MatCalc
Engineering

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

(MatCalc 6.00.0258)

P. Warczok

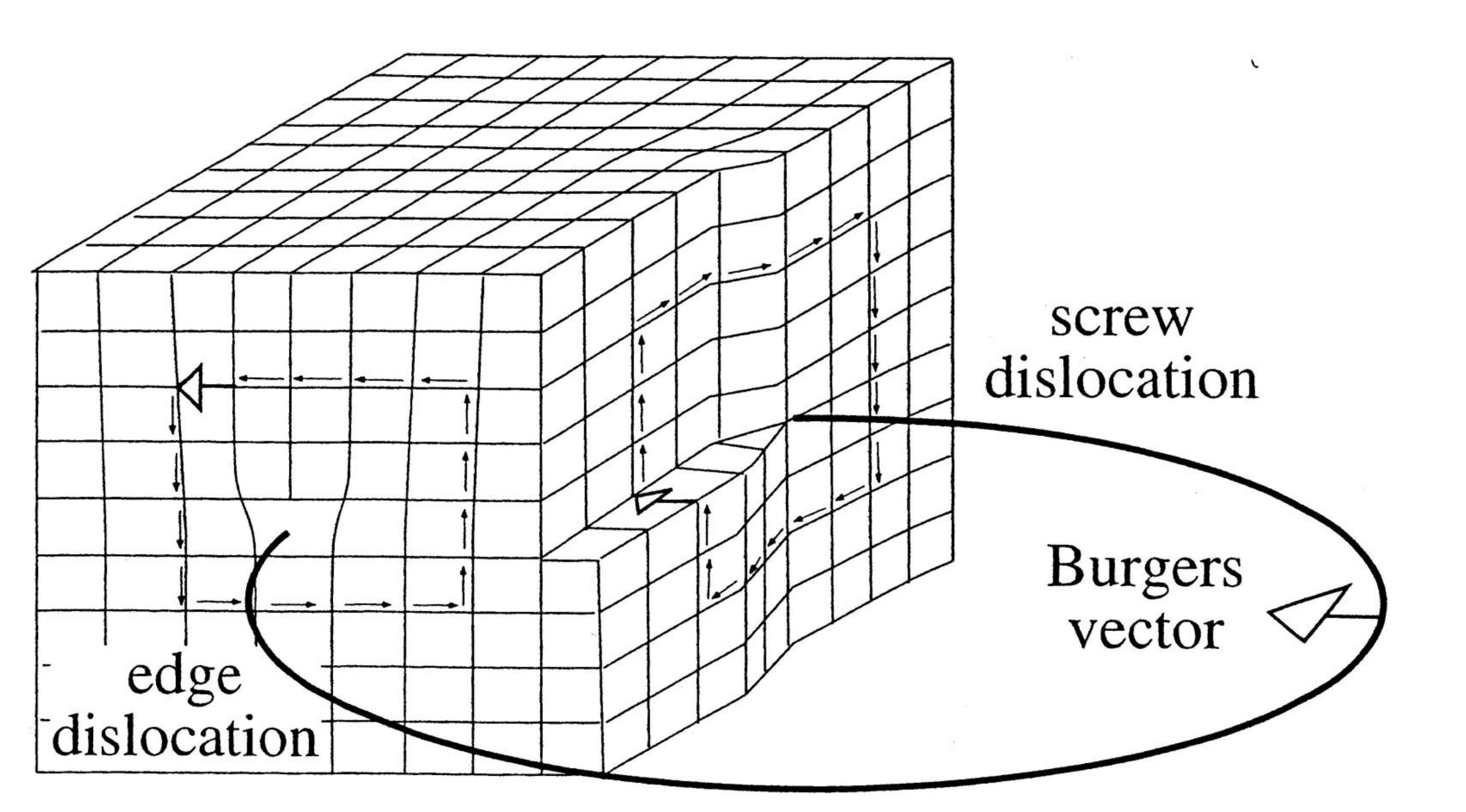
Outlook

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

Introduction to dislocations

Dislocations

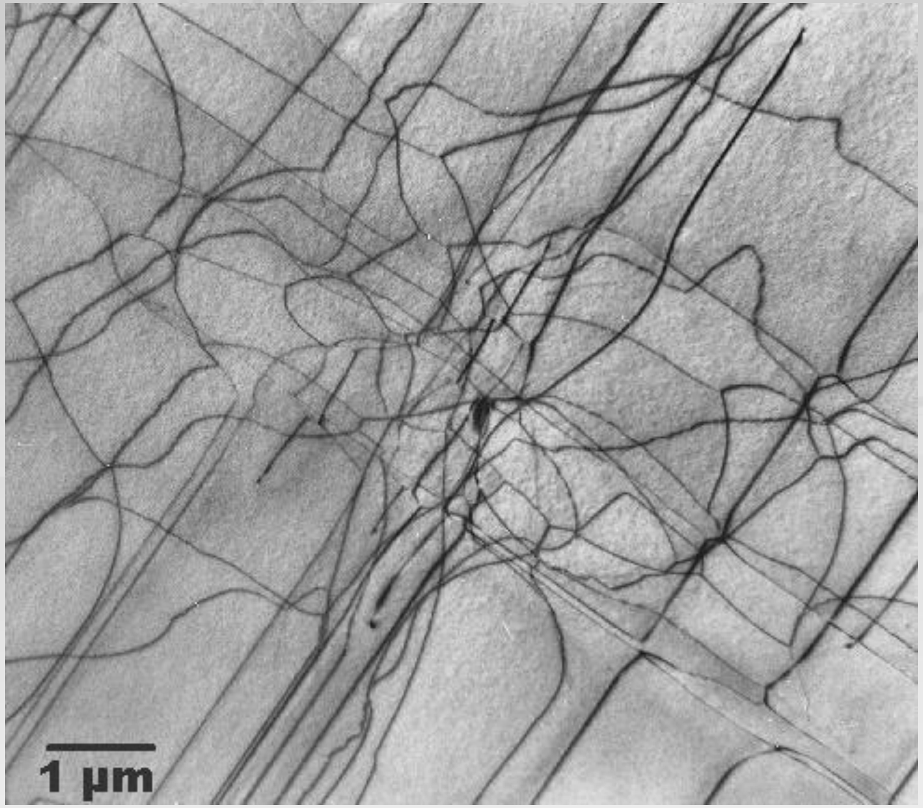
- Two geometries:
  - Edge
  - Screw



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

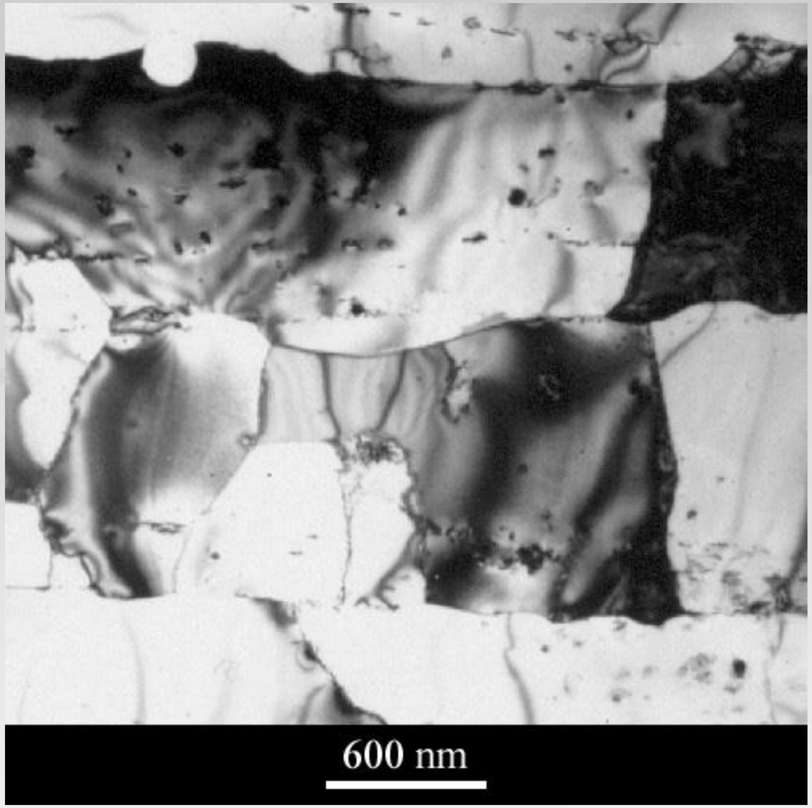
Dislocations

Internal dislocations



https://www.tf.uni-kiel.de/matwis/amat/iss/kap_5/illustr/misfit_dislocations_si.gif

Wall dislocations



https://www.flickr.com/photos/core-materials/3840257277

Dislocations & subgrains

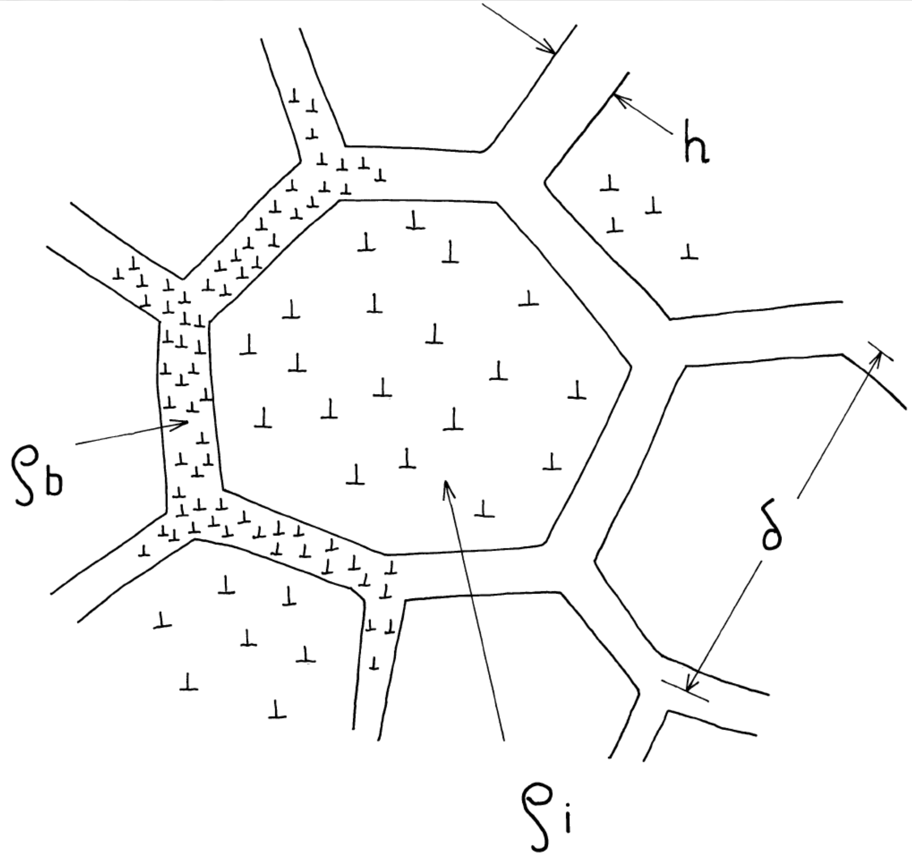


Fig. 7. A schematic representation of the microstructure; cell diameter, δ, cell wall thickness, h, cell wall dislocation density, ρ_b and dislocation density within the cells, ρ_i

