrt{\rho}$$

ρ - Dislocation density

A - A-parameter (constant)

M - Taylor factor

$\dot{\varepsilon}$ - Strain rate

b - Burgers vector

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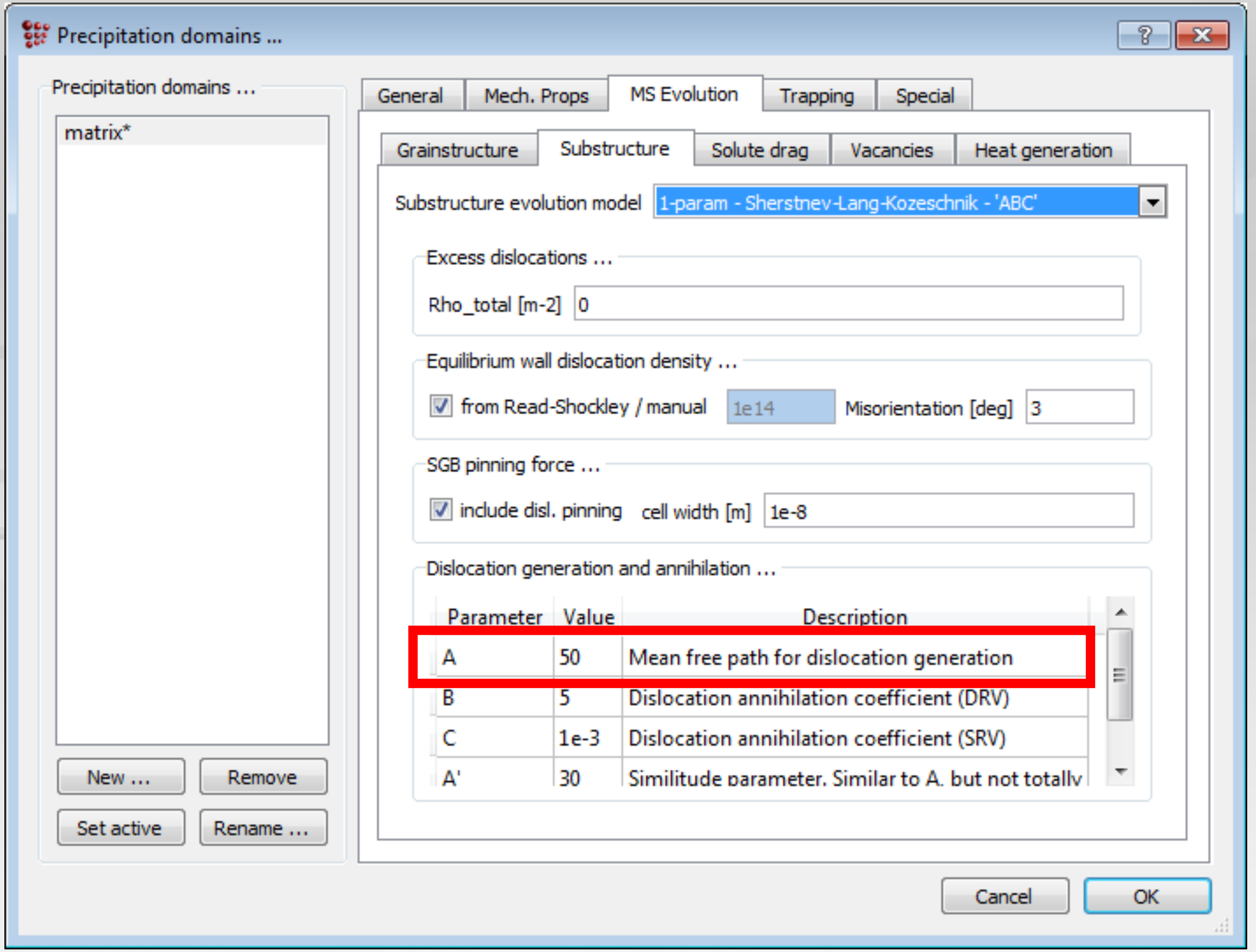
Dislocation generation (deformation)

$$\dot{\rho}_1 = \frac{M\dot{\varepsilon}}{b\boxed{A}}\sqrt{\rho}$$



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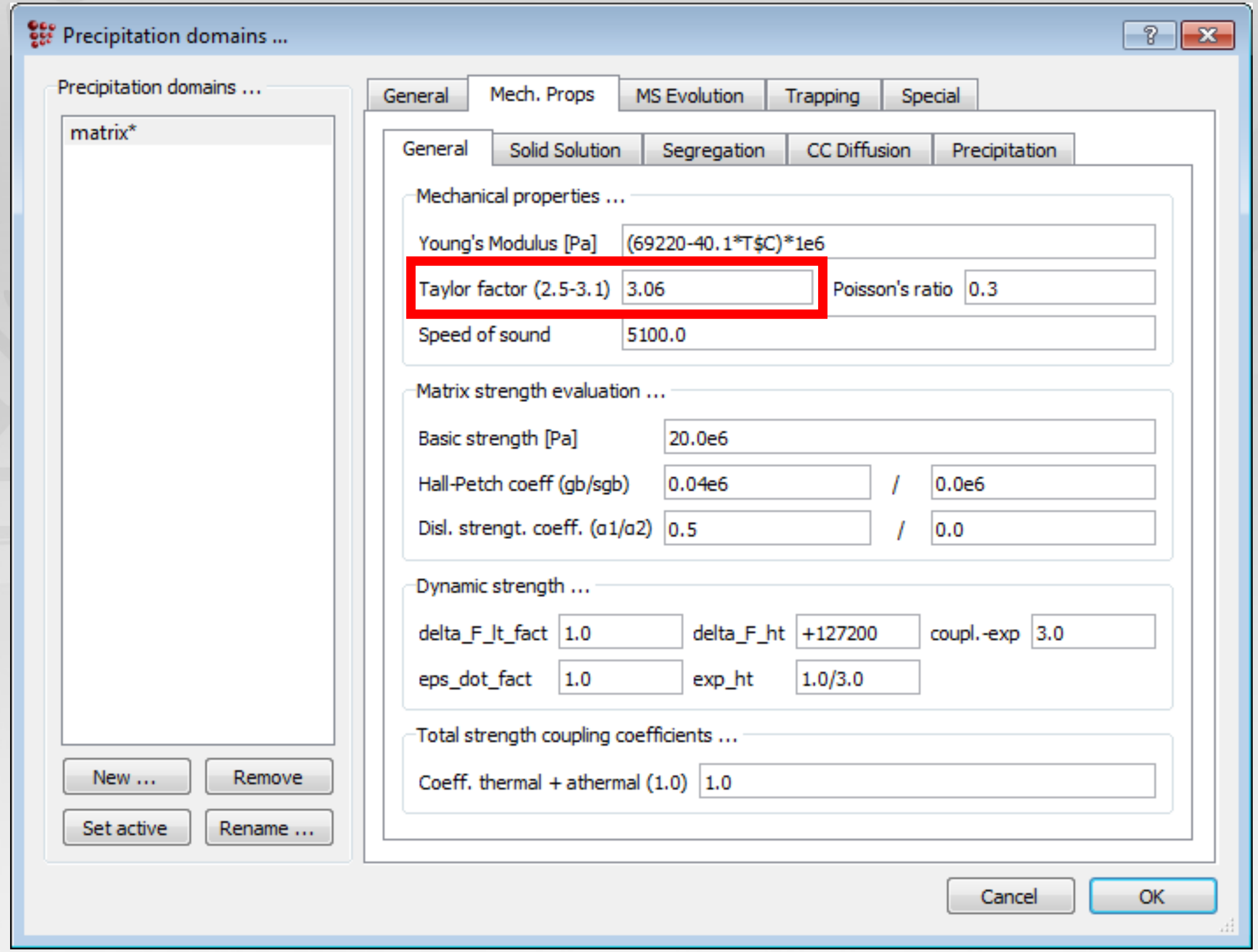

Dislocation generation (deformation)

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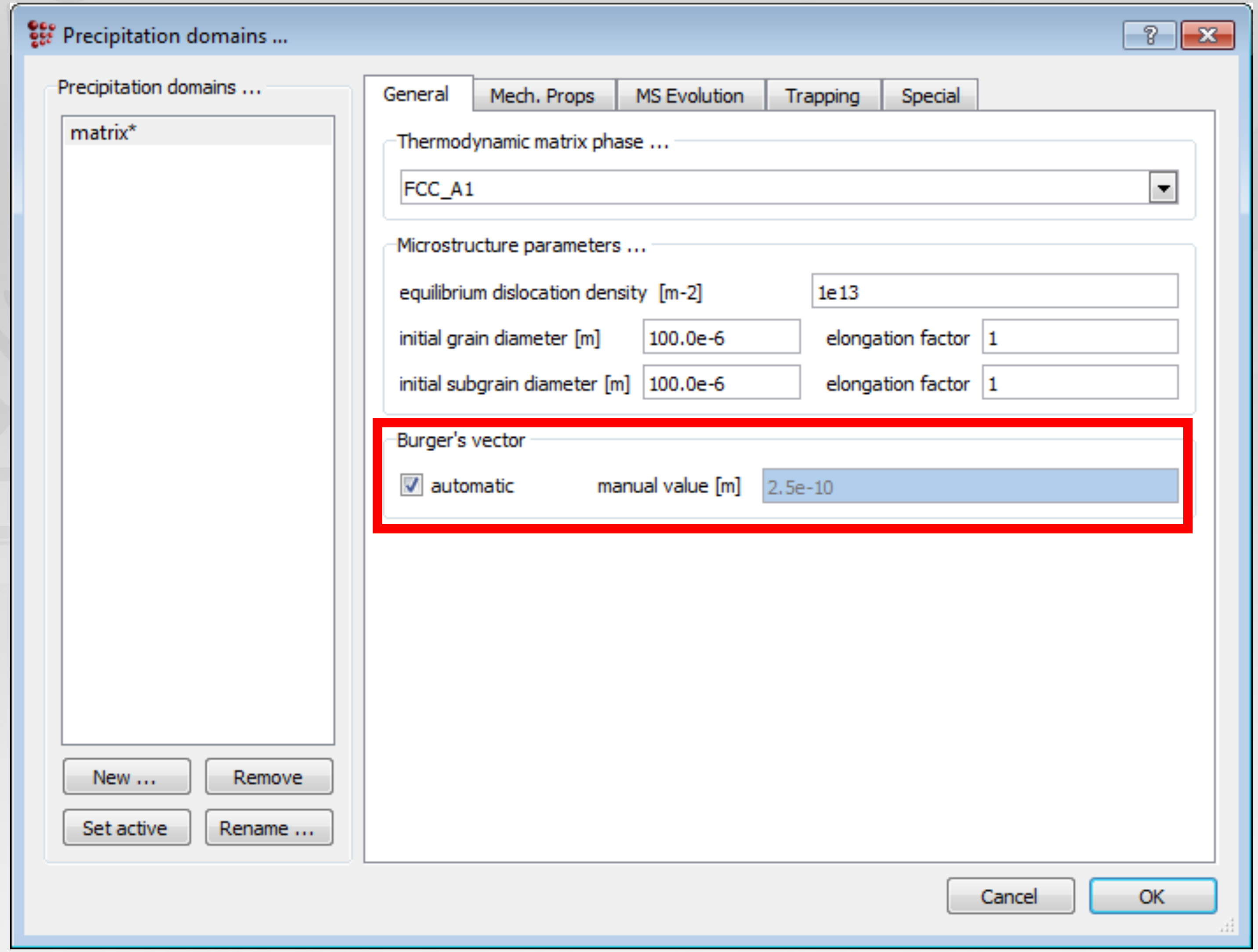

