Mathematical modeling of particle nucleation and growth in metallic alloys

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14-12-2009

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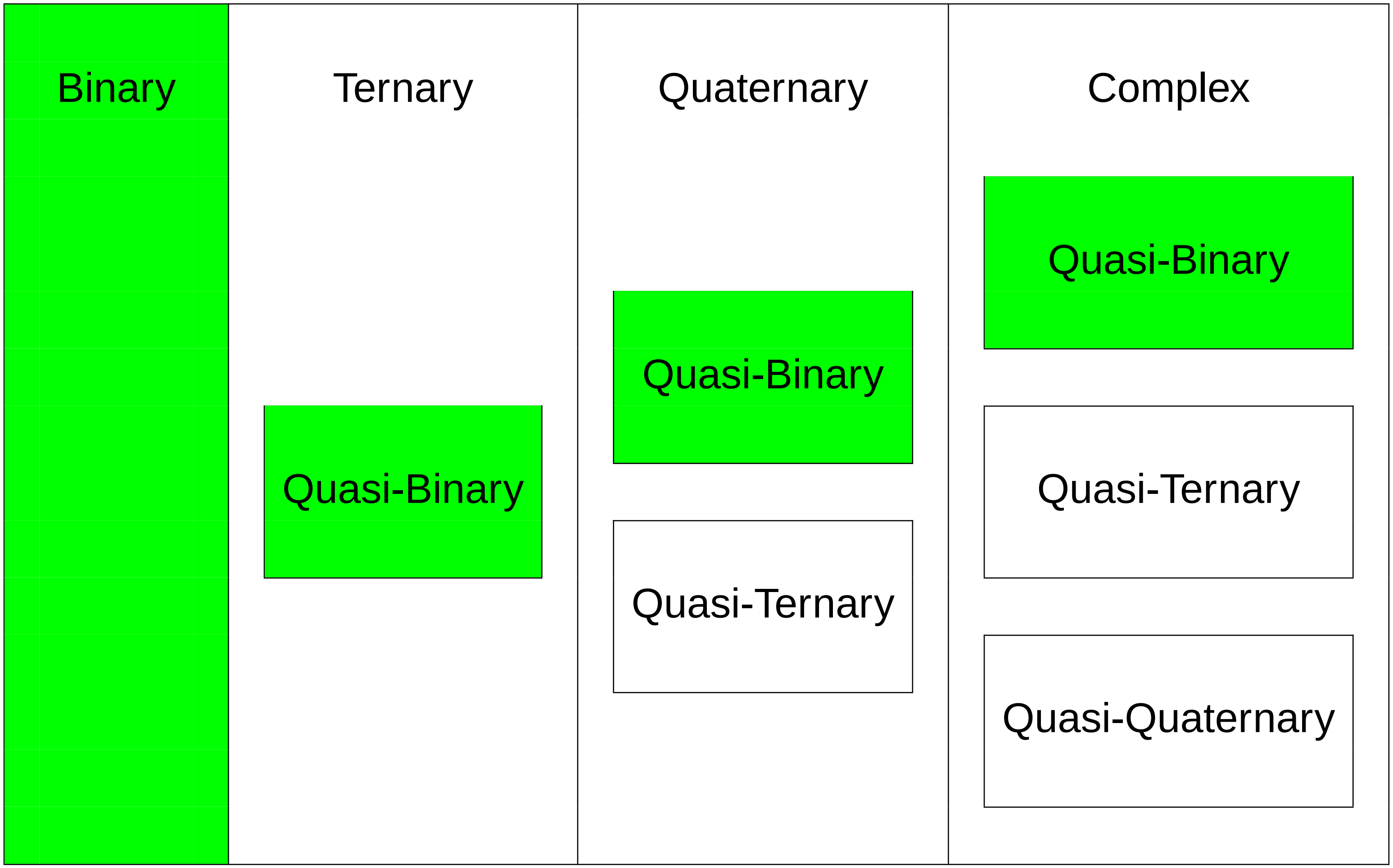
Contents

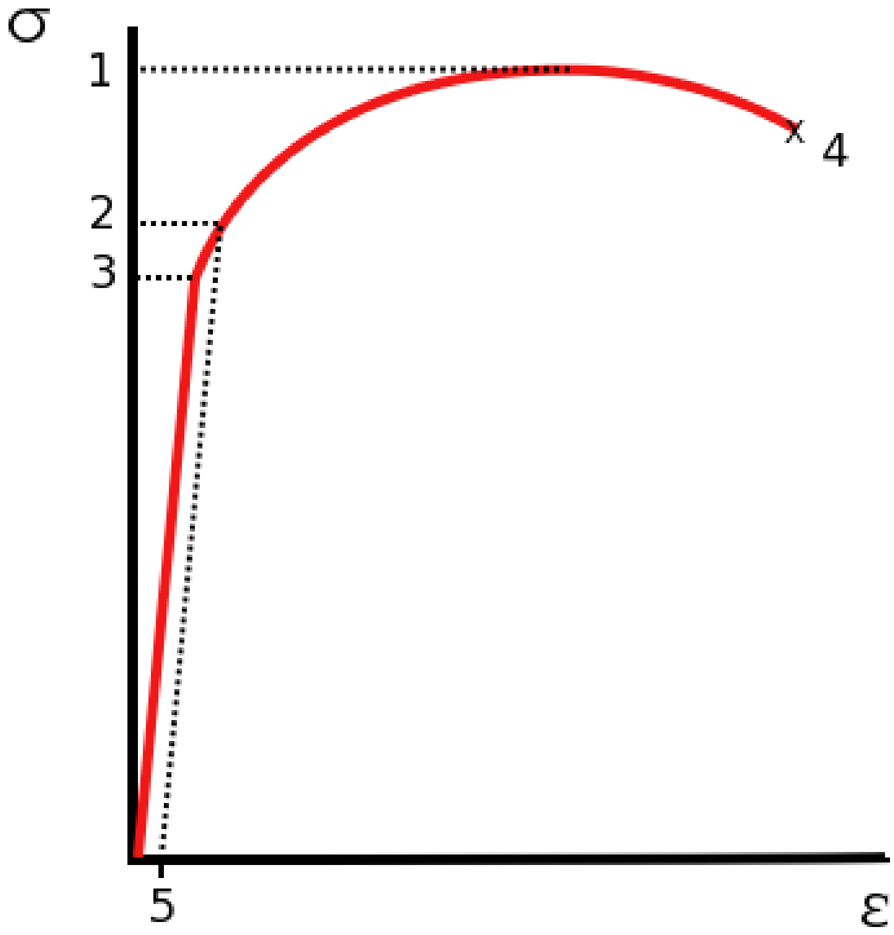
Something about alloys

Binary	Ternary	Quaternary	Complex
	Quasi-Binary	Quasi-Binary	Quasi-Binary
		Quasi-Ternary	Quasi-Ternary
			Quasi-Quaternary