E. Nes, Prog. Mater. Sci. 41 (1998) p.129-193

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

- Stress in material increases with dislocation density
- Flow curve analysis
  - Various stages in dislocation density evolution
  - Dislocation density saturation expected at some point

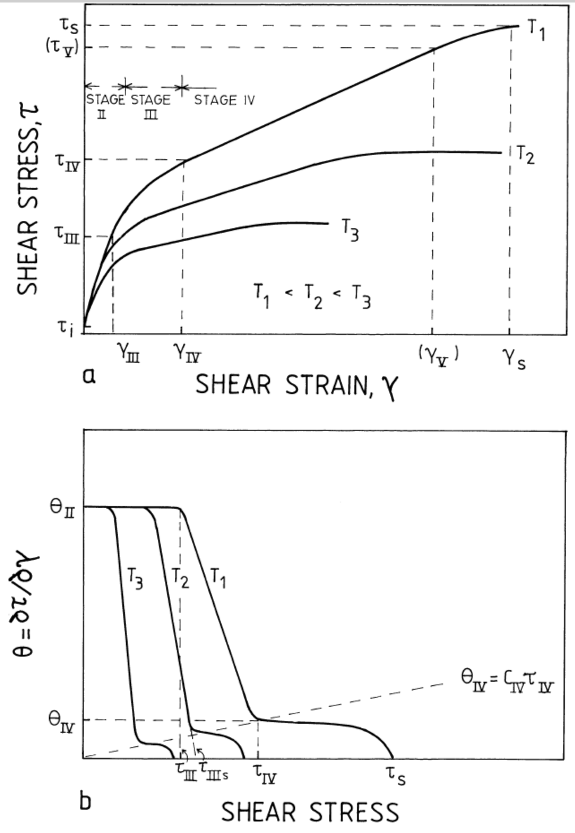
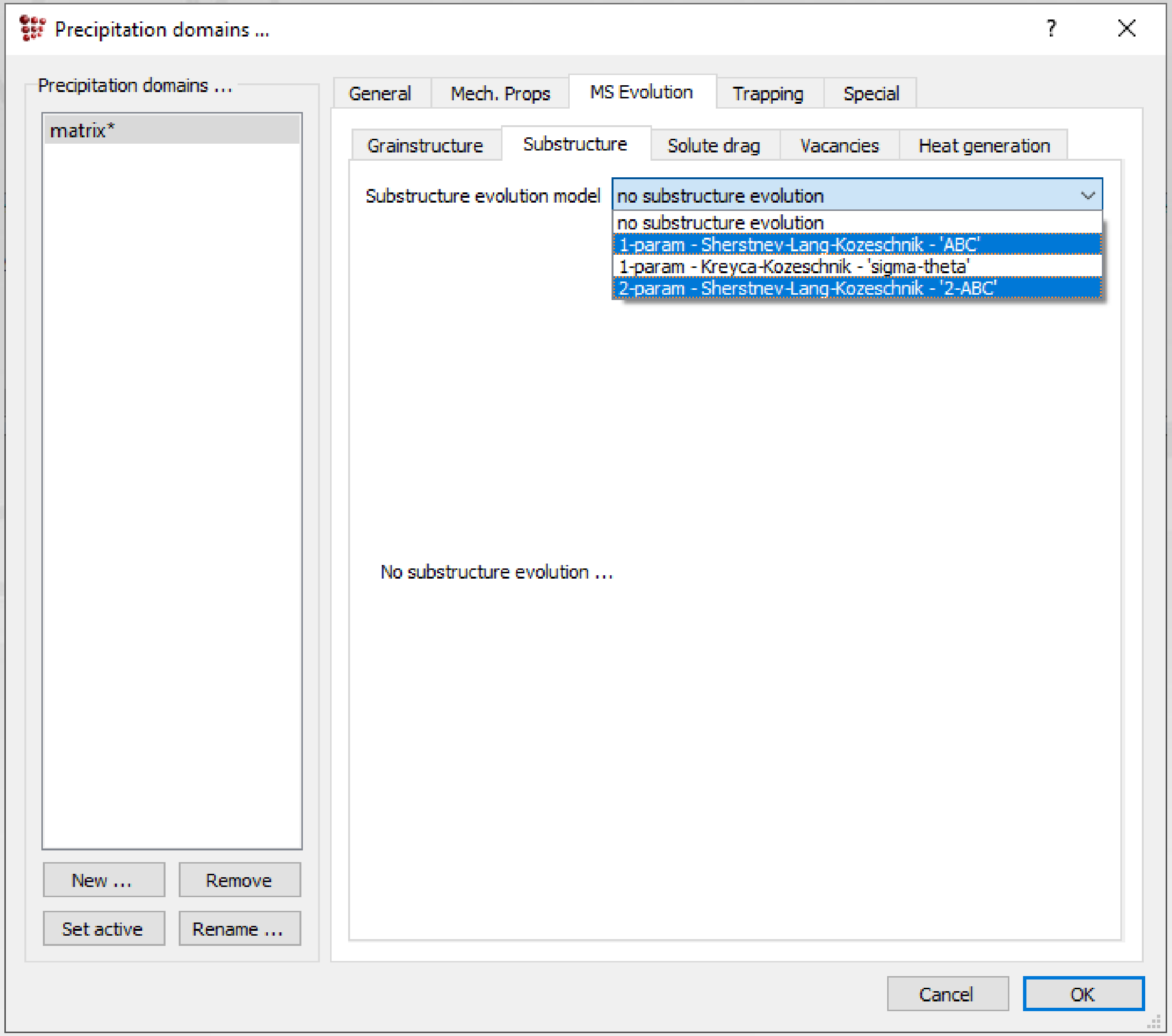


Fig. 1. (a) Schematic stress–strain curves and (b) strain hardening (θ) vs flow stress (τ) curves for fcc-metals

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 density evolution

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Dislocation generation (deformation)

$$\dot{\rho}_1 = A^{-1} \frac{M}{b} \dot{\varepsilon} \sqrt{\rho}$$

ρ - Dislocation density

A - A-parameter (constant)

M - Taylor factor

$\dot{\varepsilon}$ - Strain rate

b - Burgers vector

Dislocation generation (deformation)

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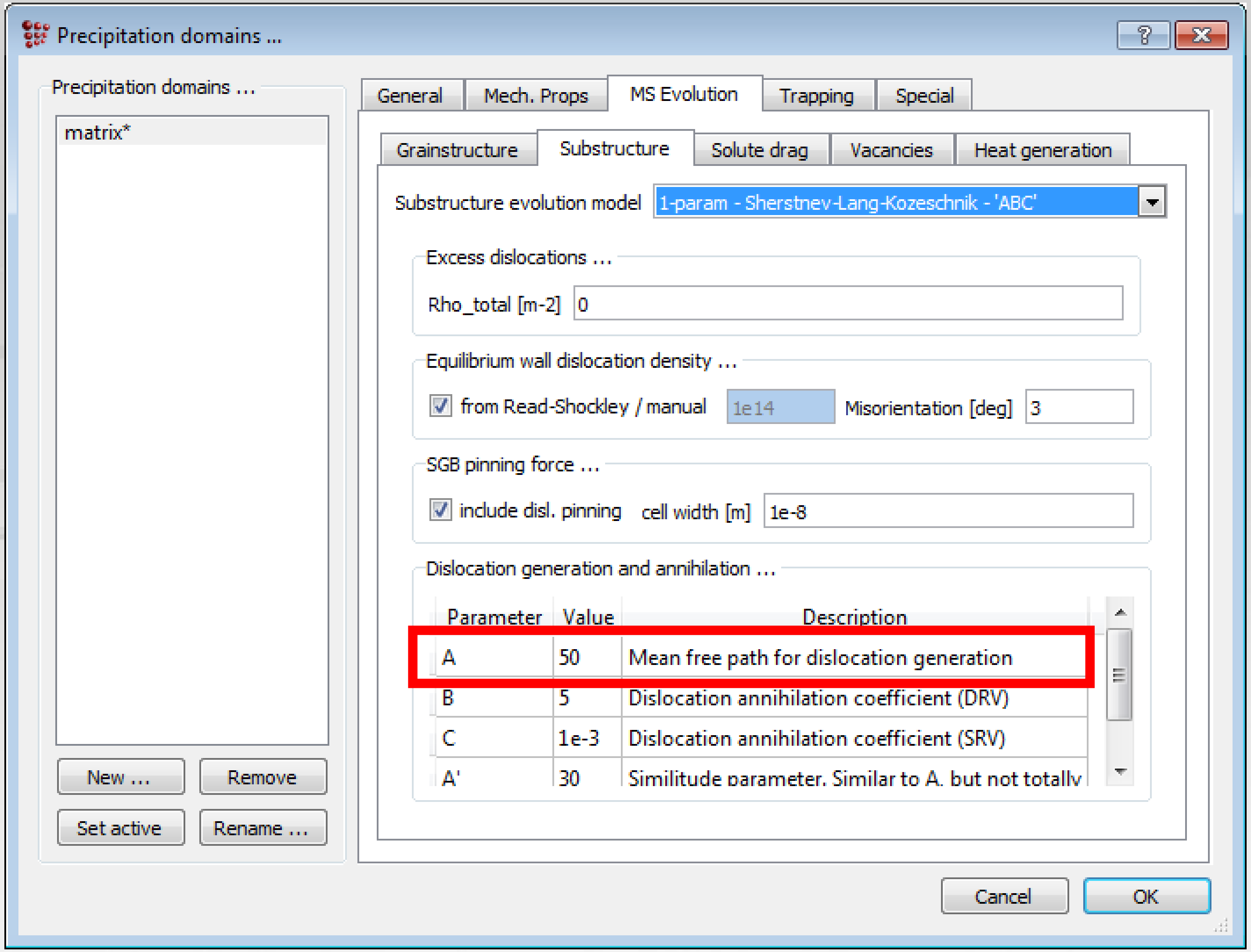