Dislocation generation (deformation)

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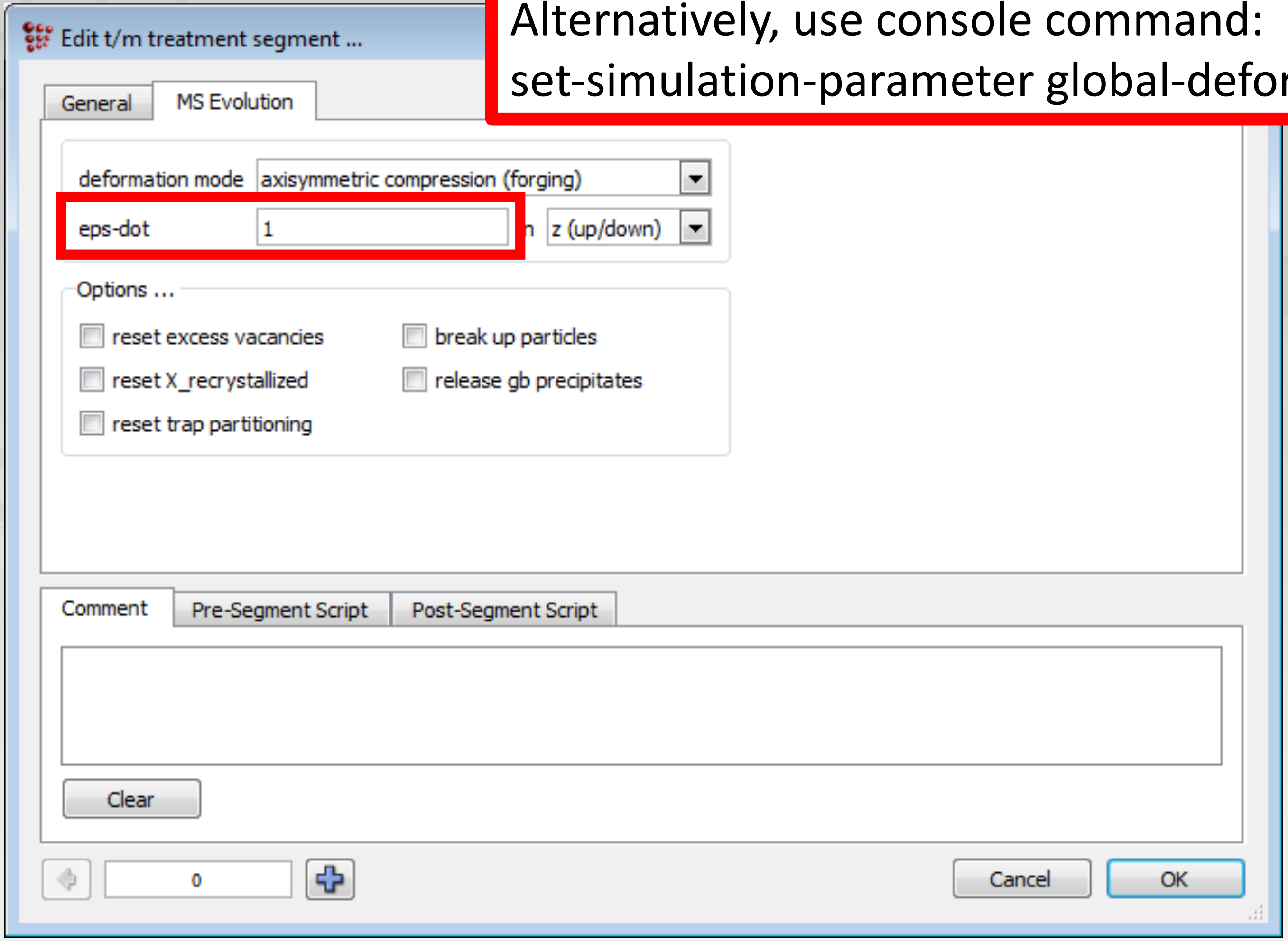

Alternatively, use console command:
set-simulation-parameter global-deformation-rate=1

M - Taylor factor

$\dot{\varepsilon}$ - Strain rate

b - Burgers vector

Dislocation annihilation (dynamic recovery)

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$$d_{ann} = \frac{G b^4 N_A}{2\pi(1-\nu) E_{Va}}$$

d_{ann} - Annihilation distance

G - Shear modulus

ν - Poisson ratio

E_{Va} - Vacancy formation energy (from thermodynamic database)

N_A - Avogadro constant

Dislocation annihilation (dynamic recovery)

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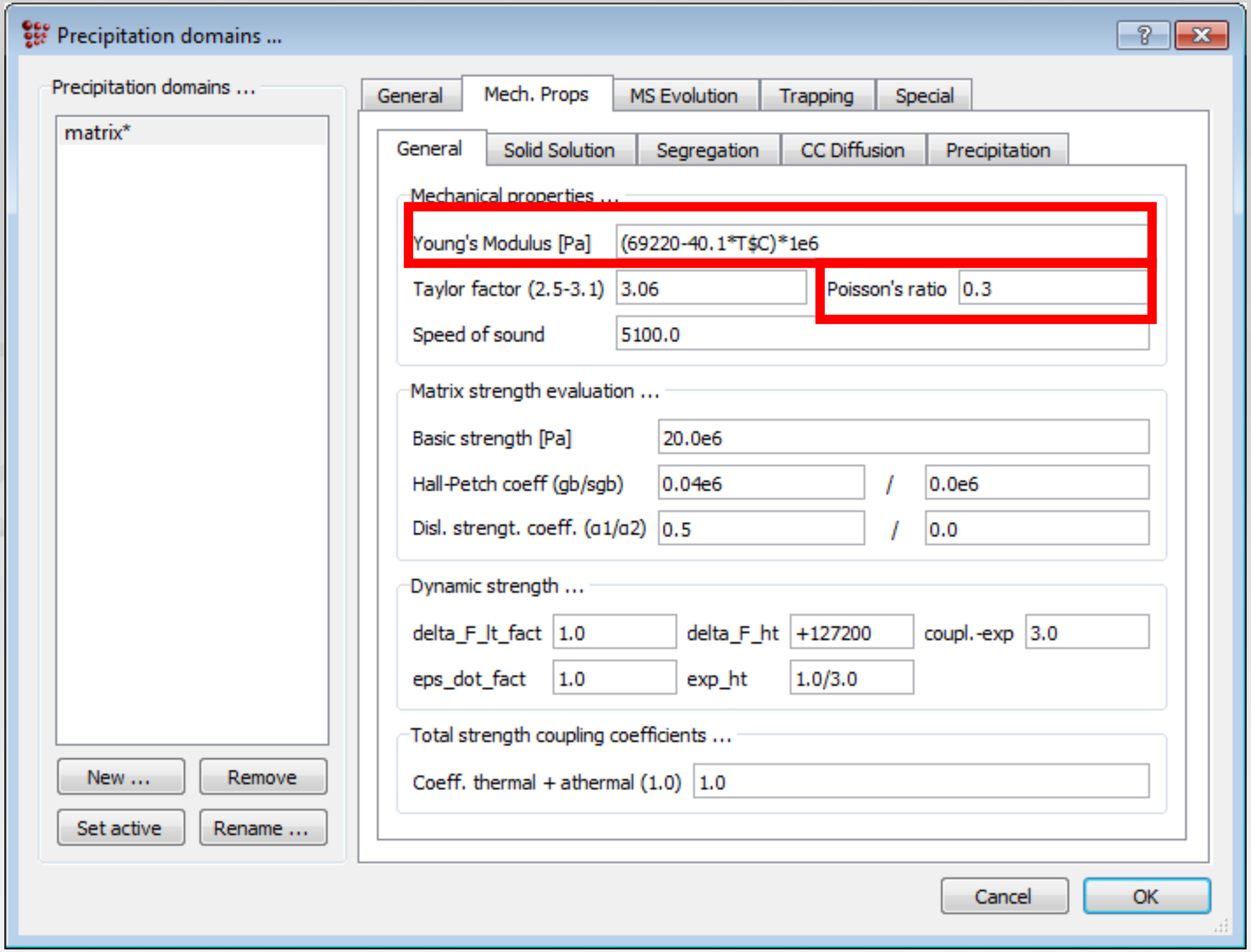

Dislocation annihilation (dynamic recovery)