Something about alloys



Something about deformations



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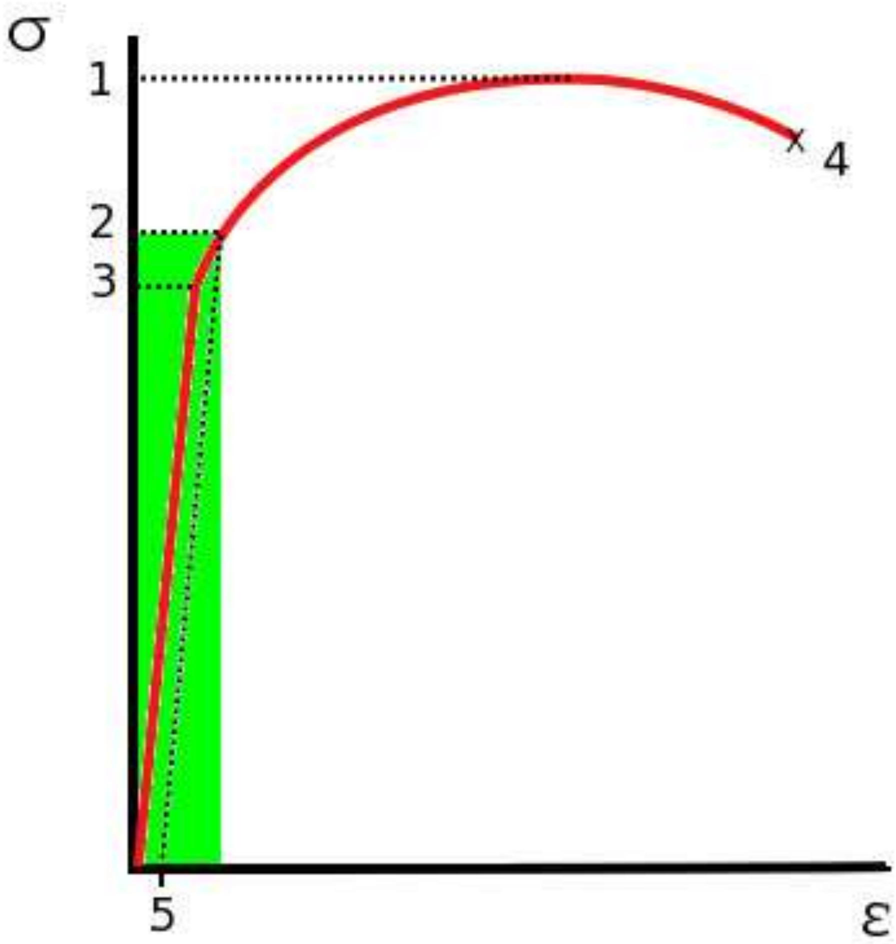

Models for nucleation

Two models, with small differences

- Myhr and Grong (2000)
- Robson et al. (2003)

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Comparison:

- Basic model == Myhr and Grong (2000)
- Adapted using Robson et al. (2003)

Governing DE

$$\begin{array}{c}\text{Change}\\ \text{in time}\end{array} = \begin{array}{c}\text{Change}\\ \text{by growth}\end{array} + \begin{array}{c}\text{Production}\\ \text{rate}\end{array}$$

Governing DE

$$\begin{array}{ccccc} \text{Change in time} & = & \text{Change by growth} & + & \text{Production rate} \\ \Downarrow & & \Downarrow & & \Downarrow \\ \dfrac{\partial N}{\partial t} & = & -\dfrac{\partial (Nv)}{\partial r} & + & S \end{array}$$