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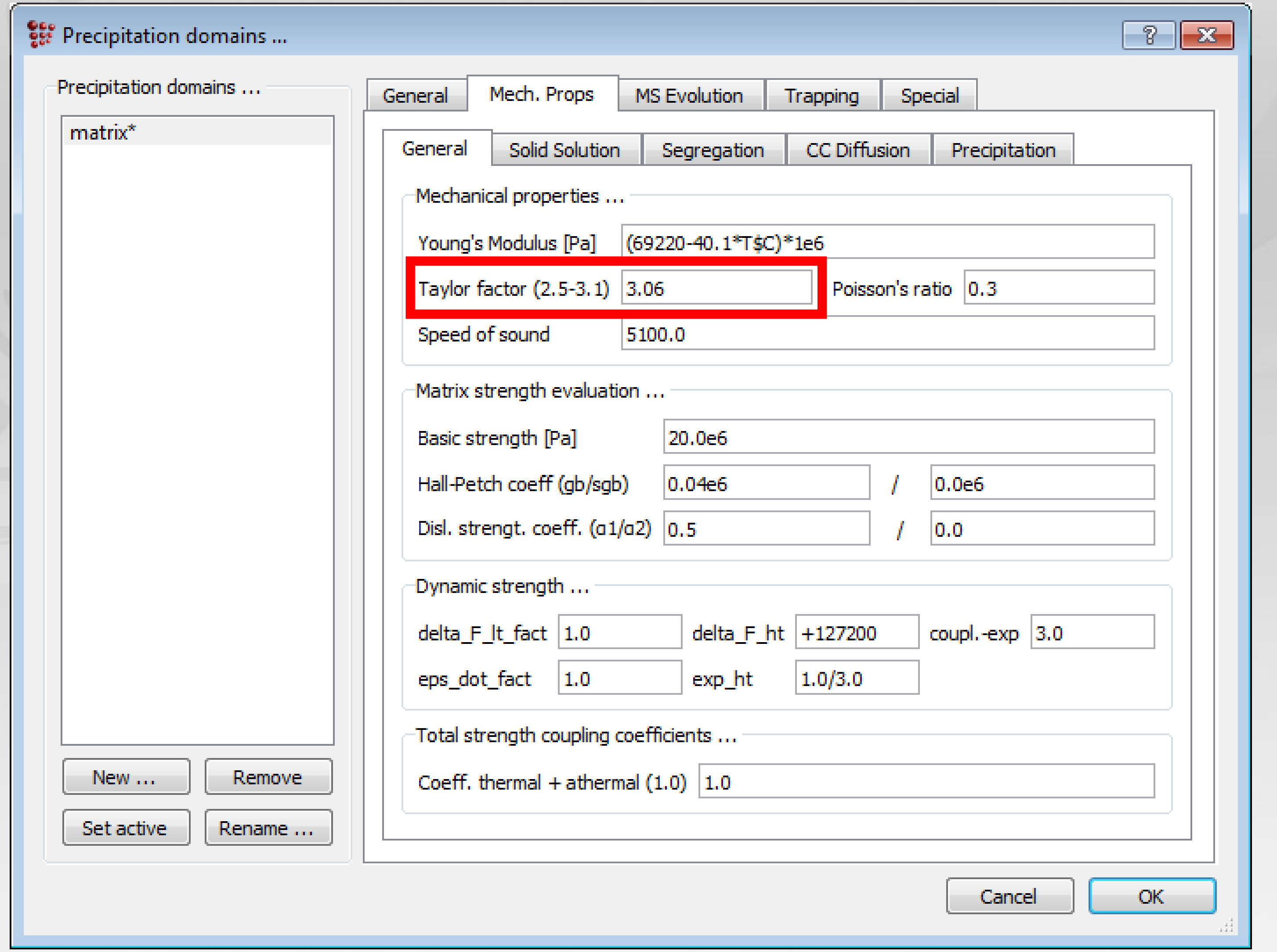

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Dislocation generation (deformation)

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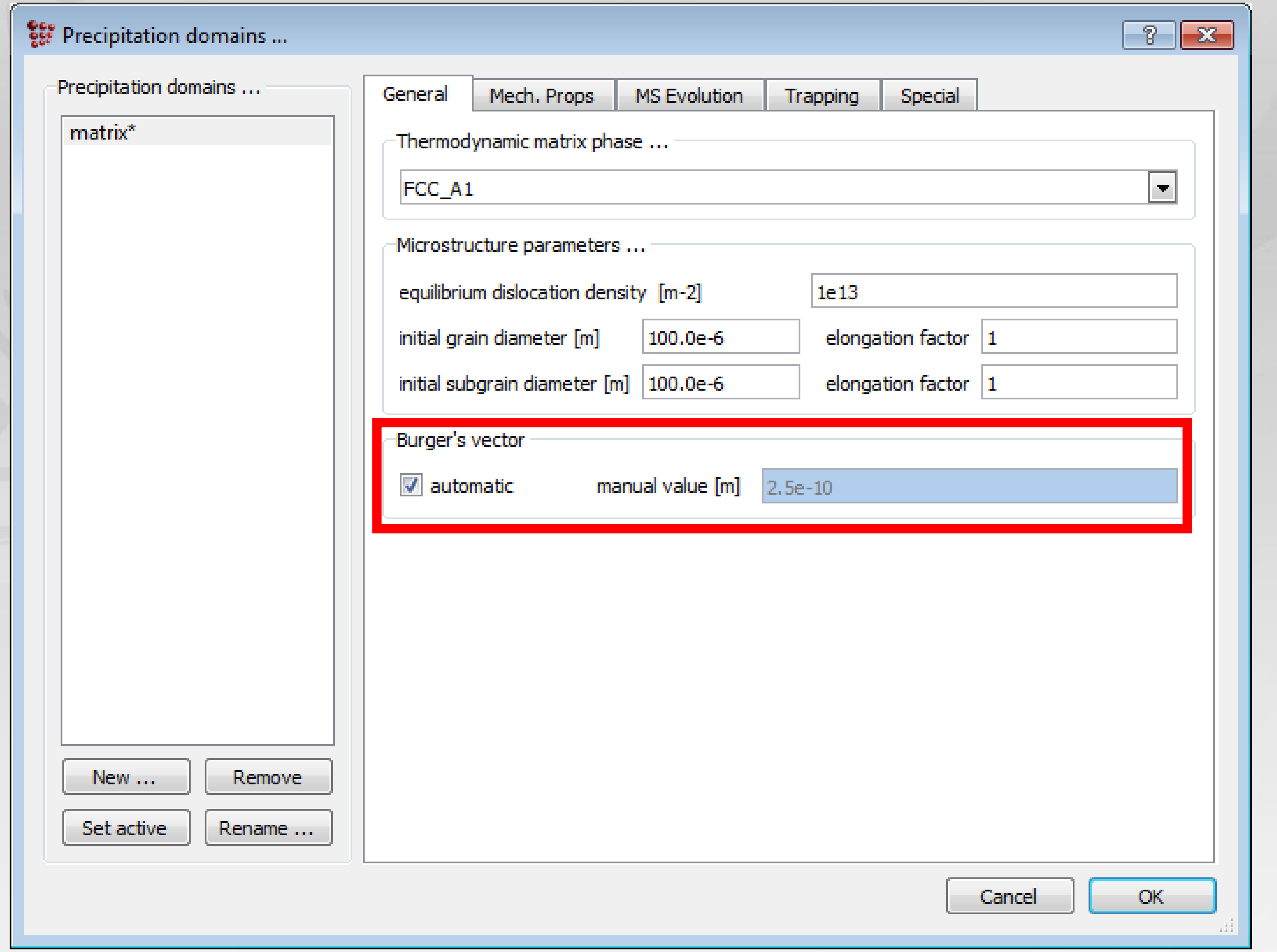

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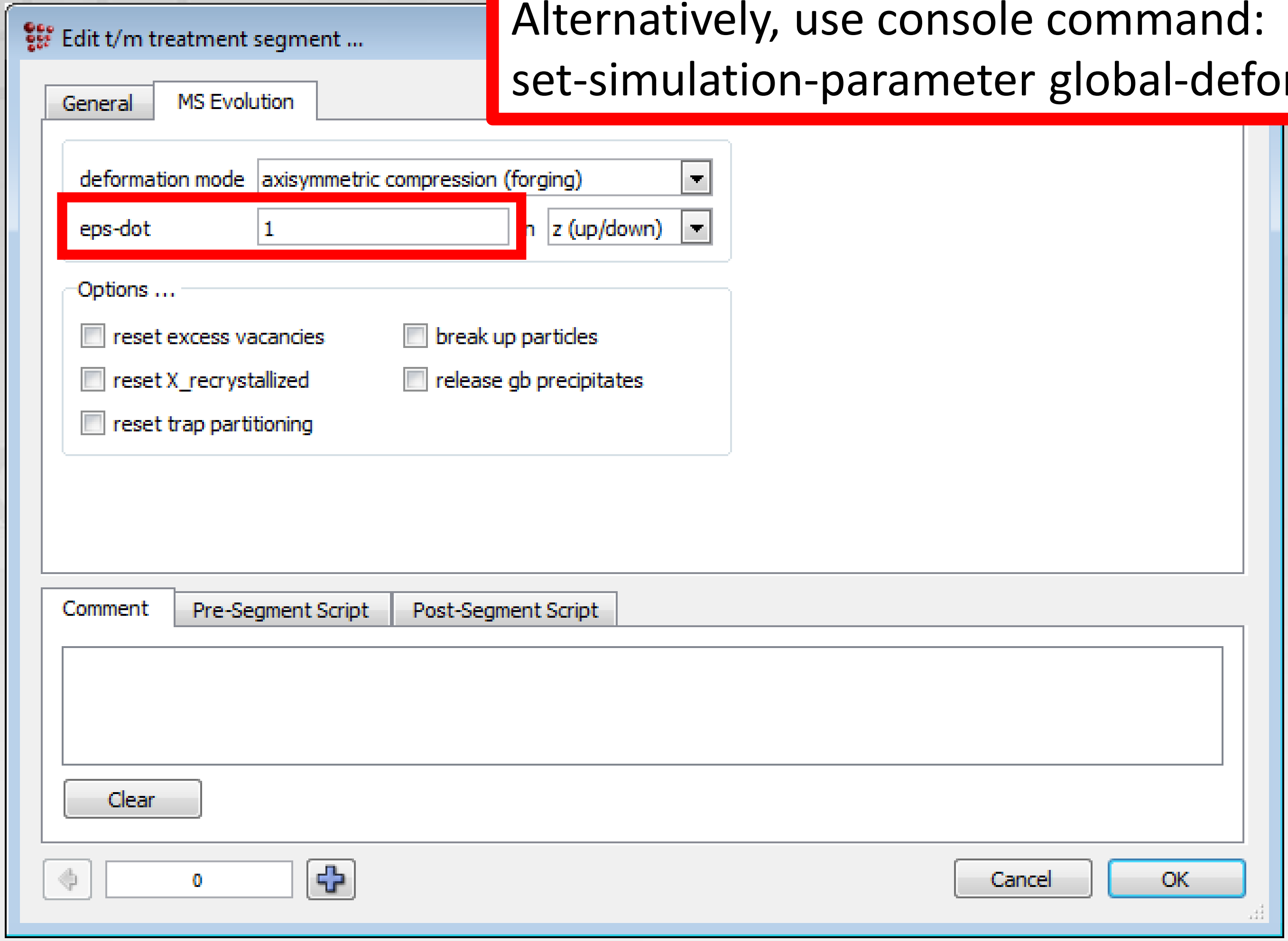
Dislocation generation (deformation)

$$\dot{\rho}_1 = A^{-1}\frac{M}{b}\dot{\varepsilon}\sqrt{\rho}$$

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



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Dislocation density evolution