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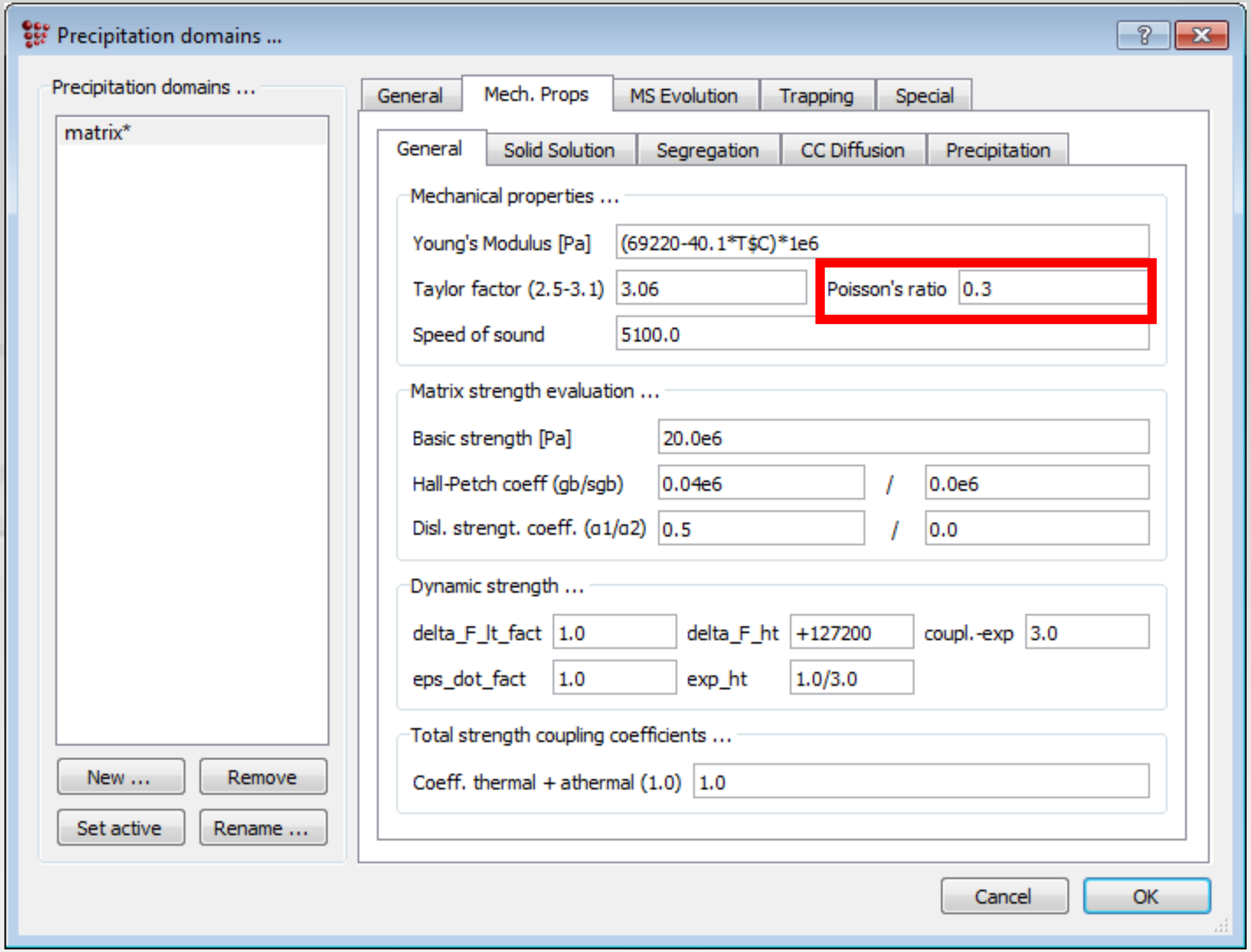

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Dislocation annihilation (dynamic recovery)

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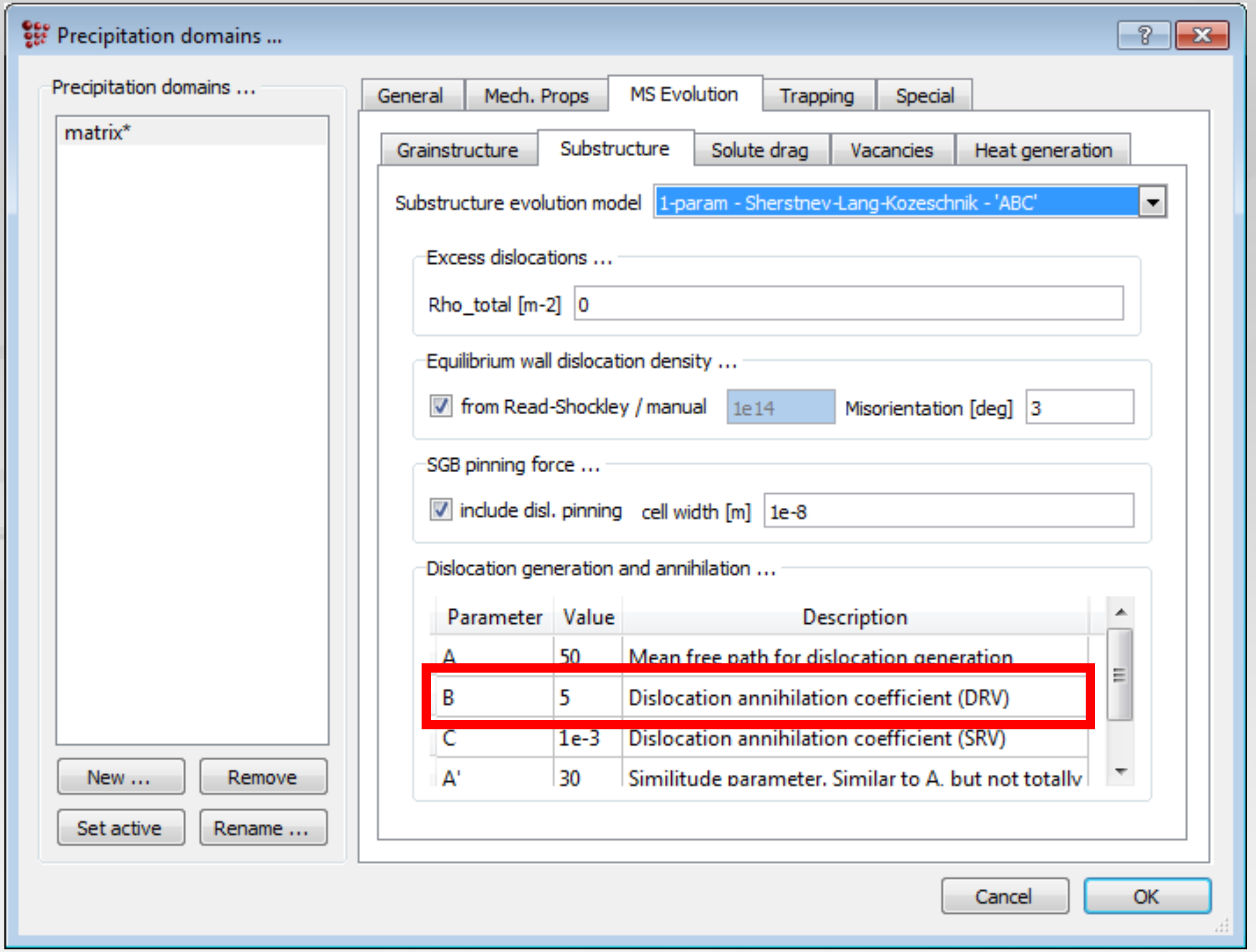
$$\dot{\rho}_2 = \frac{2M\dot{\varepsilon}d_{ann}B}{b}\rho$$

B - B-parameter (constant)



Dislocation annihilation (static recovery)

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$$\dot{\rho}_3 = \frac{2Gb^3 D_{eff} C}{k_B T}\left(\rho^2 - \rho_{eq}^2\right)$$

D_{eff} - Diffusion, incl. enhancement factors like pipe diffusion, excess vacancies, etc.

k_B - Boltzmann constant

T - Temperature

C - C-parameter (constant)

ρ_{eq} - Equilibrium dislocation density

Dislocation annihilation (static recovery)

$$\dot{\rho}_3 = \frac{2Gb^3 D_{eff}\boxed{C}}{k_B T}\left(\rho^2 - \rho_{eq}^2\right)$$

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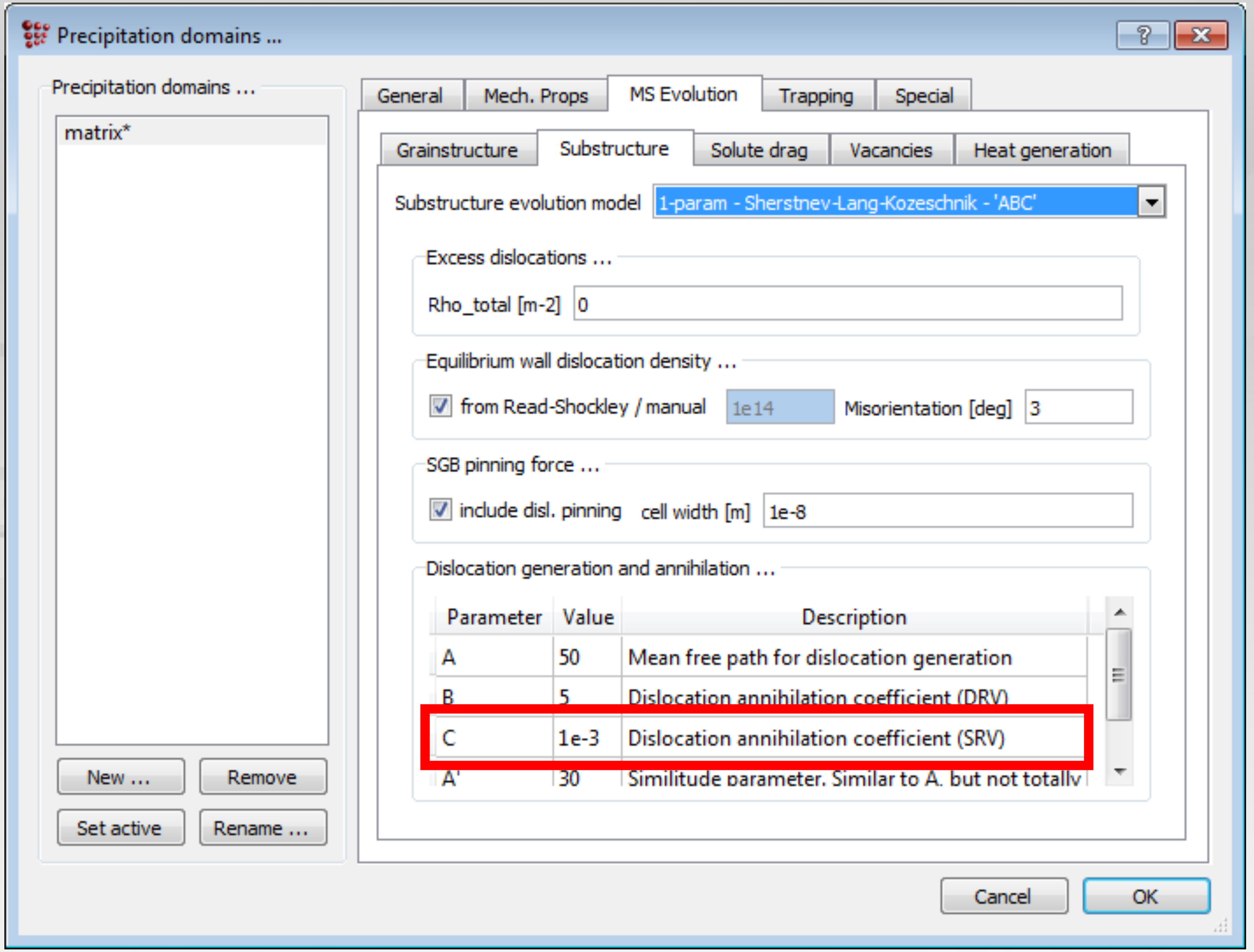