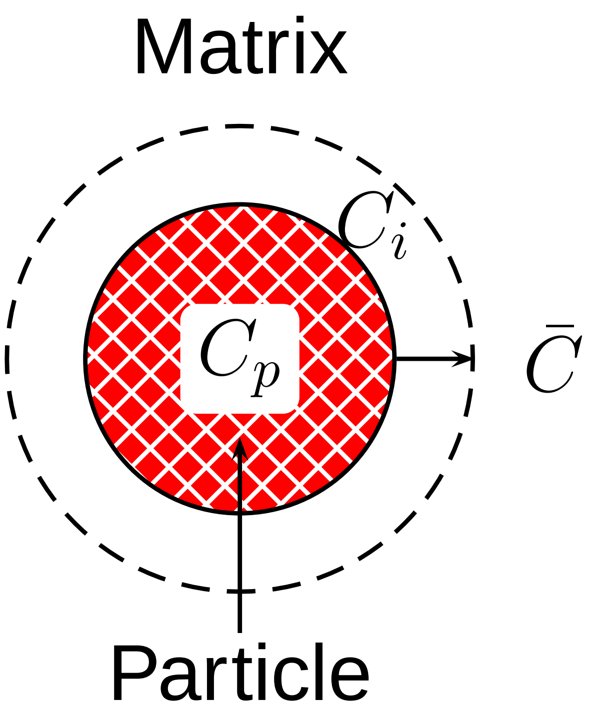
Unknowns

- Growth rate v
- Production term S

Growth of spherical particles

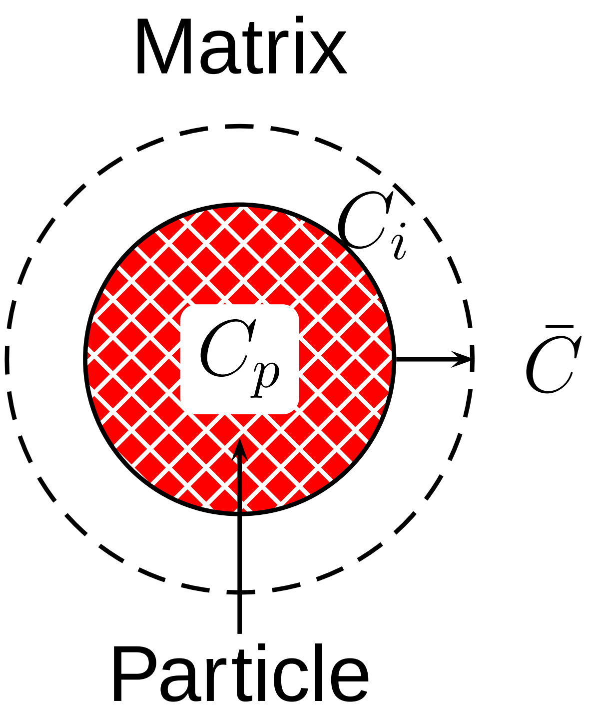
Directly influence by

- Mean concentration $\bar{C}$
- Interface concentration C_i
- Internal concentration C_p
- Diffusion coefficient D



Growth of spherical particles

$$v(r,t) = \frac{\bar{C} - C_i}{C_p - C_i} \frac{D}{r}$$



A special particle

A particle with radius r^* that will neither grow or dissolve:

$$v(r^*) = 0$$

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Solved for r^*:

$$r^* = \frac{2\gamma_{\alpha\beta}V_m}{RT}\left(\ln\left(\frac{\bar{C}}{C_e}\right)\right)^{-1}$$

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Definition: Critical particle radius

Production term

- Indicates the number of particles that nucleate over the whole domain
- Influenced by critical radius r^*
- Influenced by nucleation rate j

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Kampmann et al. (1987):

$$S(r,t) = \begin{cases} j(t) & \text{if } r = r^* + \Delta r^*, \\ 0 & \text{otherwise.} \end{cases}$$

Nucleation rate

The number of particles that nucleate with radius $r^* + \Delta r^*$:

- Influenced by diffusion
- Only if some barrier has been overcome

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$$j = j_0 \exp\left(-\frac{\mathbf{\Delta G^*_{het}}}{RT}\right) \exp\left(-\frac{\mathbf{Q_d}}{RT}\right)$$

Nucleation energy barrier

- Chemical composition
- Misfit strain energy

Nucleation energy barrier

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- Misfit strain energy

$$\Delta G^*_{\text{het}} = \frac{\tilde{A}_0^3}{(\mathbf{\Delta G_v} + \mathbf{\Delta G_s^m})^2}$$

Model overview

- Governing DE:

$$\frac{\partial N}{\partial t} = -\frac{\partial \left(Nv\right)}{\partial r} + S$$

- Source term:

$$S(r,t) = \begin{cases} j(t) & \text{if } r = r^* + \Delta r^*, \\ 0 & \text{otherwise.} \end{cases}$$

Model overview

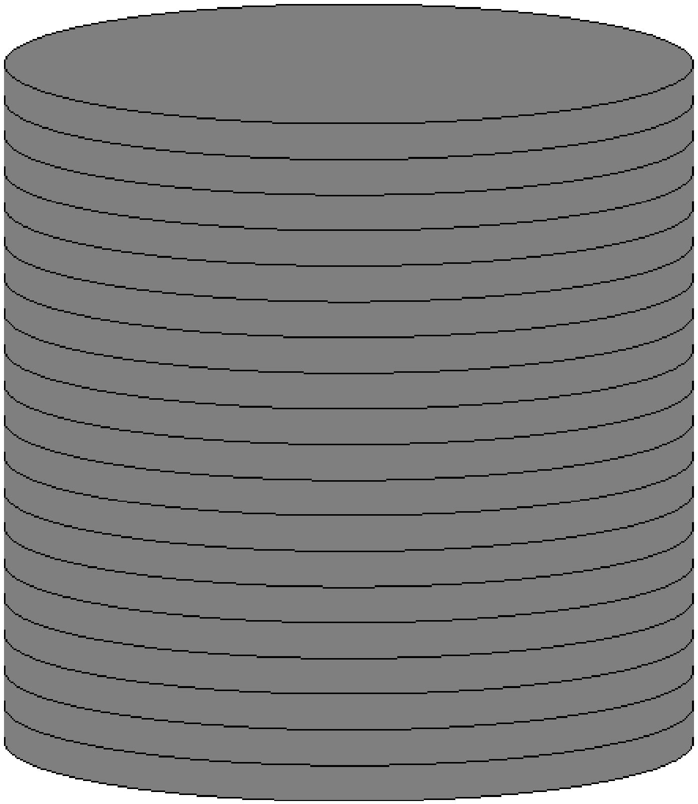
- Governing DE:

$$\frac{\partial N}{\partial t} = -\frac{\partial (Nv)}{\partial r} + S$$

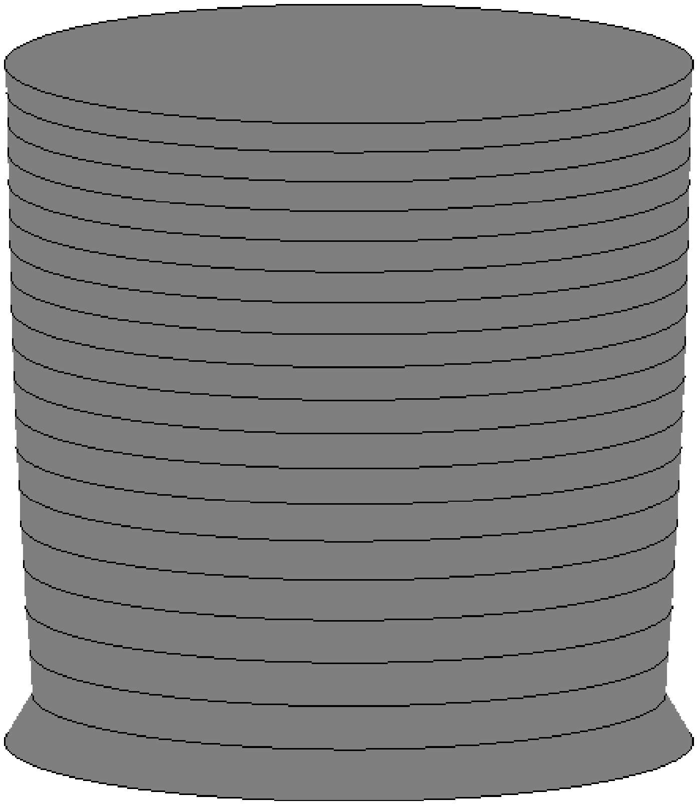
- Growth rate:

$$v = \frac{\bar{C} - C_i}{C_p - C_i}\frac{D}{r}$$

Elastic deformations



Elastic deformations



Assumptions

Rotation symmetry:

- No deformations in tangential direction
- No deformation at center axis in radial direction
- All derivatives in tangential direction vanish

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$$u_\theta = 0 \qquad u_\eta(0,\theta,z) = 0 \qquad \frac{\partial(.)}{\partial\theta} = 0$$

Strain and deformation

Chau and Wei (2000):

$$\varepsilon_{\eta\eta} = \frac{\partial u_\eta}{\partial \eta} \qquad \varepsilon_{\theta\theta} = \frac{u_\eta}{\eta}$$

$$\varepsilon_{zz} = \frac{\partial u_z}{\partial z} \qquad \varepsilon_{\eta\theta} = 0$$

$$\varepsilon_{\eta z} = \frac{1}{2}\left(\frac{\partial u_\eta}{\partial z} + \frac{\partial u_z}{\partial \eta}\right) \qquad \varepsilon_{\theta z} = 0$$

Stress and strain

Hook’s Law:

$$\sigma_{\alpha\beta} = \delta_{\alpha\beta}\lambda\left(\varepsilon_{\eta\eta} + \varepsilon_{\theta\theta} + \varepsilon_{zz}\right) + 2\mu\varepsilon_{\alpha\beta}$$

Stress and strain

Hook's Law:

$$\sigma_{\alpha\beta} = \delta_{\alpha\beta} \lambda (\varepsilon_{\eta\eta} + \varepsilon_{\theta\theta} + \varepsilon_{zz}) + 2 \mu \varepsilon_{\alpha\beta}$$

Stiffness matrix (λ) Shear modulus (μ)

Force balance

Jaeger et al. (2007):

$$\frac{\partial \sigma_{\eta\eta}}{\partial \eta} + \frac{\partial \sigma_{\eta z}}{\partial z} + \frac{\sigma_{\eta\eta} - \sigma_{\theta\theta}}{\eta} + b_\eta = 0$$

$$\frac{\partial \sigma_{\eta z}}{\partial \eta} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{\sigma_{\eta z}}{\eta} + b_z = 0$$

Boundary conditions

- Symmetry condition:

$$u_\eta(0, \theta, z) = 0$$

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$$u_\eta(0, \theta, z) = 0$$

- Fixed boundaries:

$$u_\alpha(\eta, \theta, z) = 0$$

- Moving boundaries:

$$\left(\underline{\underline{\boldsymbol{\sigma}}}(\eta, \theta, z)\right)_\alpha \cdot \boldsymbol{n} = f_\alpha(\eta, \theta, z)$$

Coupling the models

Remember the nucleation energy barrier:

$$\Delta G^*_{\text{het}} = \frac{\tilde{A}_0^3}{\left(\Delta G_v + \Delta G_s^m\right)^2}$$

Misfit strain energy

Coupling the models

Remember the nucleation energy barrier:

$$\Delta G^*_{\text{het}} = \frac{\tilde{A}_0^3}{\left(\Delta G_v + \Delta G_s^m\right)^2}$$

Misfit strain energy

Question:

Is there something like elastic strain energy?

Coupling the models (2)

Answer:

YES!!!

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YES!!!

Solution:

$$\Delta G_s^{el} = \frac{1}{2}\underline{\underline{\boldsymbol{\sigma}}} : \underline{\underline{\boldsymbol{\varepsilon}}}$$

Coupling the models (2)

Answer:

YES!!!

Solution:

$$\Delta G_s^{el} = \frac{1}{2}\underline{\underline{\boldsymbol{\sigma}}} : \underline{\underline{\boldsymbol{\varepsilon}}}$$

and:

$$\Delta G^*_{\text{het}} = \frac{\tilde{A}_0^3}{\left(\Delta G_v + \Delta G_s^m + \Delta G_s^{el}\right)^2}$$

Coupling the models (3)

Question:

Is there also a reverse coupling?

Coupling the models (3)

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Answer:

YES !!!

Coupling the models (3)

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Solution by Pal (2005):

$$\mu = \mu_m + \left(\frac{15(1-\nu_m)(\mu_p - \mu_m)}{2\mu_p(4-5\nu_m) + \mu_m(7-5\nu_m)} \right) \mu_m f$$

$$E = E_m + \left(10\beta_1(1+\nu_m) + \beta_2(1-2\nu_m)\right) E_m f$$

$$\lambda = \mu \frac{E - 2\mu}{3\mu - E}$$

Recap

Two models:

- Nucleation model
- Elastic model

Two couplings:

- From elastic to nucleation
- From nucleation to elastic

Numerical methods

Nucleation model:

- Upwind scheme
- IMEX-θ method with $\theta = \frac{1}{2}$

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Nucleation model:

- Upwind scheme
- IMEX-θ method with $\theta = \frac{1}{2}$

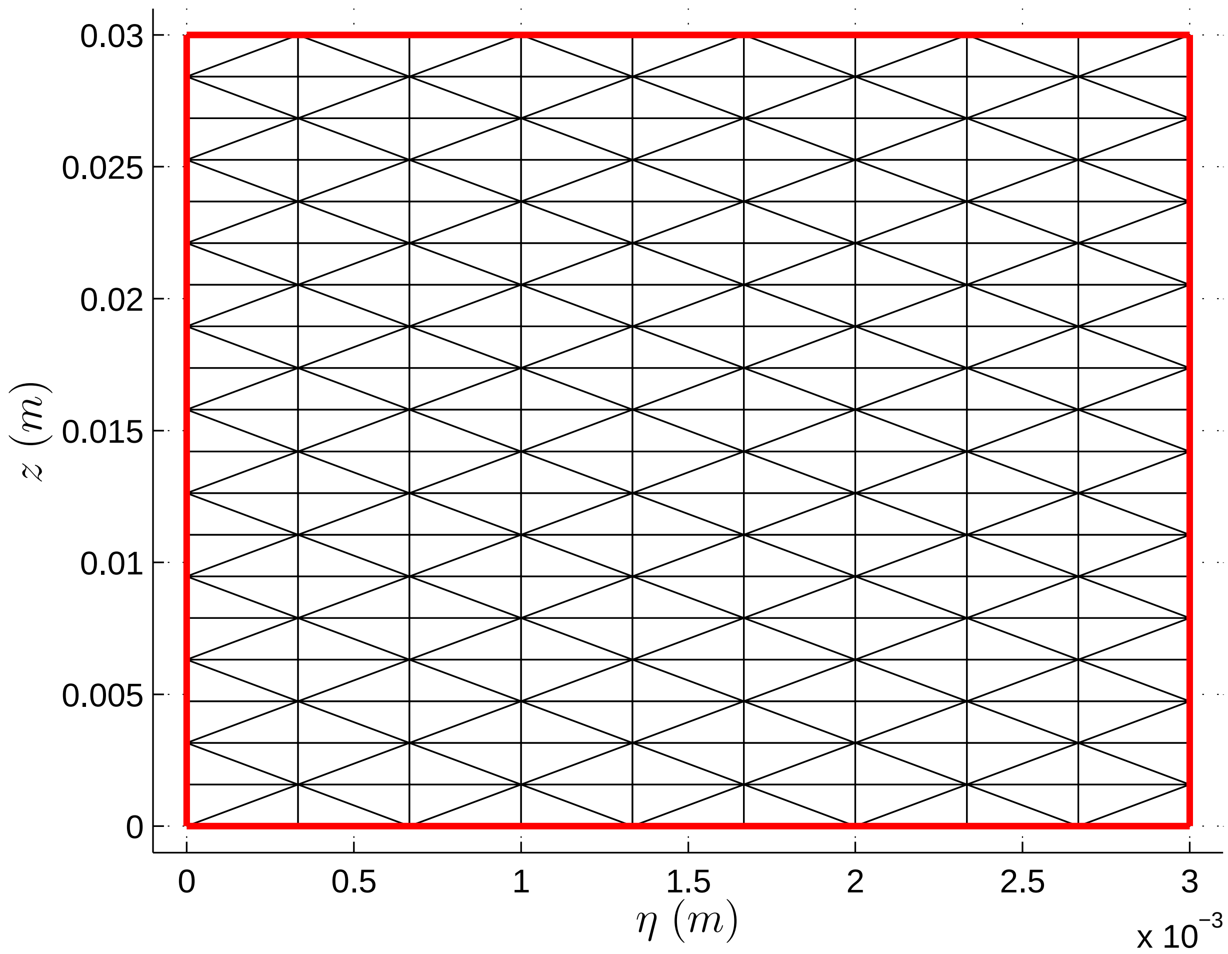
$$\left(I - \frac{1}{2}\frac{\Delta t}{\Delta r}A^n\right)\vec{N}^{n+1} = \left(I + \frac{1}{2}\frac{\Delta t}{\Delta r}A^n\right)\vec{N}^n + \Delta t\vec{S}^n$$

Numerical methods (2)

Elastic model:

- Finite Element Method
- Linear elements
- Use of rotation symmetry

Numerical methods (2)



Numerical methods (2)

Equation:

$$\begin{bmatrix} S_{\eta\eta} & S_{\eta z} \\ S_{z\eta} & S_{zz} \end{bmatrix} \begin{bmatrix} u_\eta \\ u_z \end{bmatrix} = \begin{bmatrix} q_\eta \\ q_z \end{bmatrix}$$

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Algorithm:

1. Set all constants;
2. Set all initial values;

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1. Set all constants;
2. Set all initial values;
3. For each time step:
   (a) Calculate elastic parameters;
   (b) Build matrices for elastic deformation;
   (c) Calculate elastic deformations;
   (d) Calculate elastic strain energy;

Numerical methods

Algorithm:

. . .

3. For each time step:

   . . .

   (e) For each point:

      i. Calculate nucleation parameters;
      ii. Calculate matrices for nucleation;
      iii. Calculate nucleation.

Simulation

Material:

- Aluminum alloy AA 6082
- Mg_2Si particles

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Shape:

- Cylindrical
- Height 30 millimeter
- Radius 3 millimeter

Simulation (2)