$$\dot{\rho} = \dot{\rho_1} - \dot{\rho_2} - \dot{\rho_3}$$

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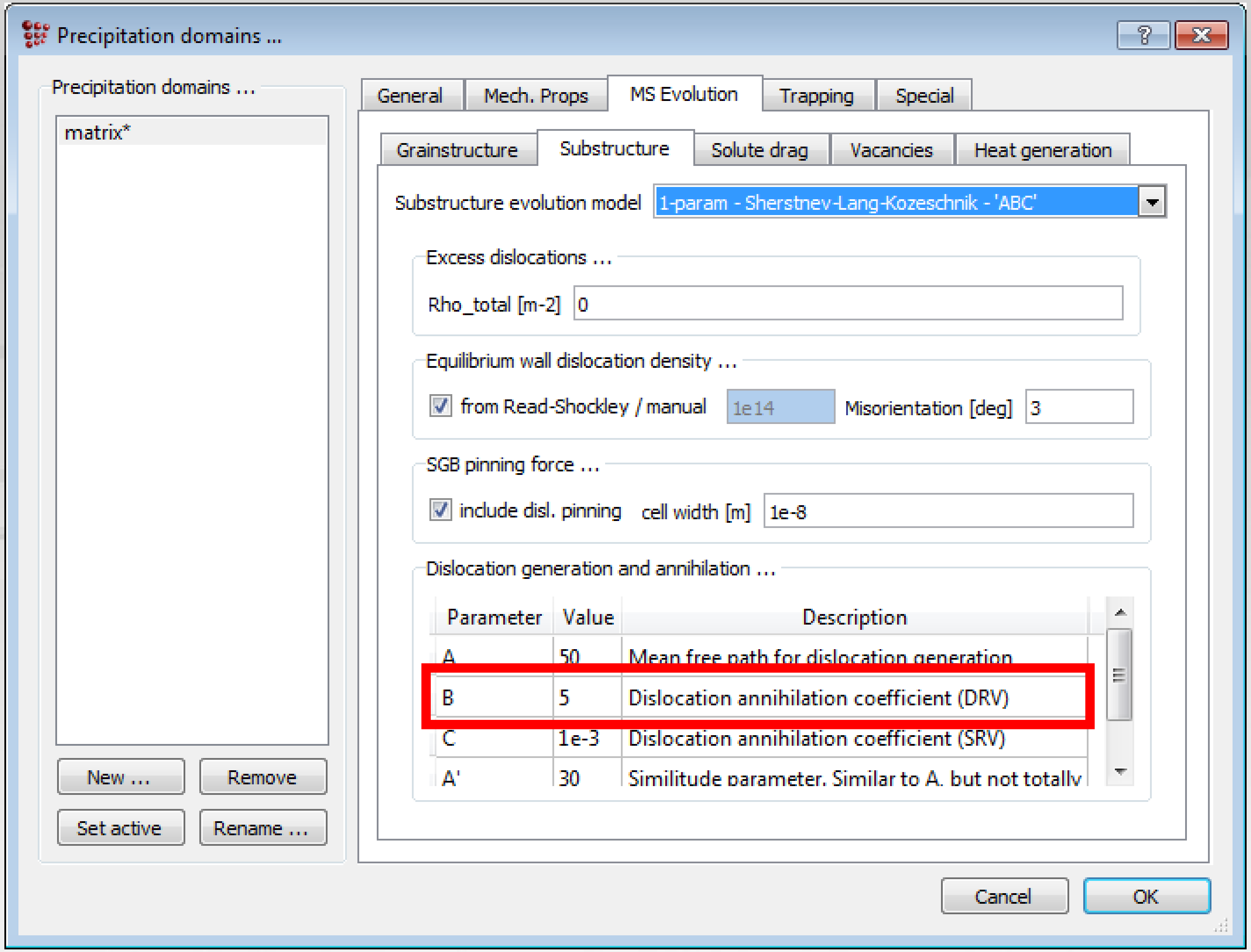
  - Dynamic recovery (dislocations with antiparallel Burgers vectors hit each other) → $\dot{\rho_2}$
  - Static recovery (dislocation climb) → $\dot{\rho_3}$

Dislocation annihilation (dynamic recovery)

$$\dot{\rho}_2 = \boxed{B} \frac{2Md_{ann}}{b} \dot{\varepsilon}\rho$$

B - B-parameter (constant)

d_{ann} - Annihilation distance



Dislocation annihilation (dynamic recovery)

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

d_{ann} - Annihilation distance

G - Shear modulus

ν - Poisson ratio

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

N_A - Avogadro constant

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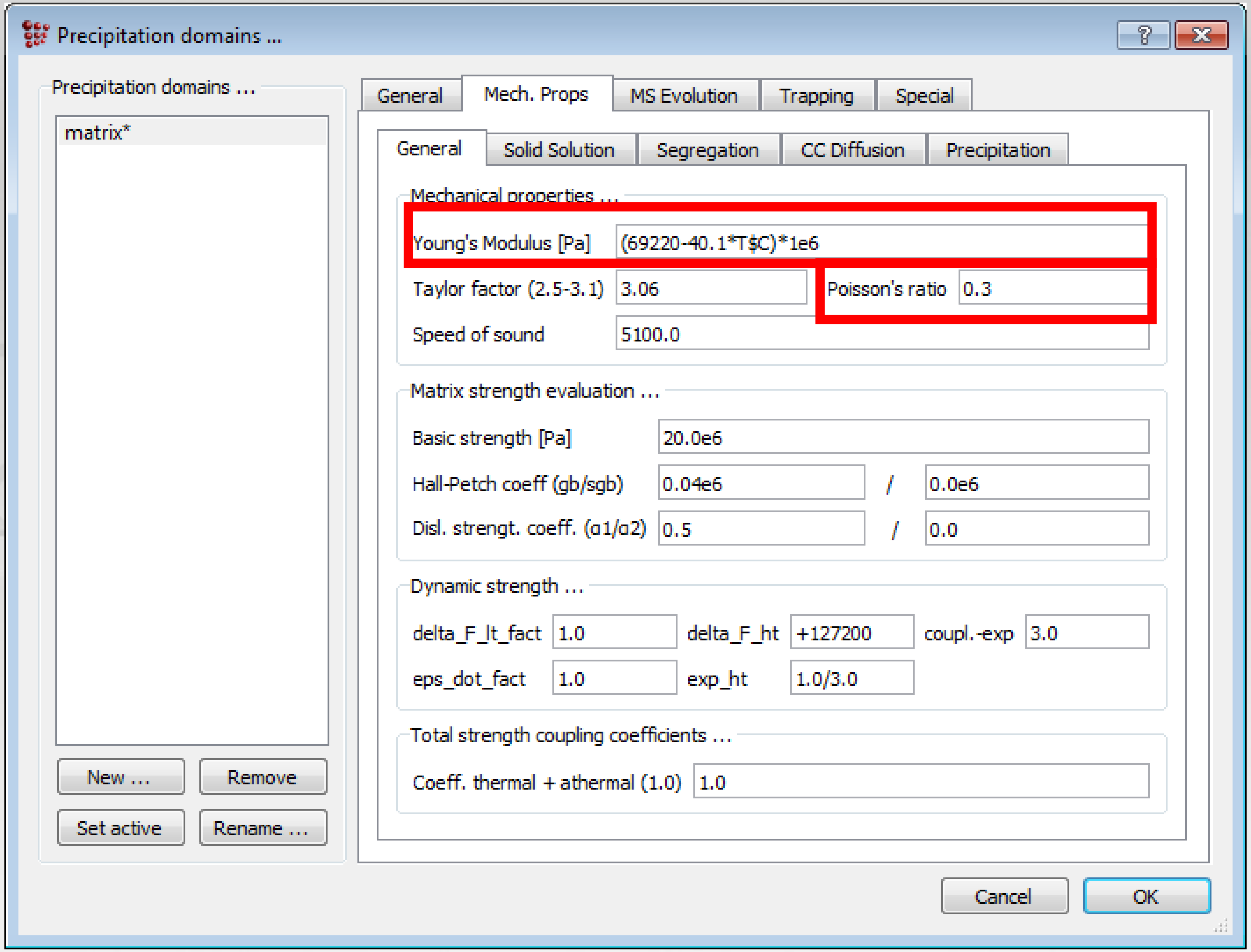
Dislocation annihilation (dynamic recovery)

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



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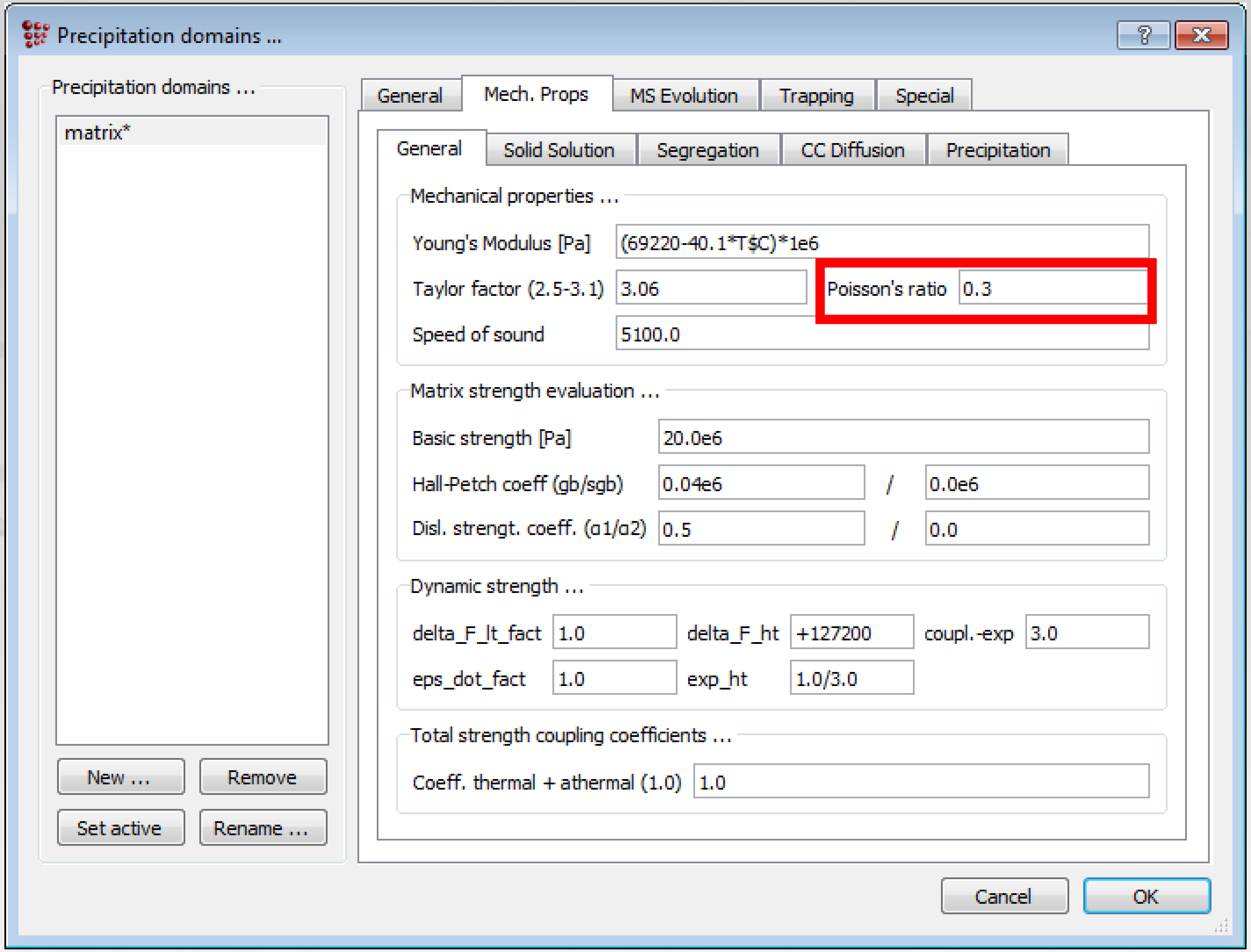