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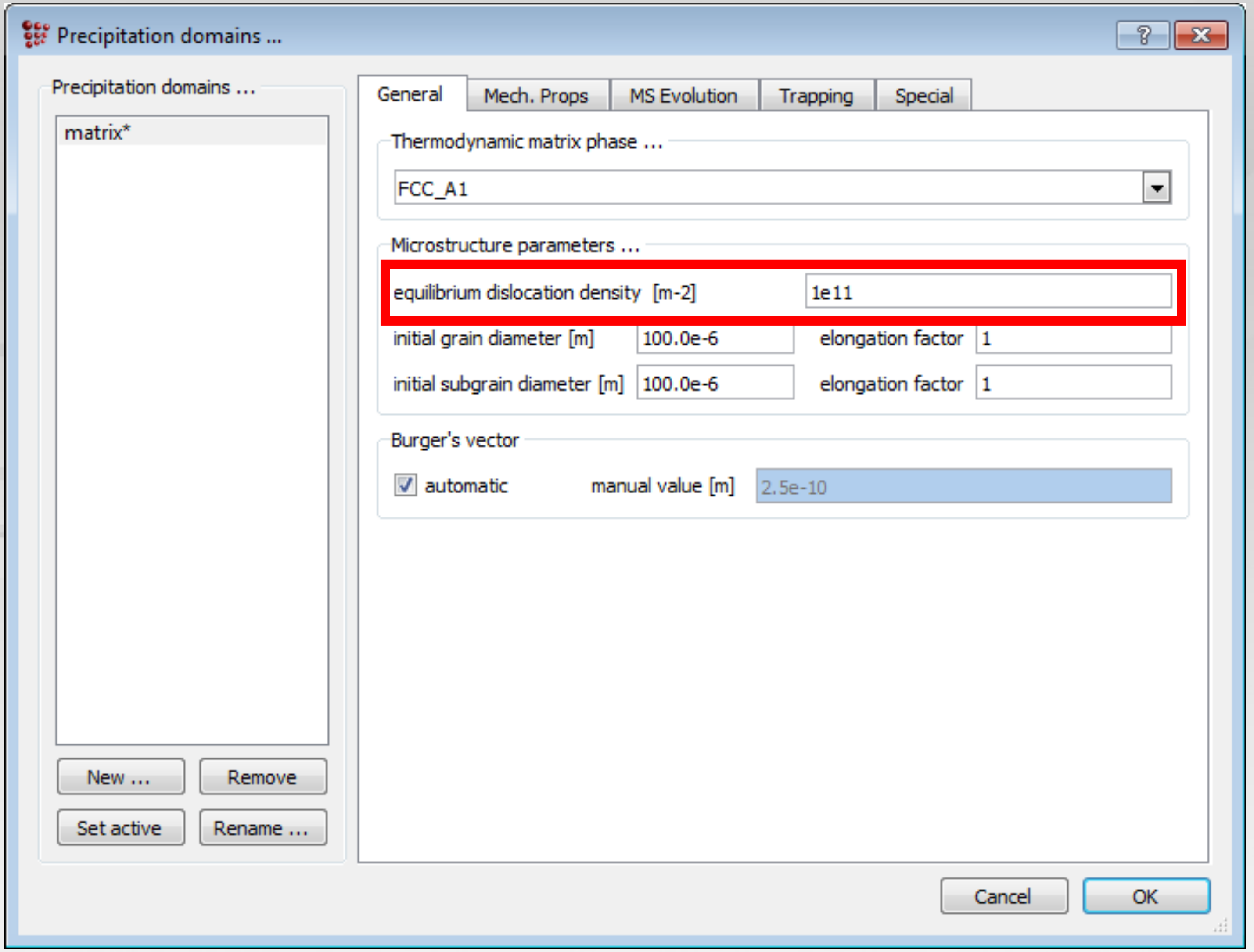

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Dislocation annihilation (static recovery)

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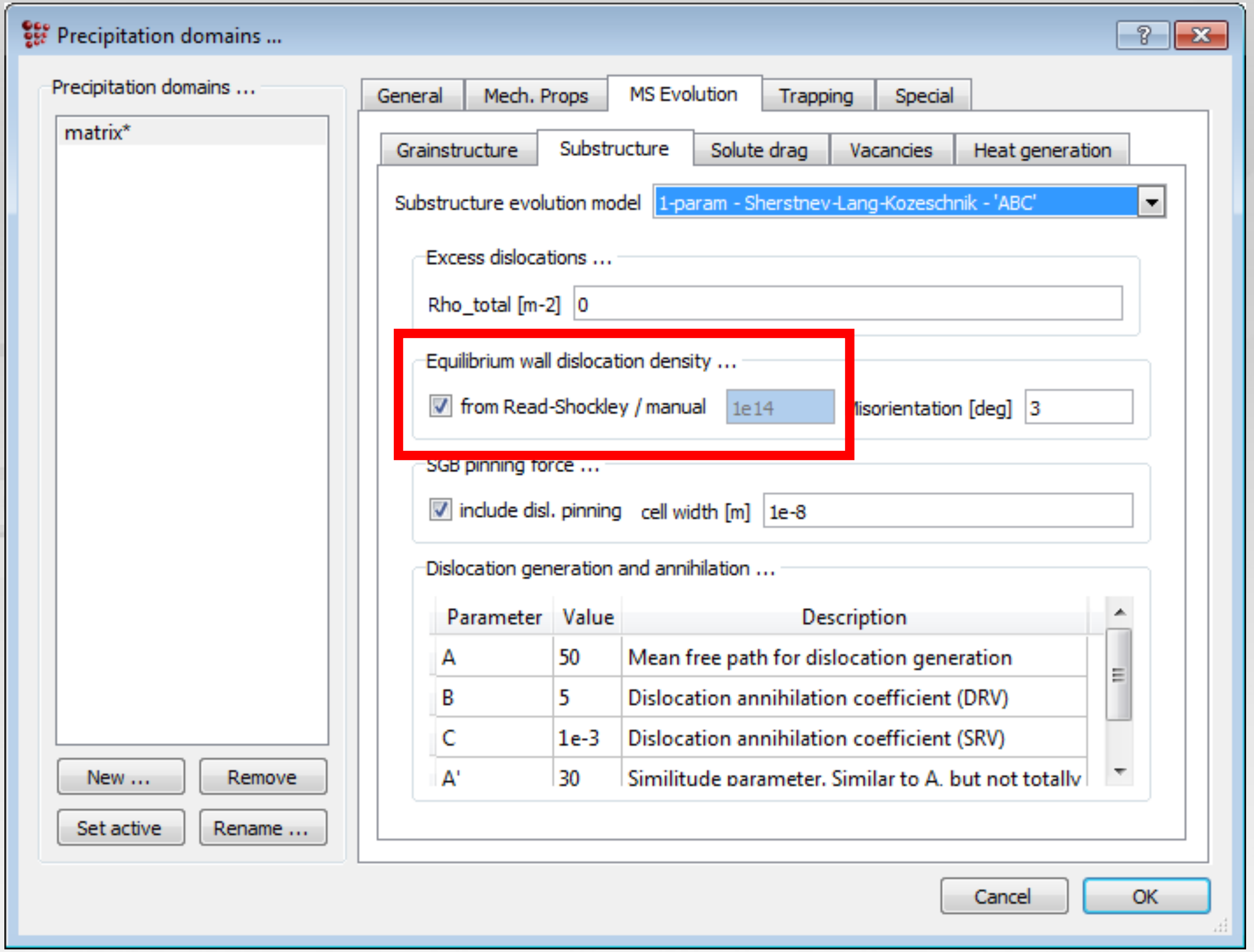
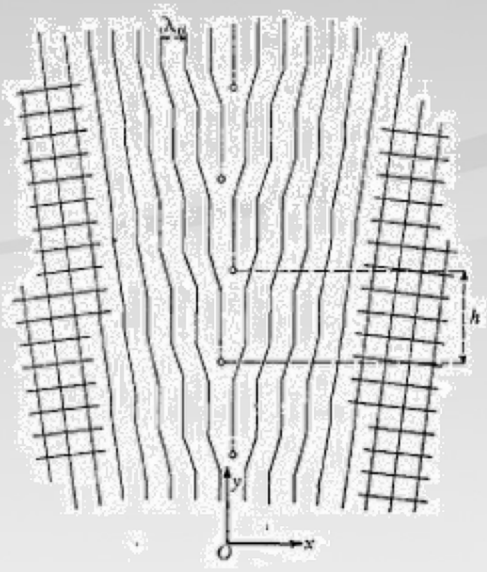


Read-Shockley dislocation density

- Read-Shockley dislocation density → necessary amount to fulfill geometrical constraint