Time

- Total of 3000 seconds
- Time step of 0.5 seconds

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- Total of 3000 seconds
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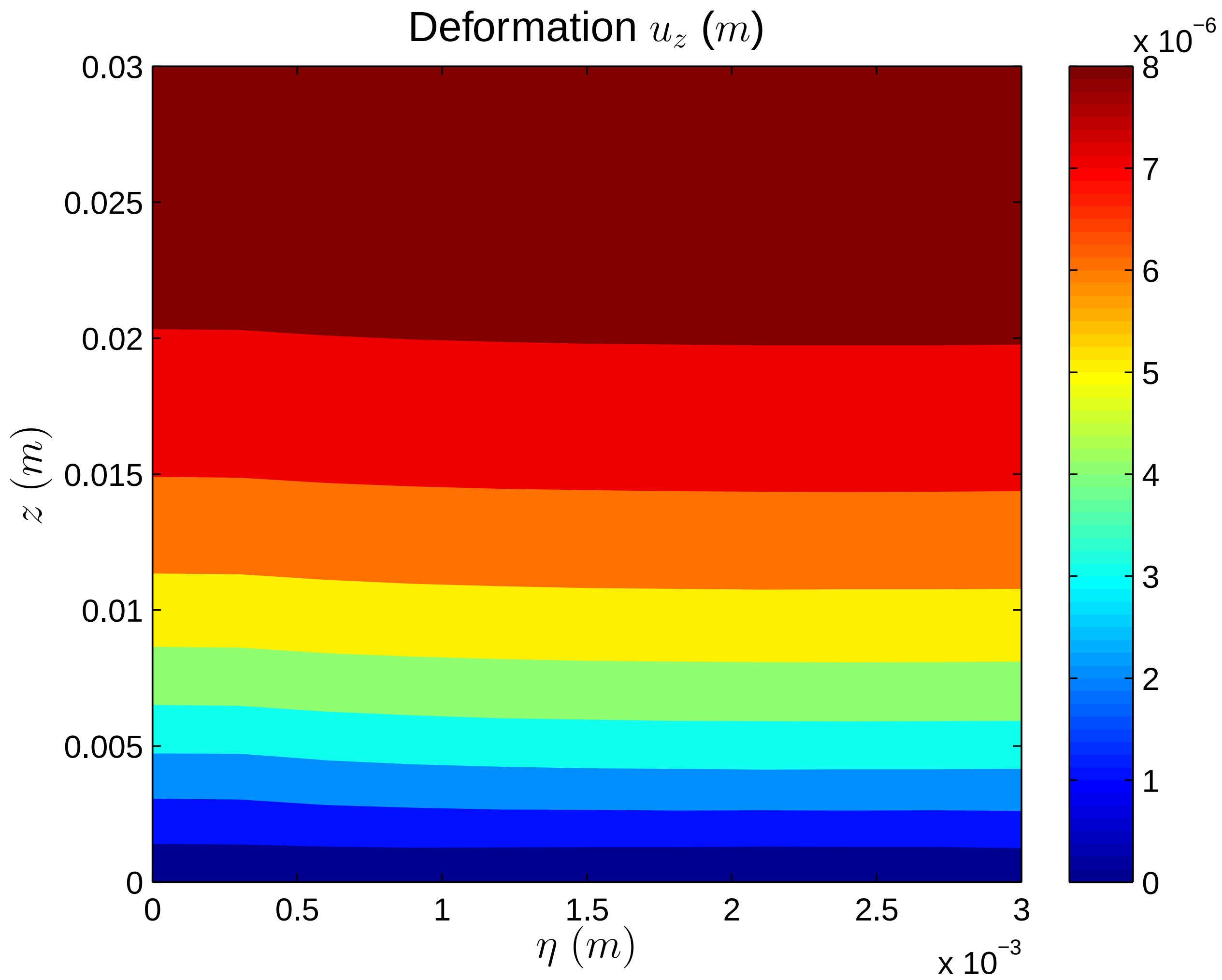
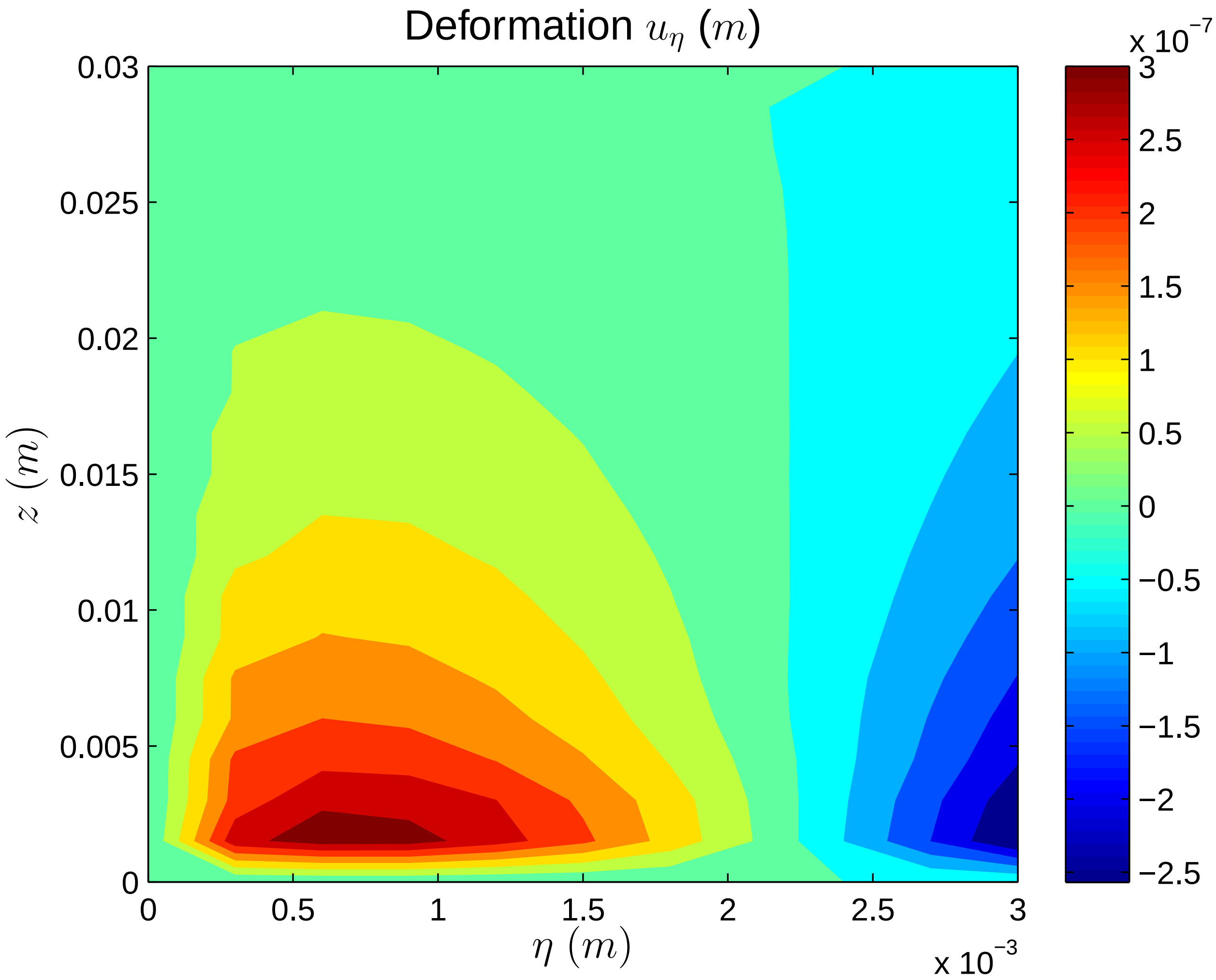
Test:

- Tensile test
- Bottom axial and radial fixed
- Top radial fixed
- Axial force at top of 6 million N/m^2
- Sides free

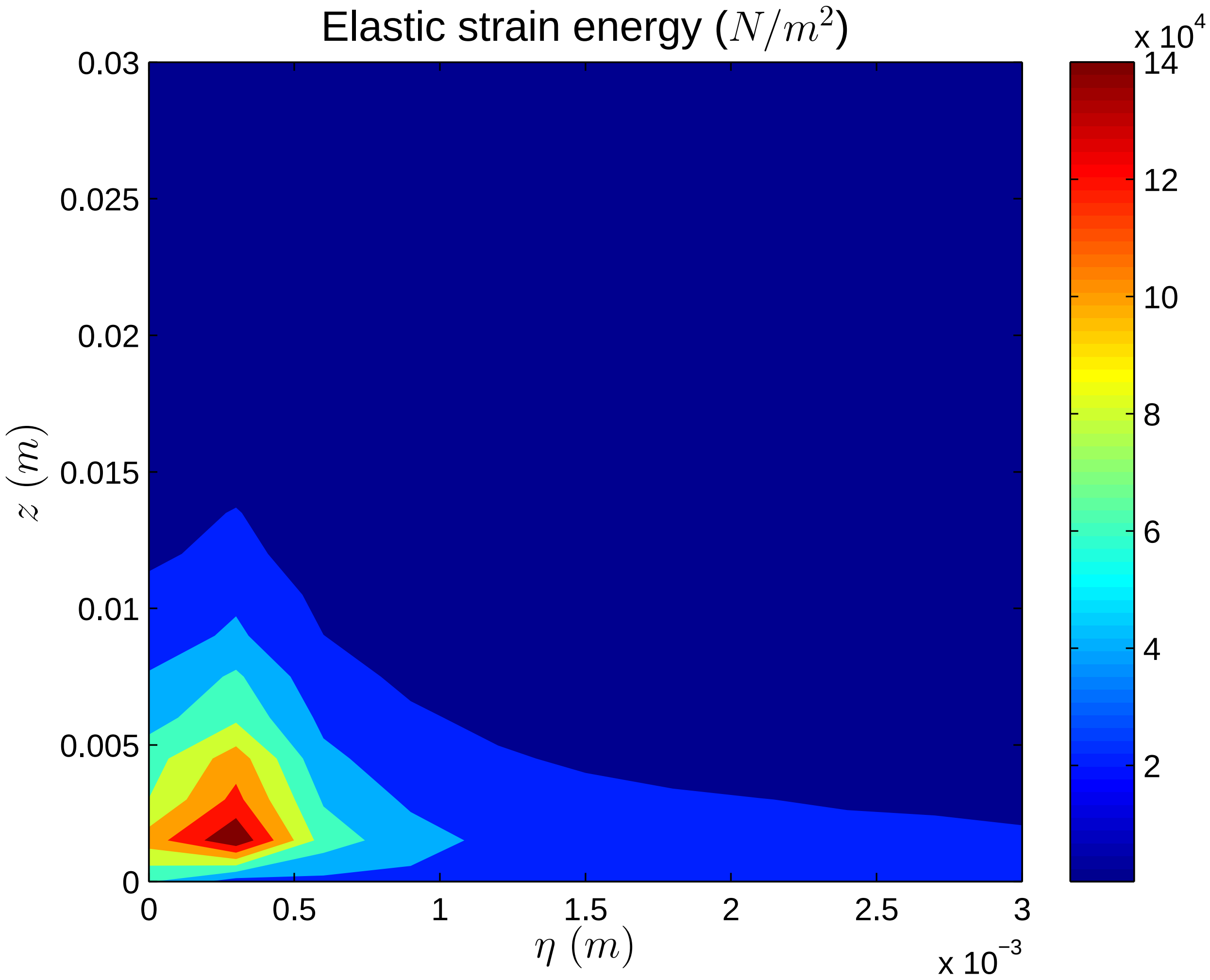