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Dislocation density evolution

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Dislocation annihilation (static recovery)

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

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

k_B - Boltzmann constant

T - Temperature

C - C-parameter (constant)

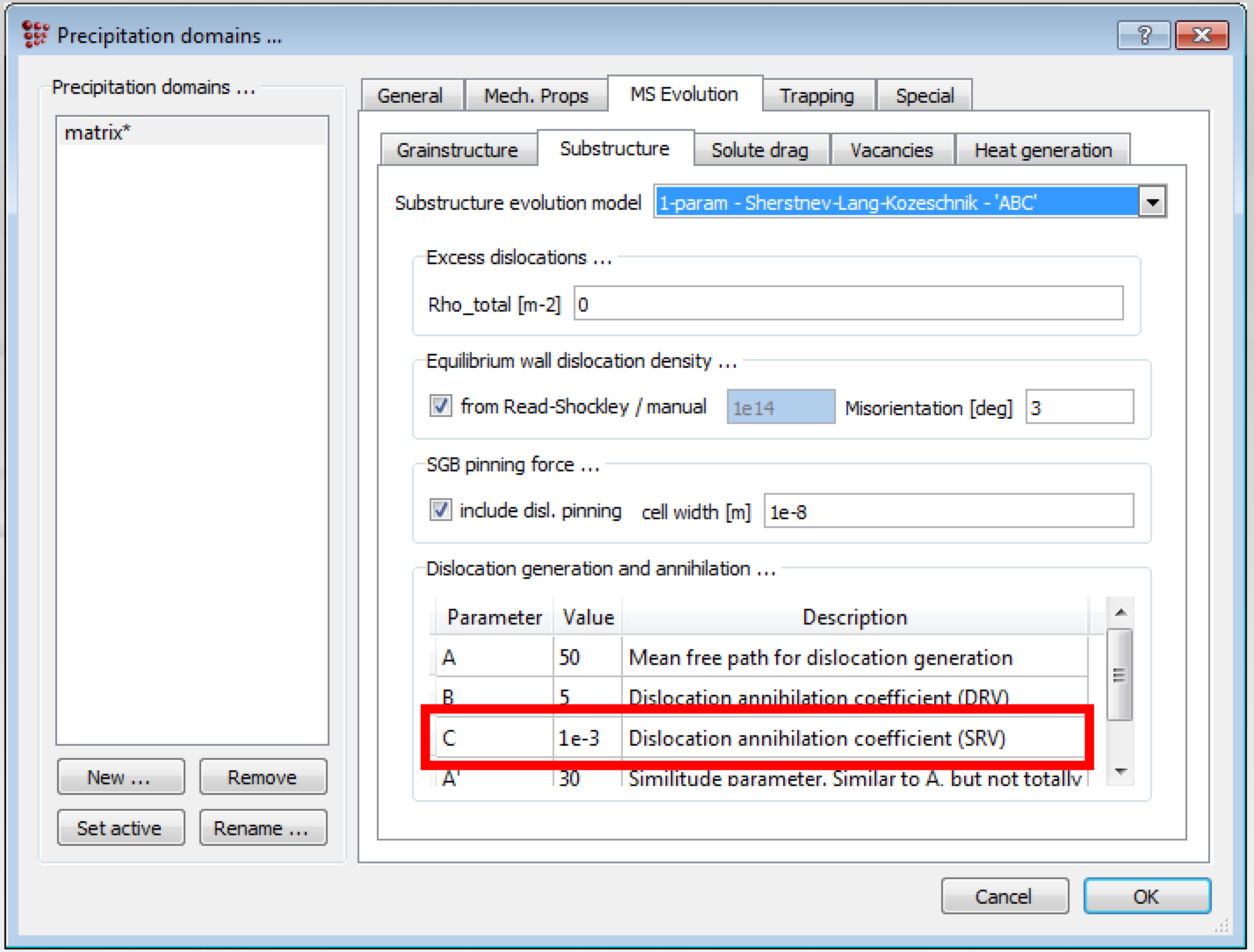
ρ_{eq} - Equilibrium dislocation density

Dislocation annihilation (static recovery)

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

C - C-parameter (constant)

ρ_{eq} - Equilibrium dislocation density (sum of equilibrium values for intrinsic and wall dislocations)



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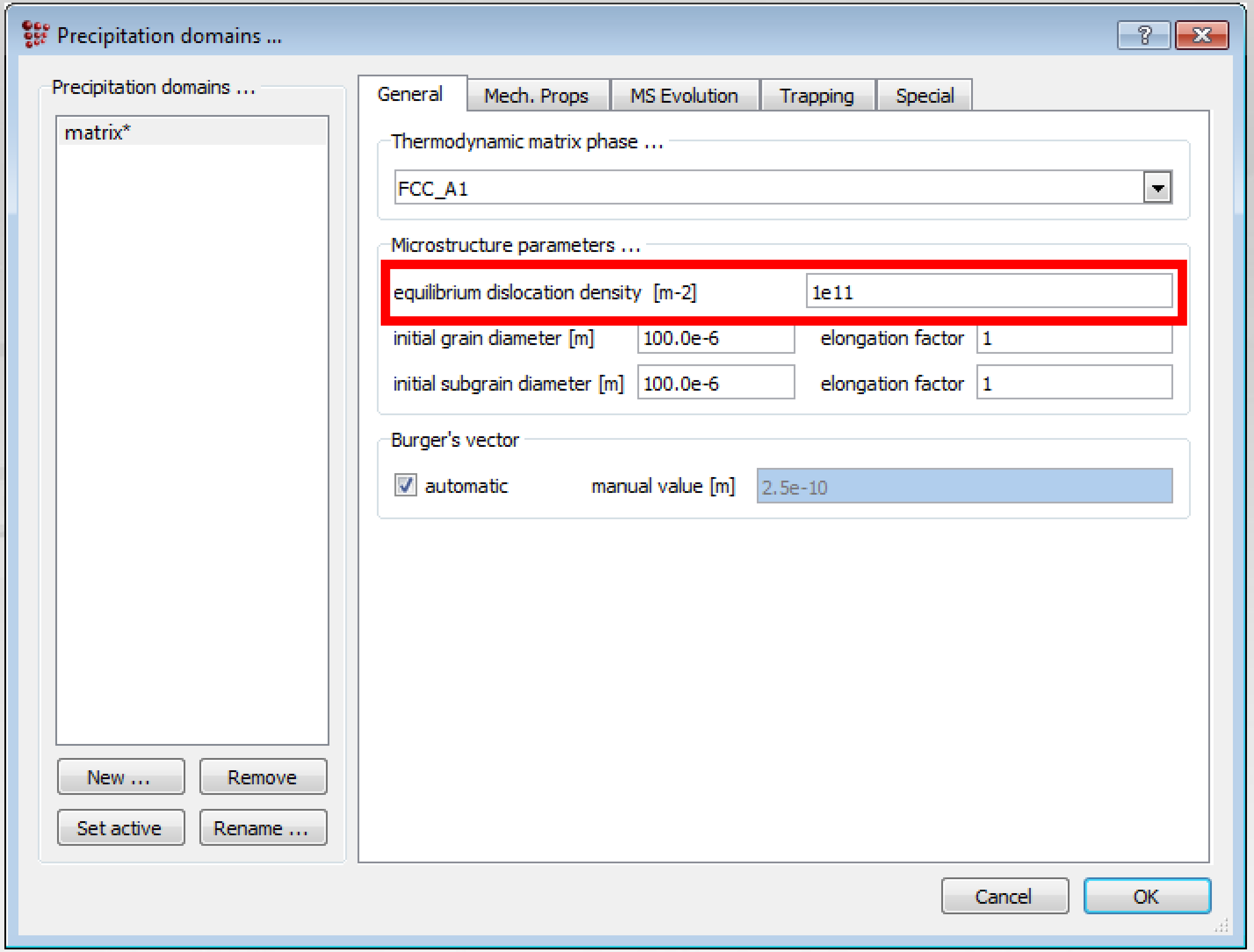

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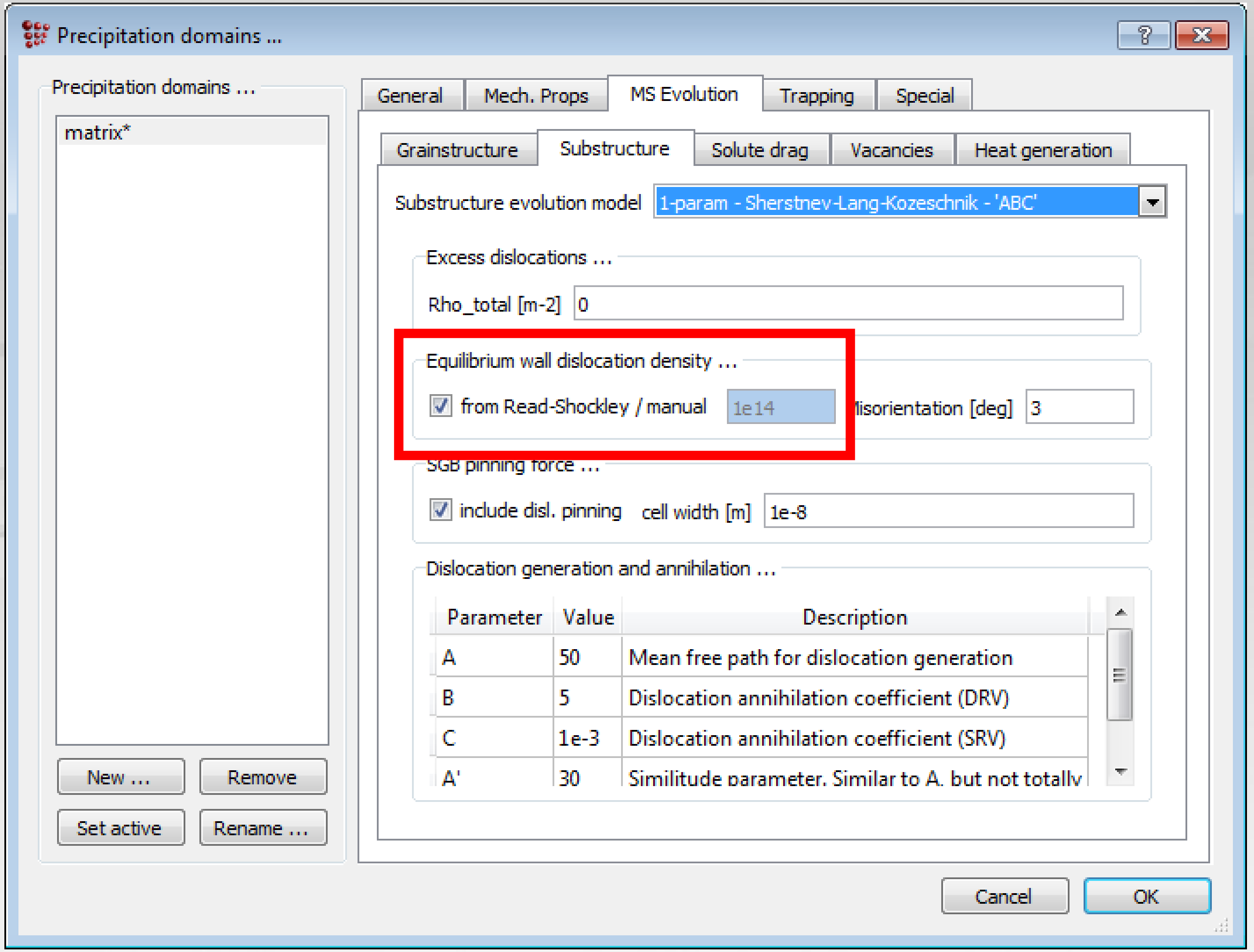