$$\rho_{RS} = \frac{tan\theta}{\delta b}$$

θ - Misorientation angle



Burgers, J.M., Proc. Phys. Soc. 52 (1940) 23-33

Read-Shockley dislocation density

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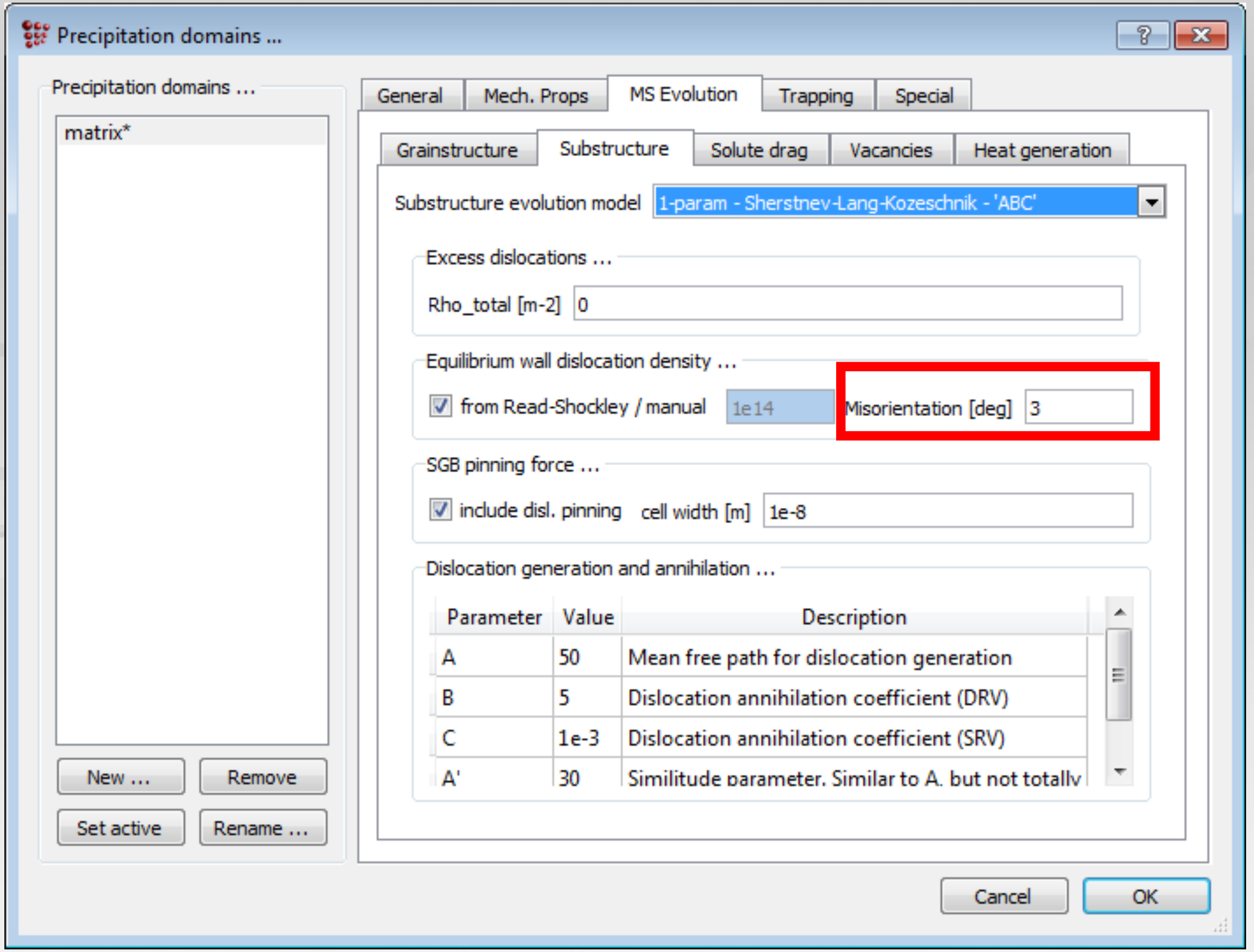

Subgrain size evolution

Subgrain size evolution

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$$\dot{\delta} = \dot{\delta}_1 - \dot{\delta}_2$$

- Subgrains grow to minimize the subgrain boundary area (minimize the boundary energy) → $\dot{\delta}_1$
- Subgrain walls shrink with increasing dislocation density (more wall dislocations available) → $\dot{\delta}_2$

Subgrain growth

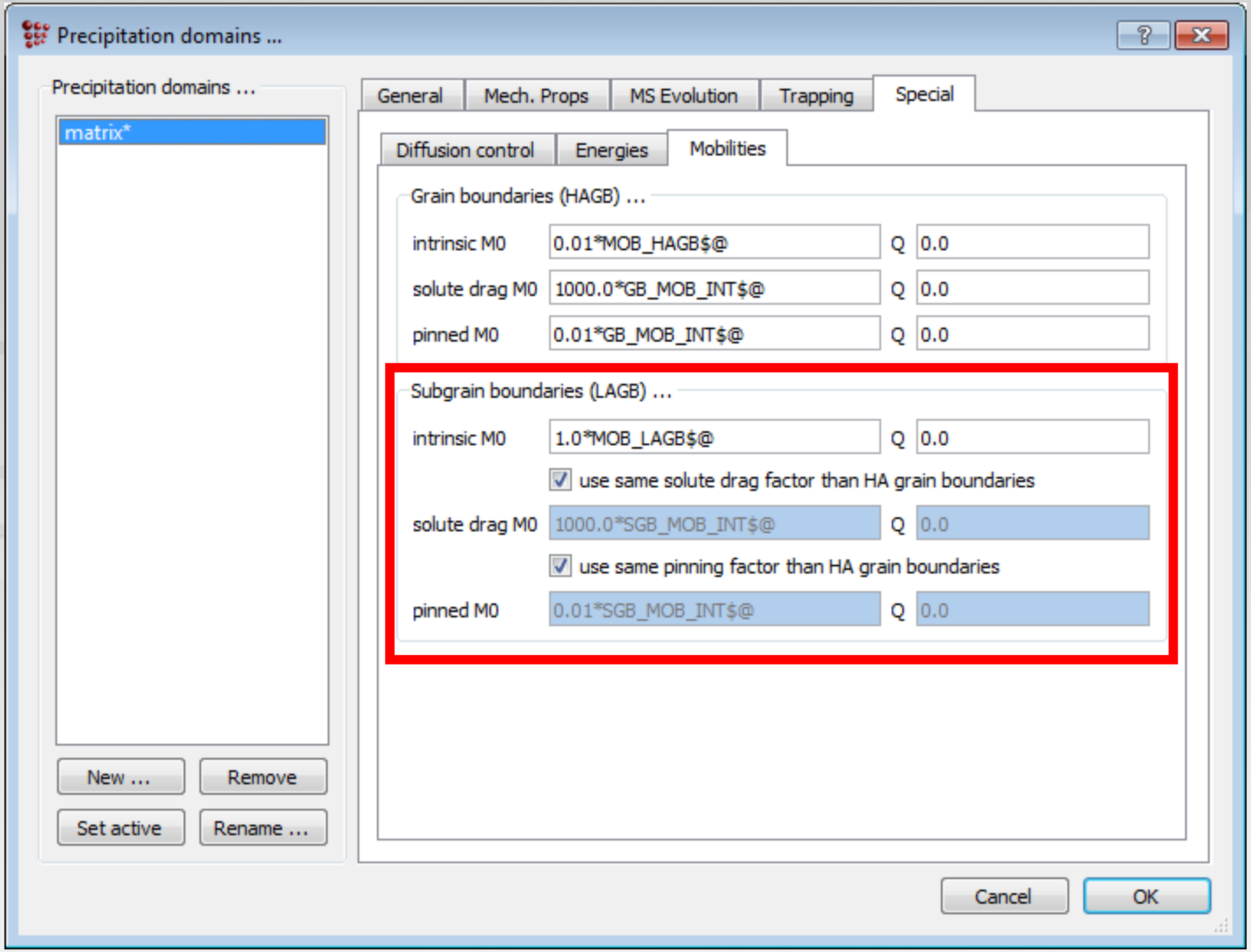
$$\dot{\delta}_1 = MP_D$$

- Subgrain growth model same as for grain growth → product of mobility and driving force
- Same models for   as for grain boundary mobility → same effects for precipitate pinning and solute drag

Subgrain growth

$$\dot{\delta}_1 = \boxed{M} P_D$$

- Same models as for grain boundary mobility → same effects for precipitate pinning and solute drag



Subgrain growth

- Driving force – balance between Laplace pressure and dislocation pinning of subgrain walls

$$P_D = \frac{4\gamma_{sgb}}{\delta} - \frac{Gb^2}{\sqrt{w\rho}}\sqrt{\rho - \rho_{RS}}$$

γ_{sgb} - Subgrain boundary energy

δ - Subgrain size

w - Cell width for dislocation pinning

ρ_{RS} - Read-Shockley dislocation density

Subgrain growth

- Driving force – balance betw

  dislocation pinning of subgra

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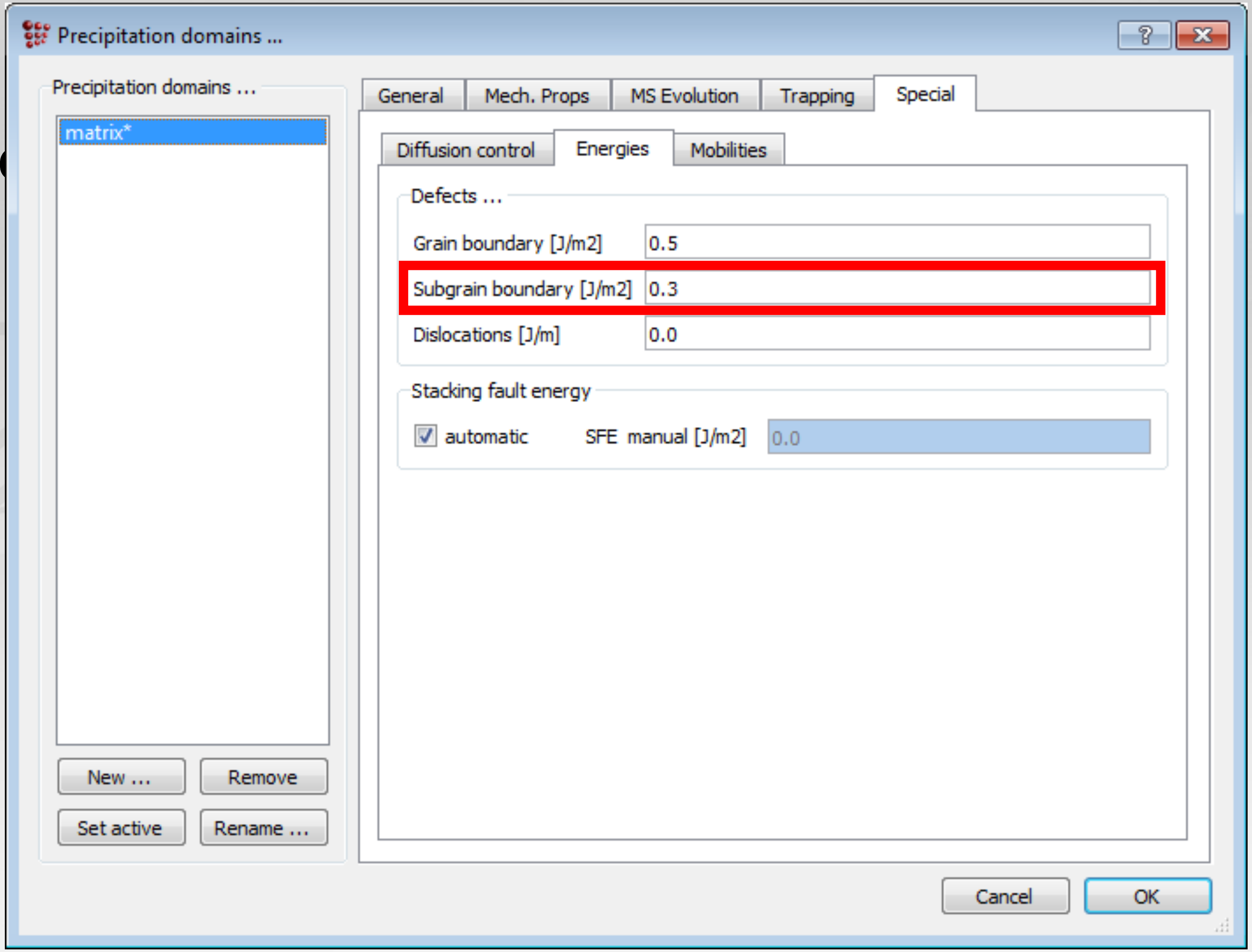

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Subgrain growth

- Driving force – balance betv
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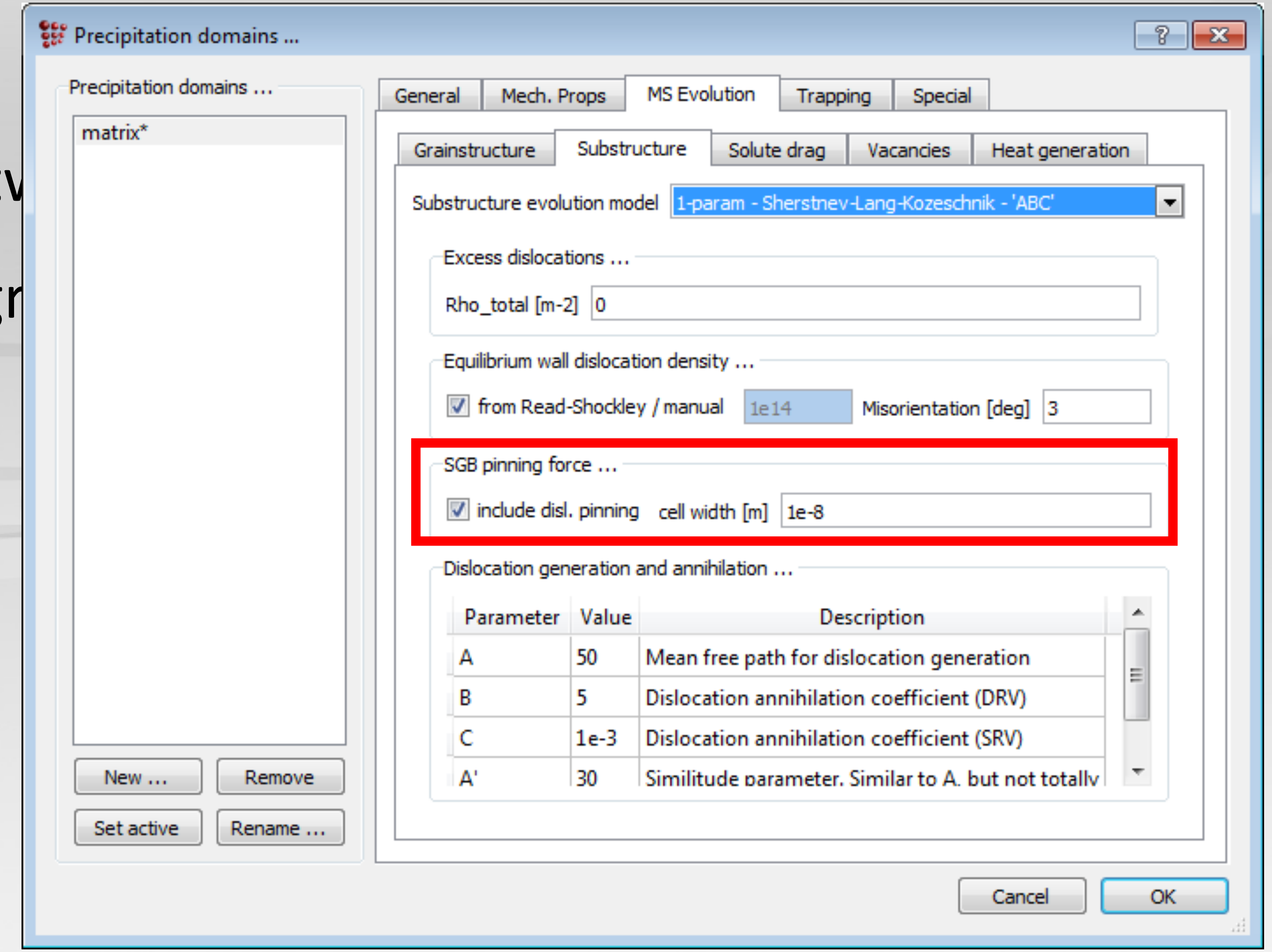
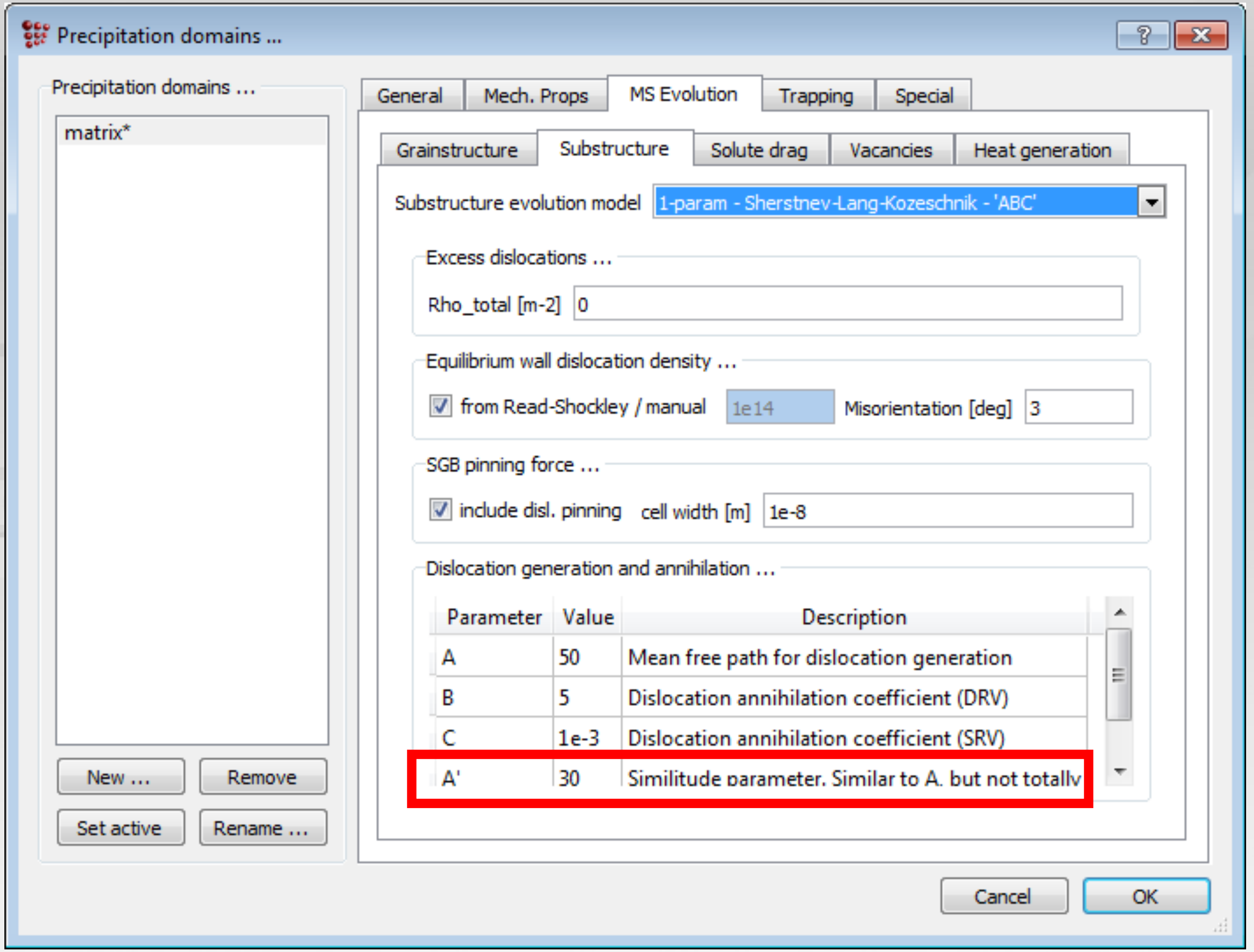


Subgrain shrinkage

$$\dot{\delta}_2 = \frac{\delta^3}{2(\boxed{A'})^2}\dot{\rho}_1$$

A' - A'-parameter (constant)



Model demonstration

1-parameter model

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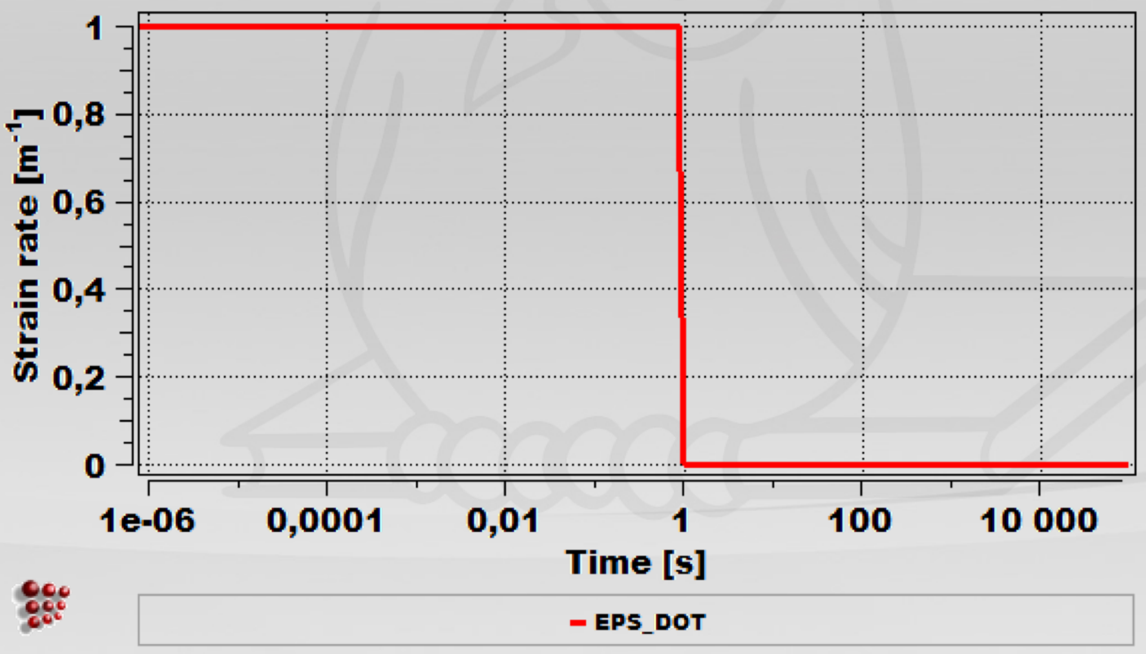