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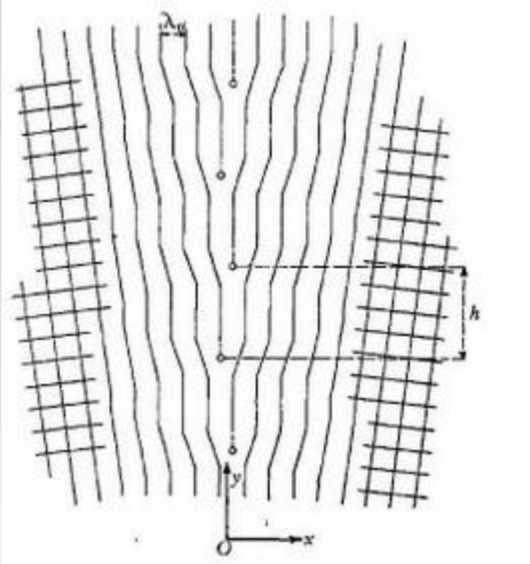
Wall dislocation density (1-parameter model)

- Taken as Read-Shockley dislocation density → necessary amount to fulfill geometrical constraint for subgrains with a given misorientation angle and size

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

θ - Misorientation angle

δ - Subgrain diameter



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

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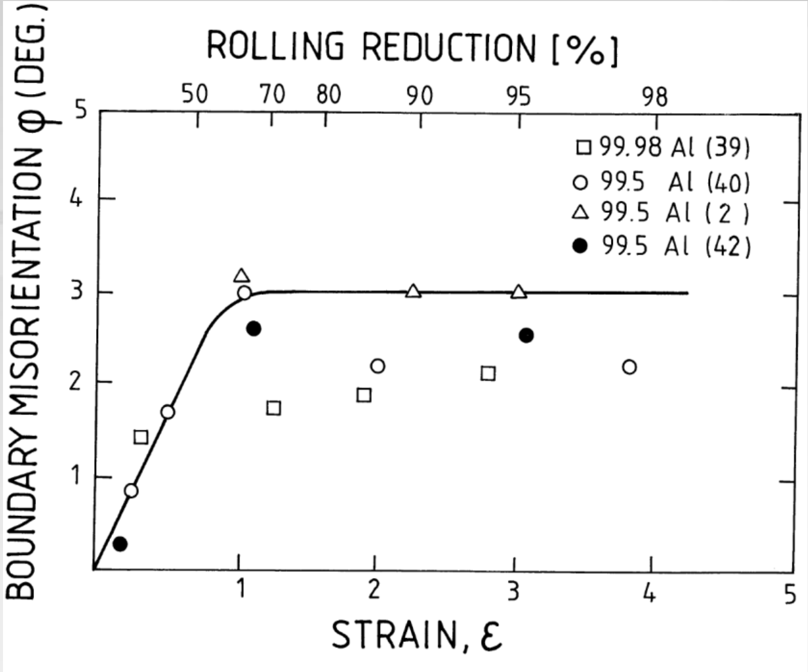

Fig. 6. Sub-boundary misorientation vs strain(2)

E. Nes, Prog. Mater. Sci. 41 (1998) p.129-193

Read-Shockley dislocation density

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

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

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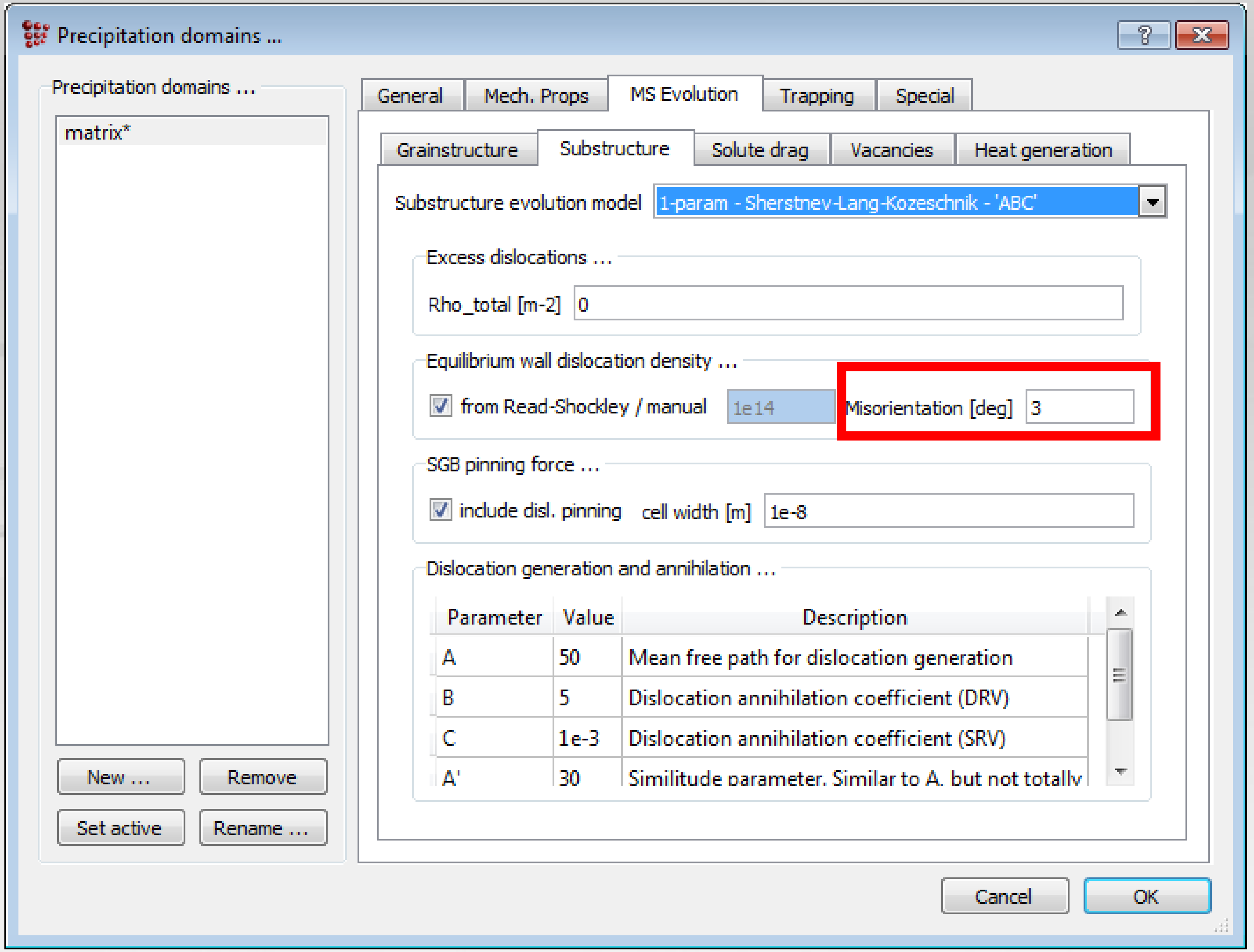

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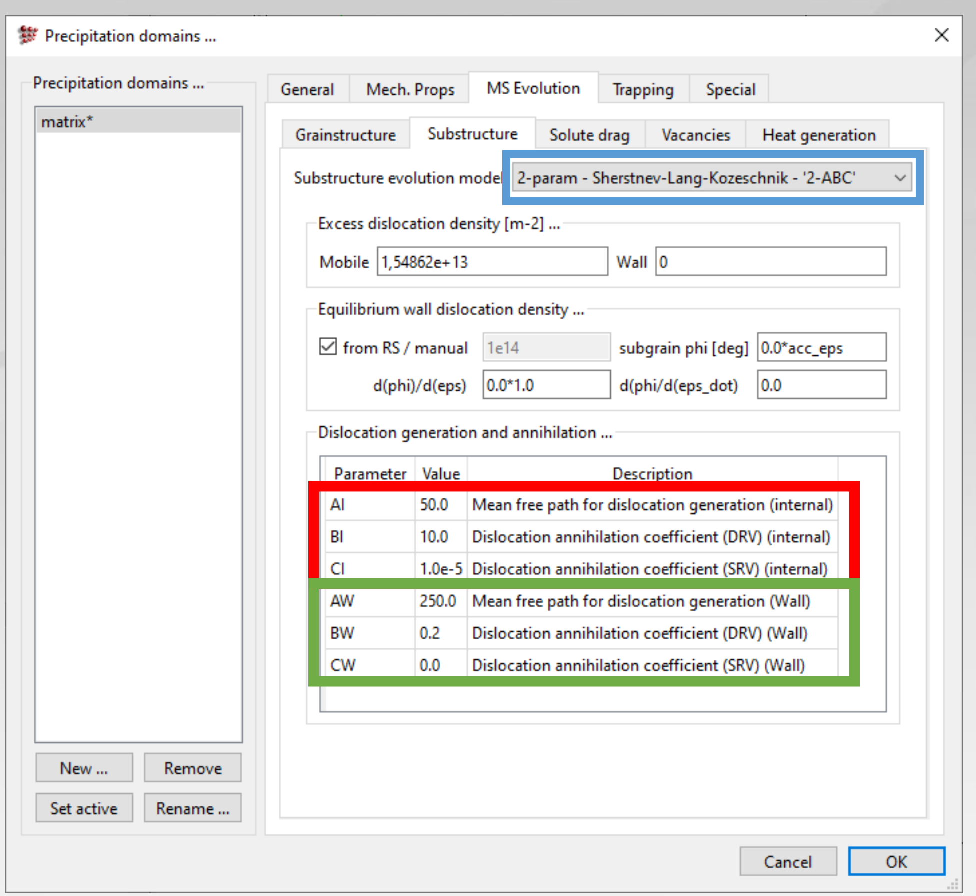
Wall dislocation density (2-parameter model)

- Separate equations for internal and wall dislocations
  - Internal dislocations

$$\dot{\rho}_i = \dot{\rho}_{i,1} - \dot{\rho}_{i,2} - \dot{\rho}_{i,3}$$

  - Wall dislocations

$$\dot{\rho}_w = \dot{\rho}_{w,1} - \dot{\rho}_{w,2} - \dot{\rho}_{w,3}$$



Subgrain size evolution

(only when a subgrain evolution model is active)

Subgrain size evolution

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

- 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 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 growth inhibition as for grain boundary mobility → same effects for precipitate pinning and solute drag

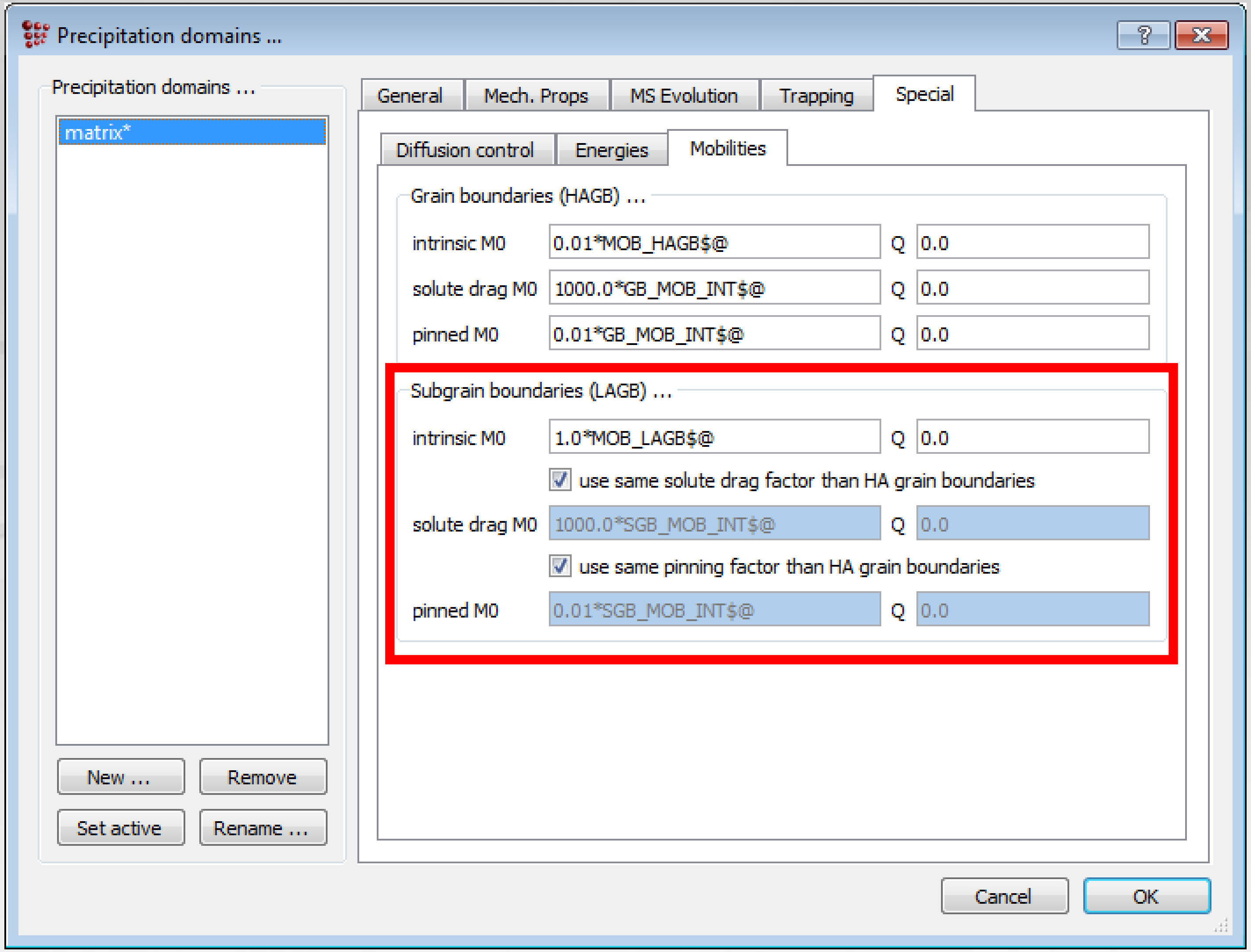
Subgrain growth

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

$$M = \eta_f \frac{D_b b^2}{k_b T}$$

D_b - Bulk diffusion coefficient

η_f - Scaling factor



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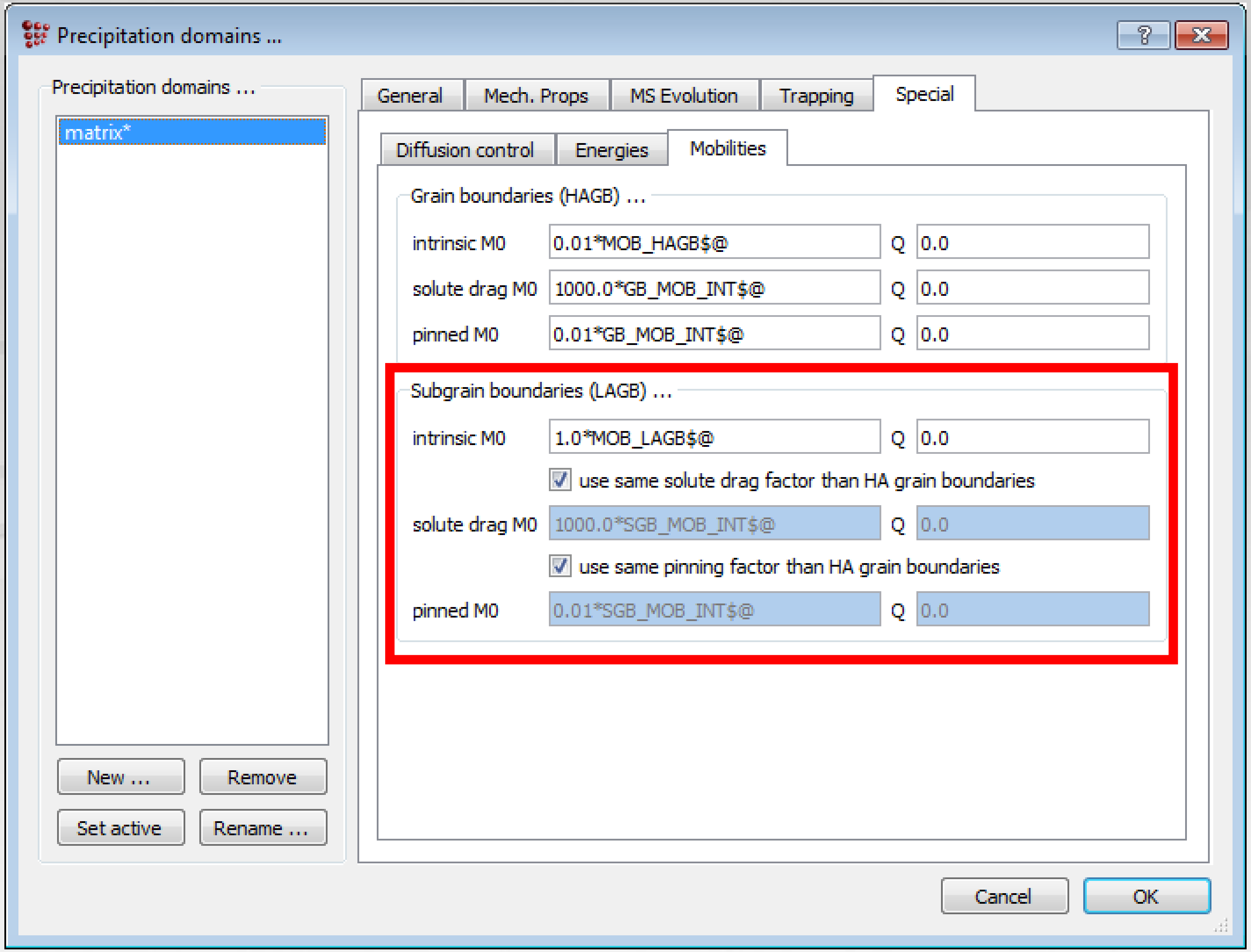
Subgrain growth

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



Same models as for grain boundary mobility

→ same effects for precipitate pinning and solute drag

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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

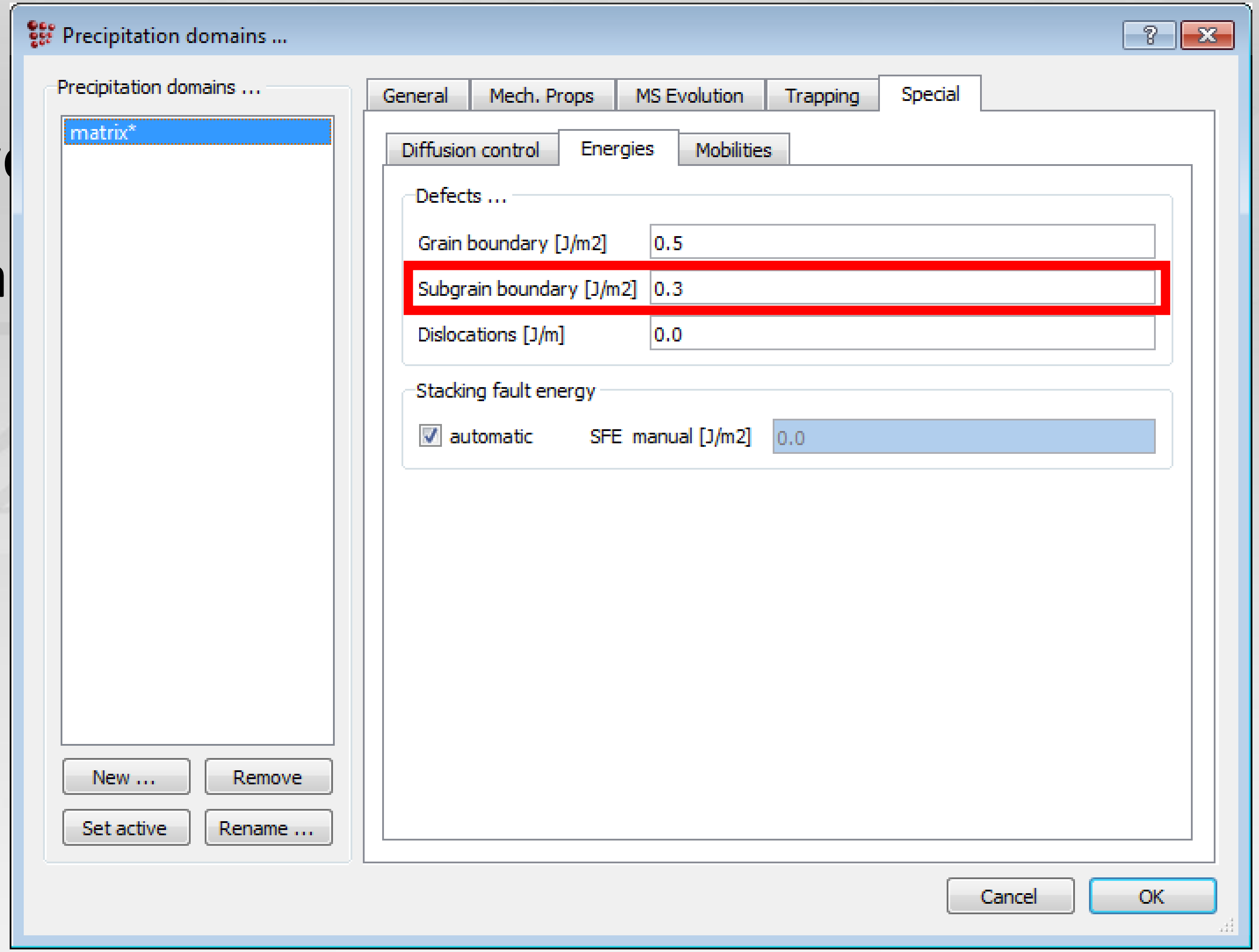
ρ_{RS} - Read-Shockley dislocation density