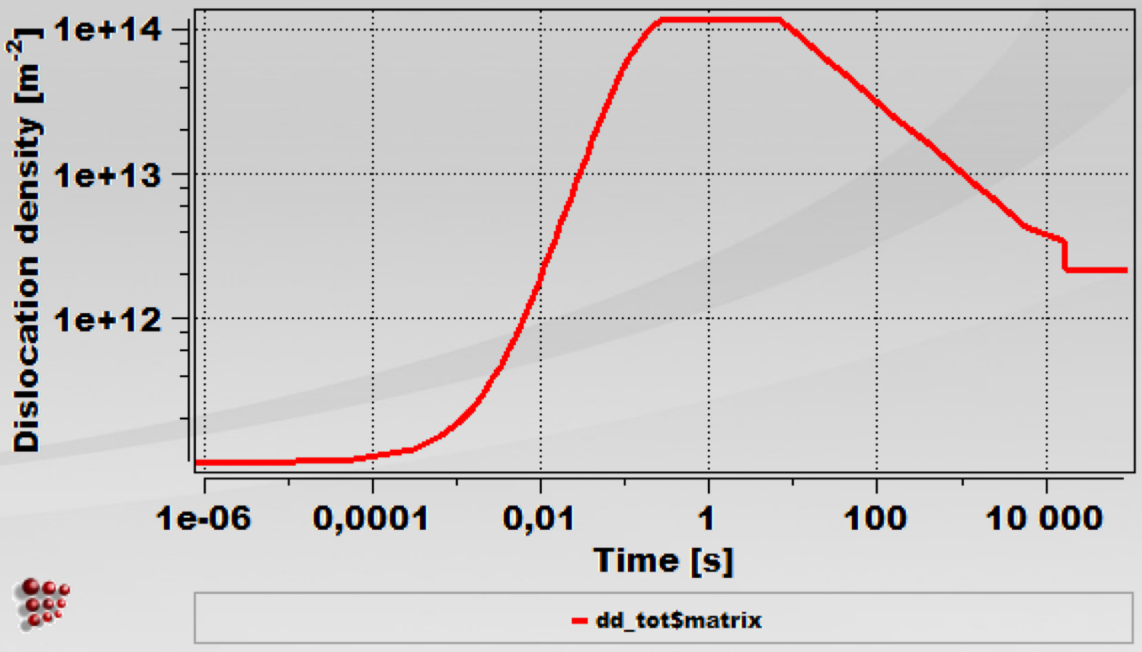

Al, 400°C isothermal, A=50, B=5, C=1e-3 (default values)

1-parameter model

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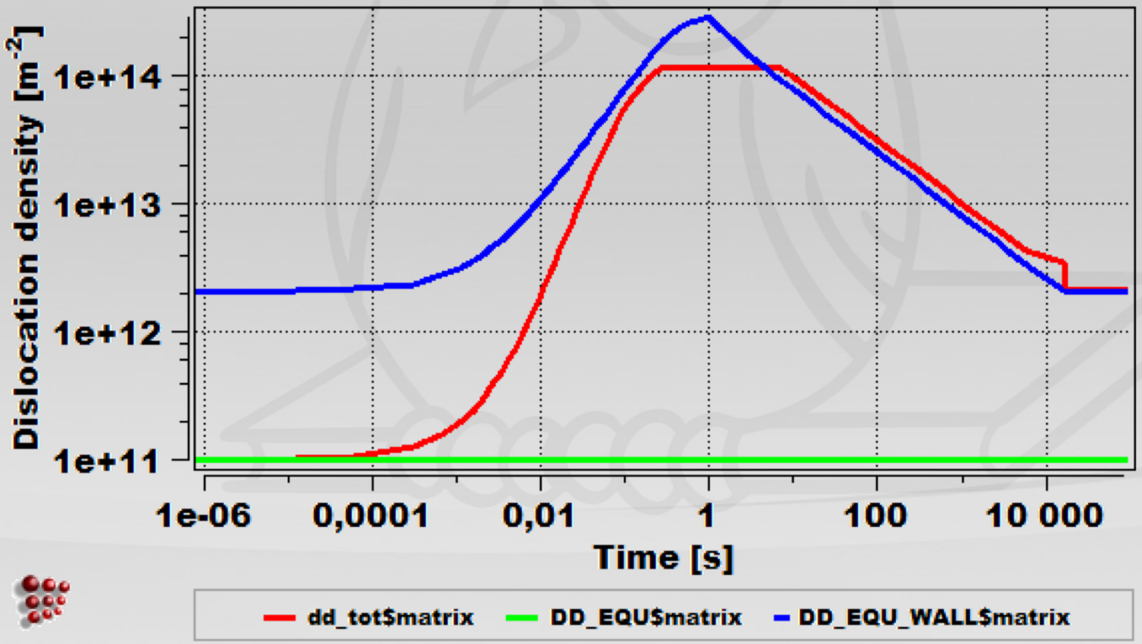

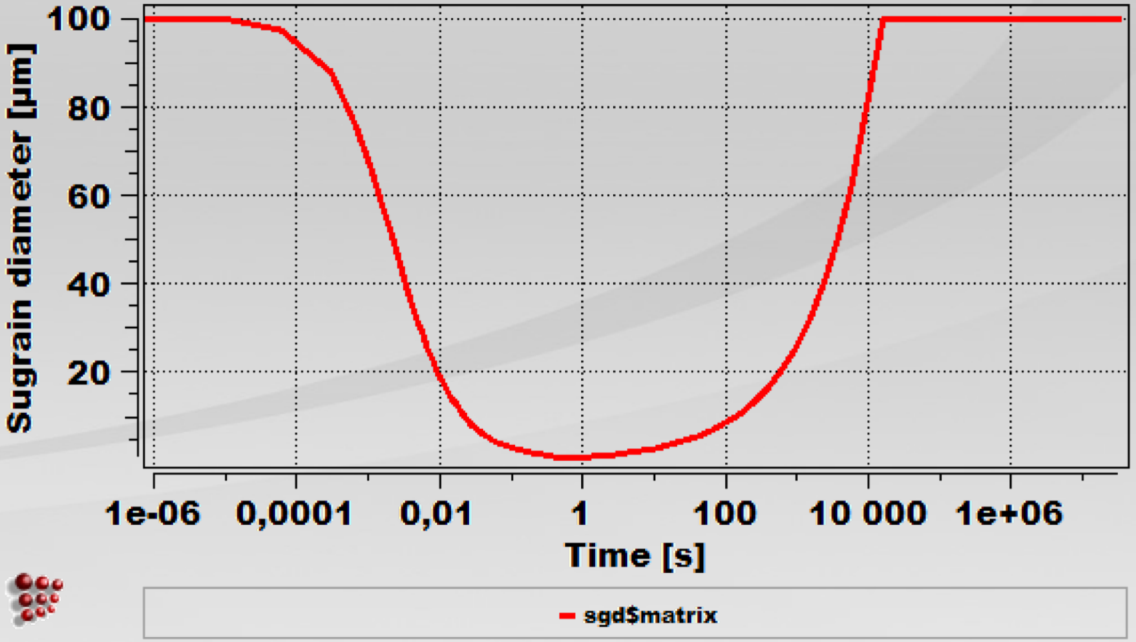

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2-parameters model

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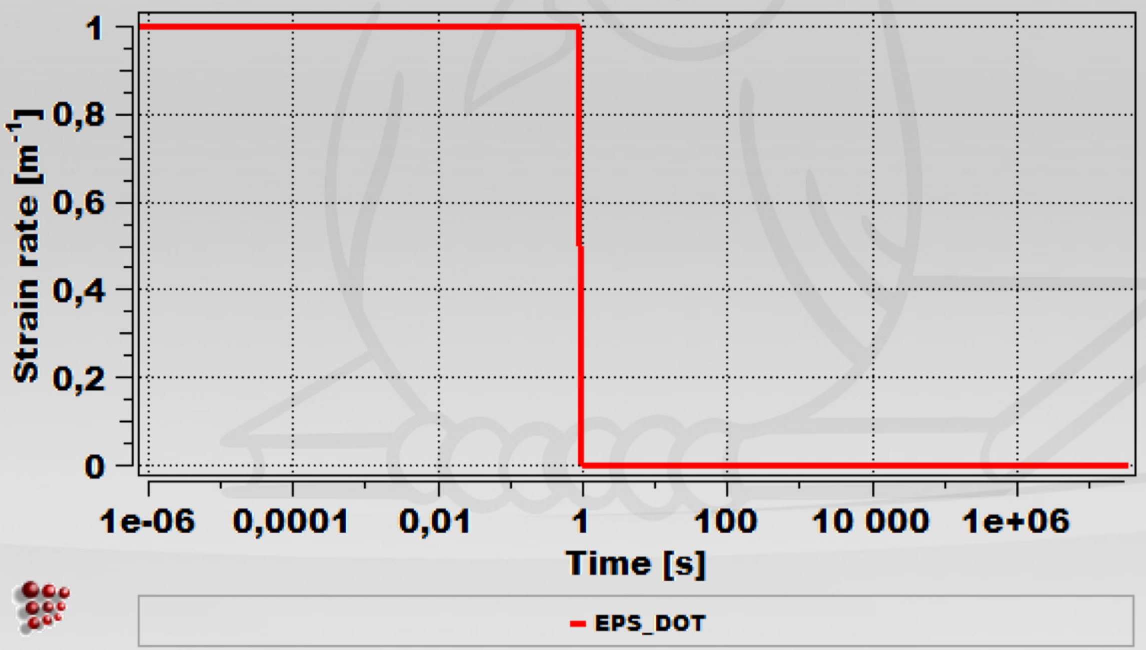