Subgrain growth

- Driving force – balance betw

dislocation pinning of subgra

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



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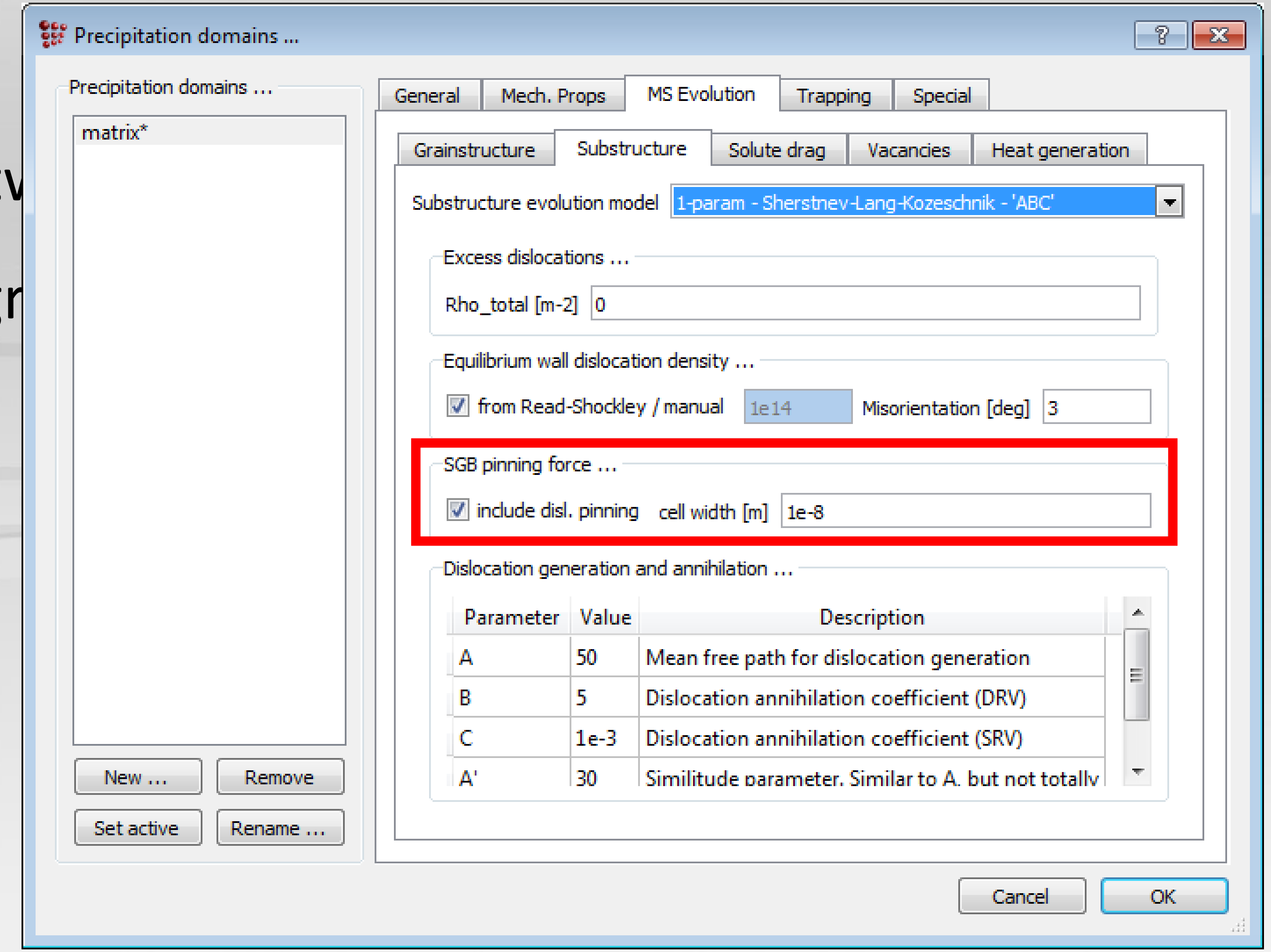


Subgrain size evolution

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

- 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 shrinkage

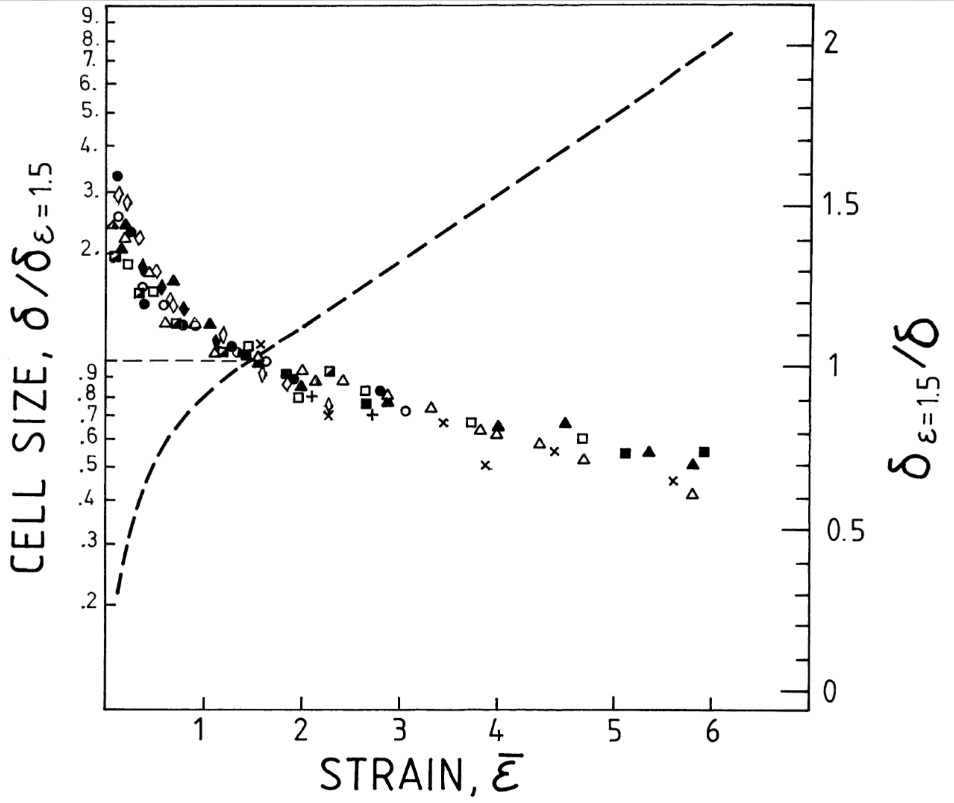
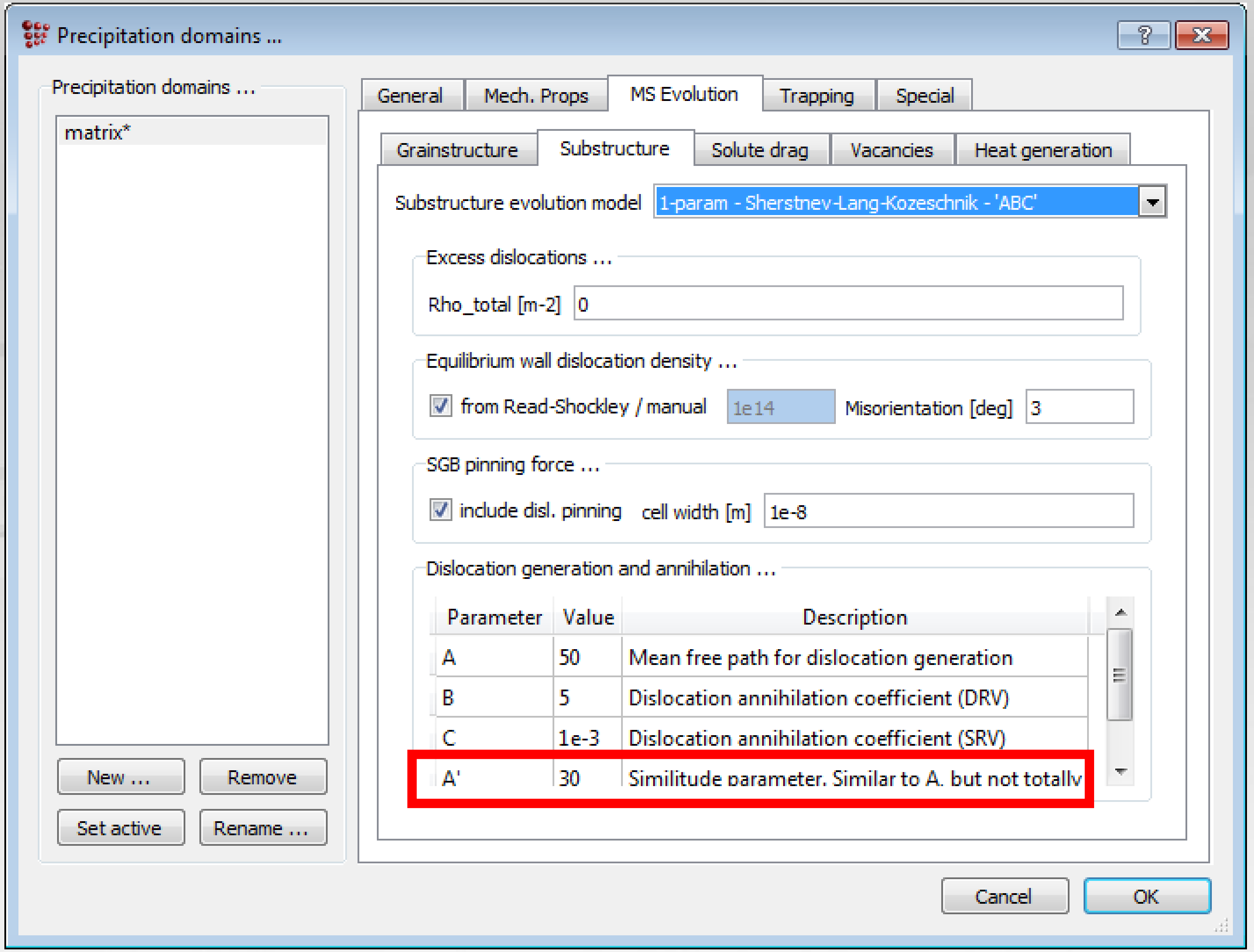


Fig. 4. Subgrain/cell size as a function of equivalent strain, from Ref.[34]

E. Nes, Prog. Mater. Sci. 41 (1998) p.129-193

Subgrain shrinkage

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



A' - A'-parameter (constant)

Acknowledgments

- Yao Shan
- Heinrich Buken

Thank you for

your attention!