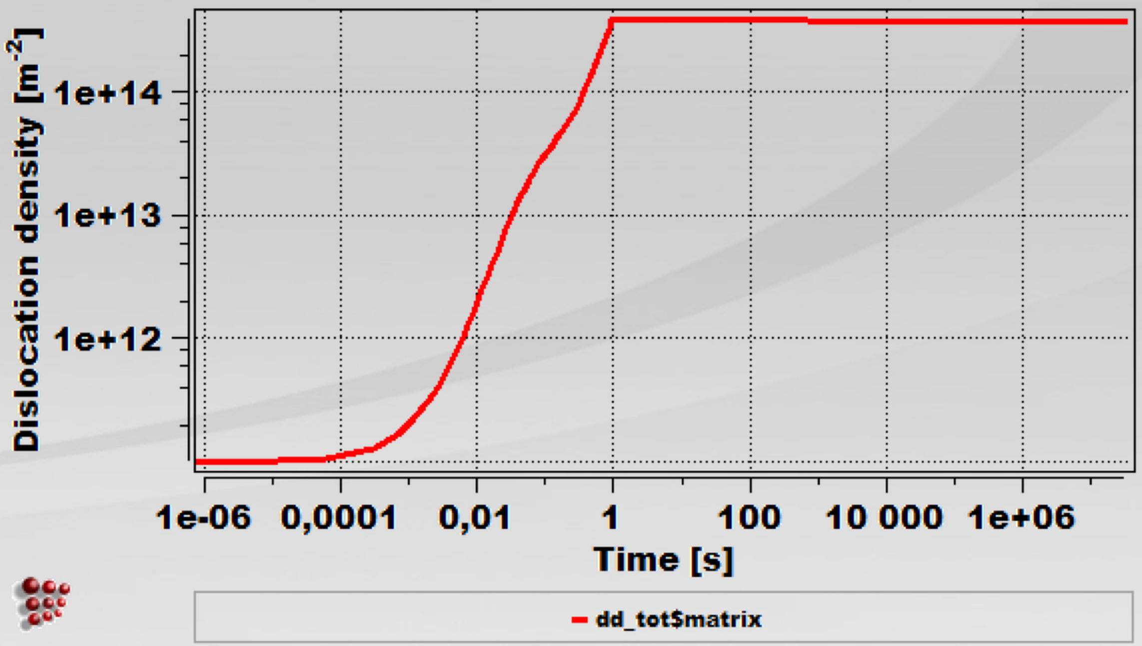

Al, 400°C isothermal, A=50, B=5, C=1e-3, Aw=250, Bw=2e-1, Cw=0 (default values)

2-parameters model

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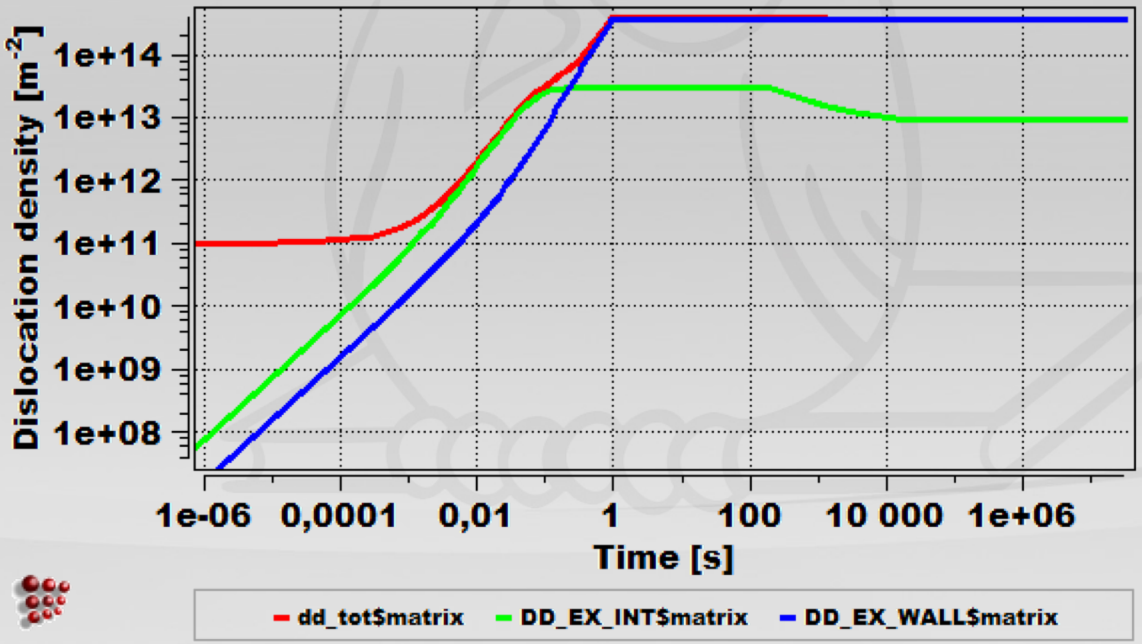

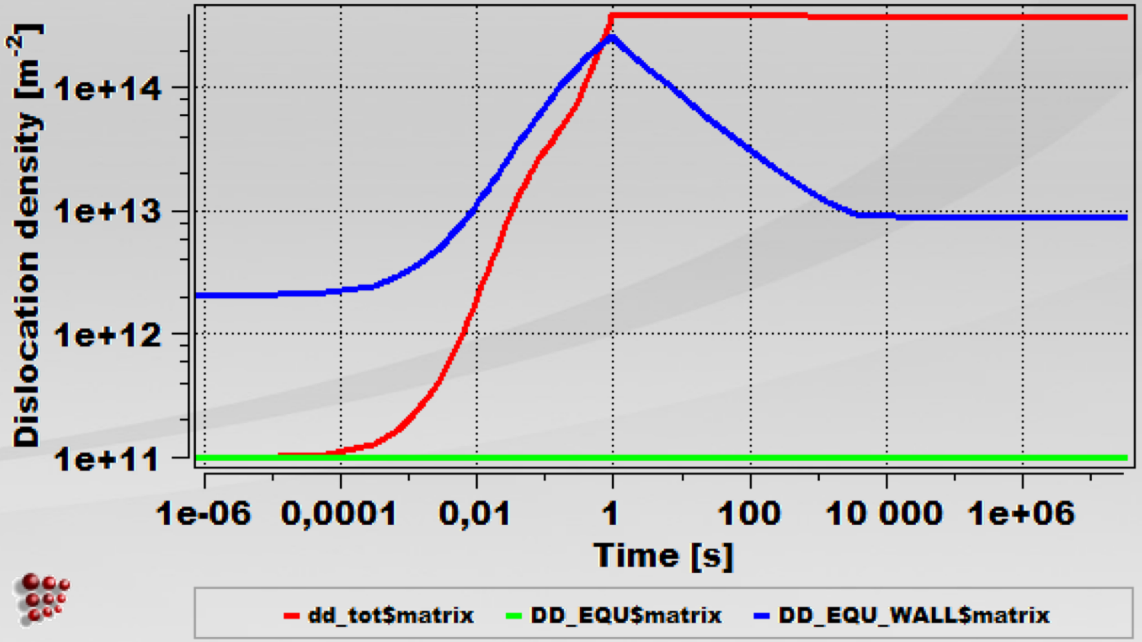

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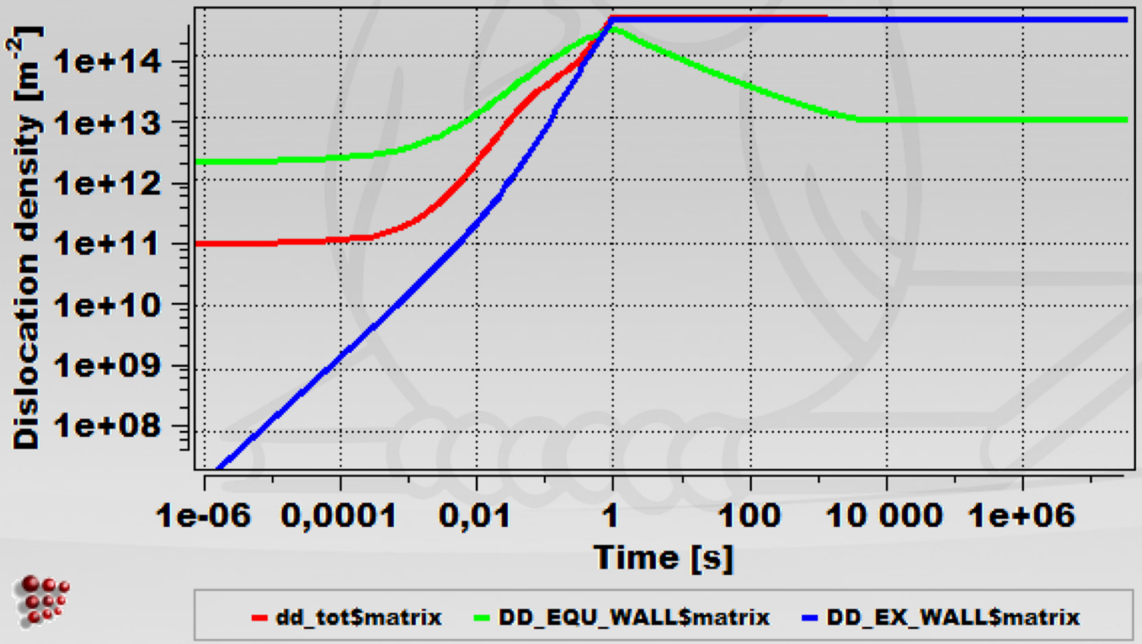

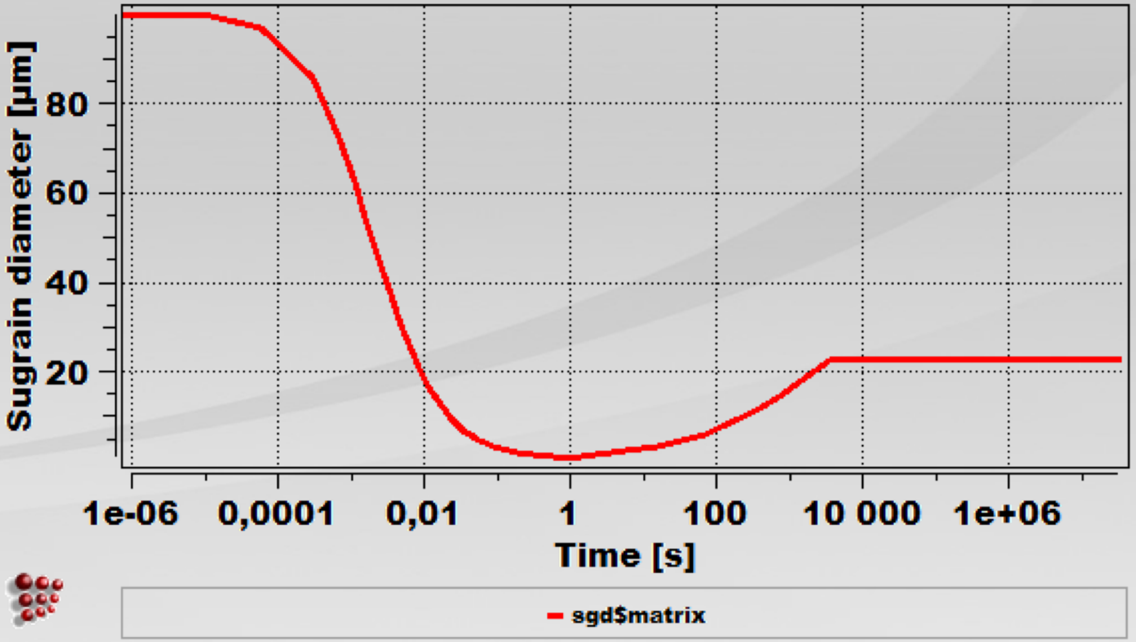

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Acknowledgments

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