Typical deformations: Axial



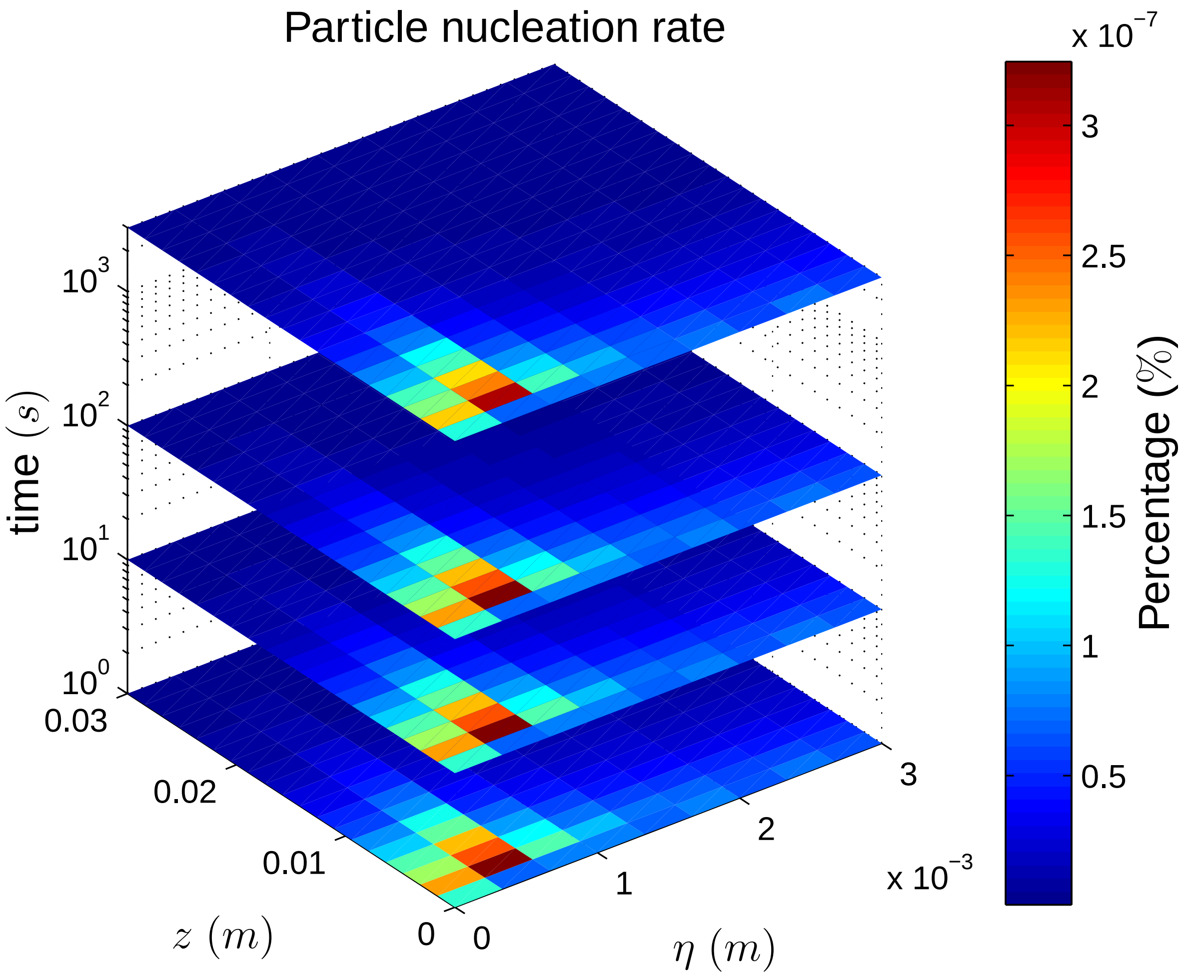
Typical deformations: Radial



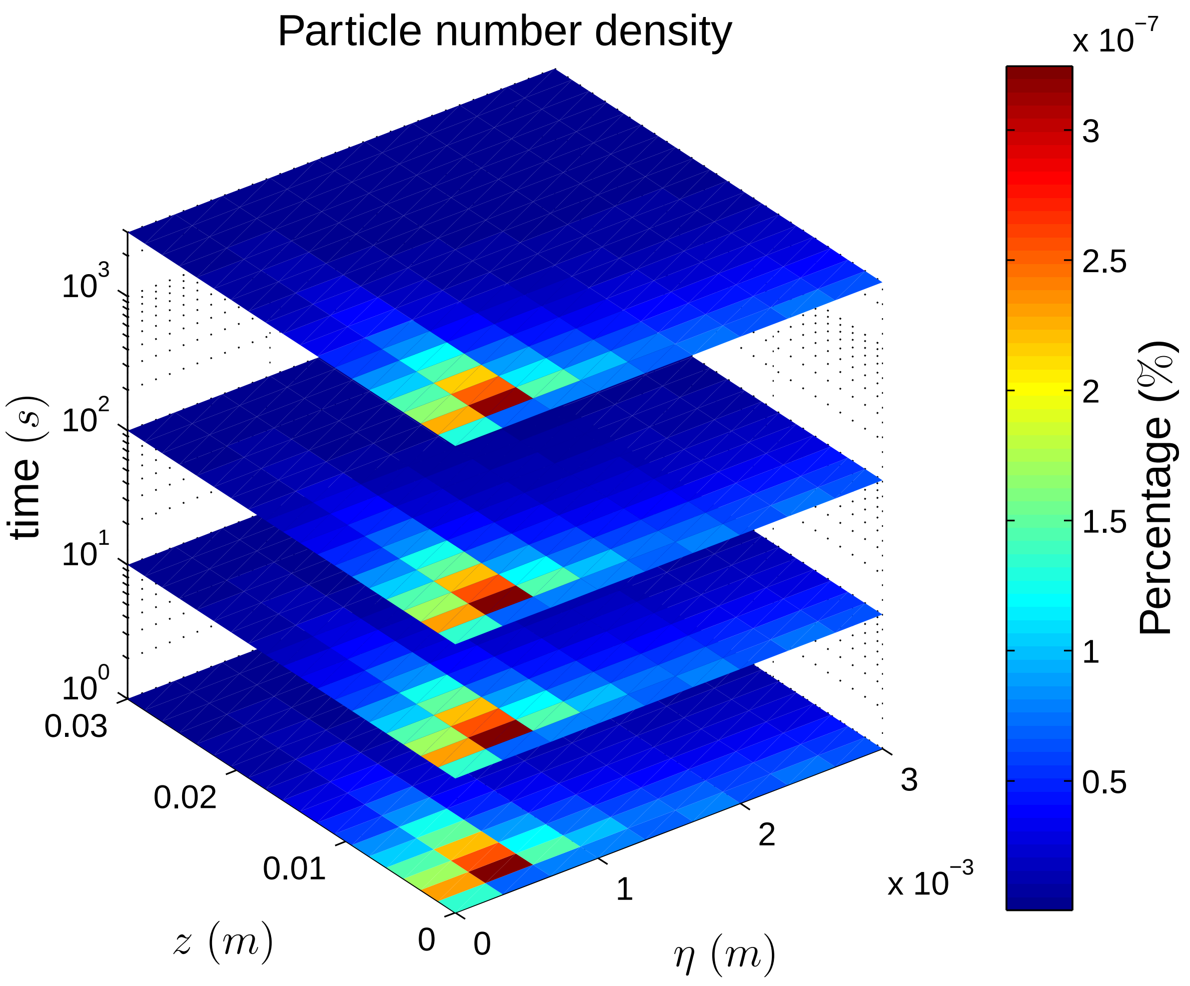
Typical deformations: Energy



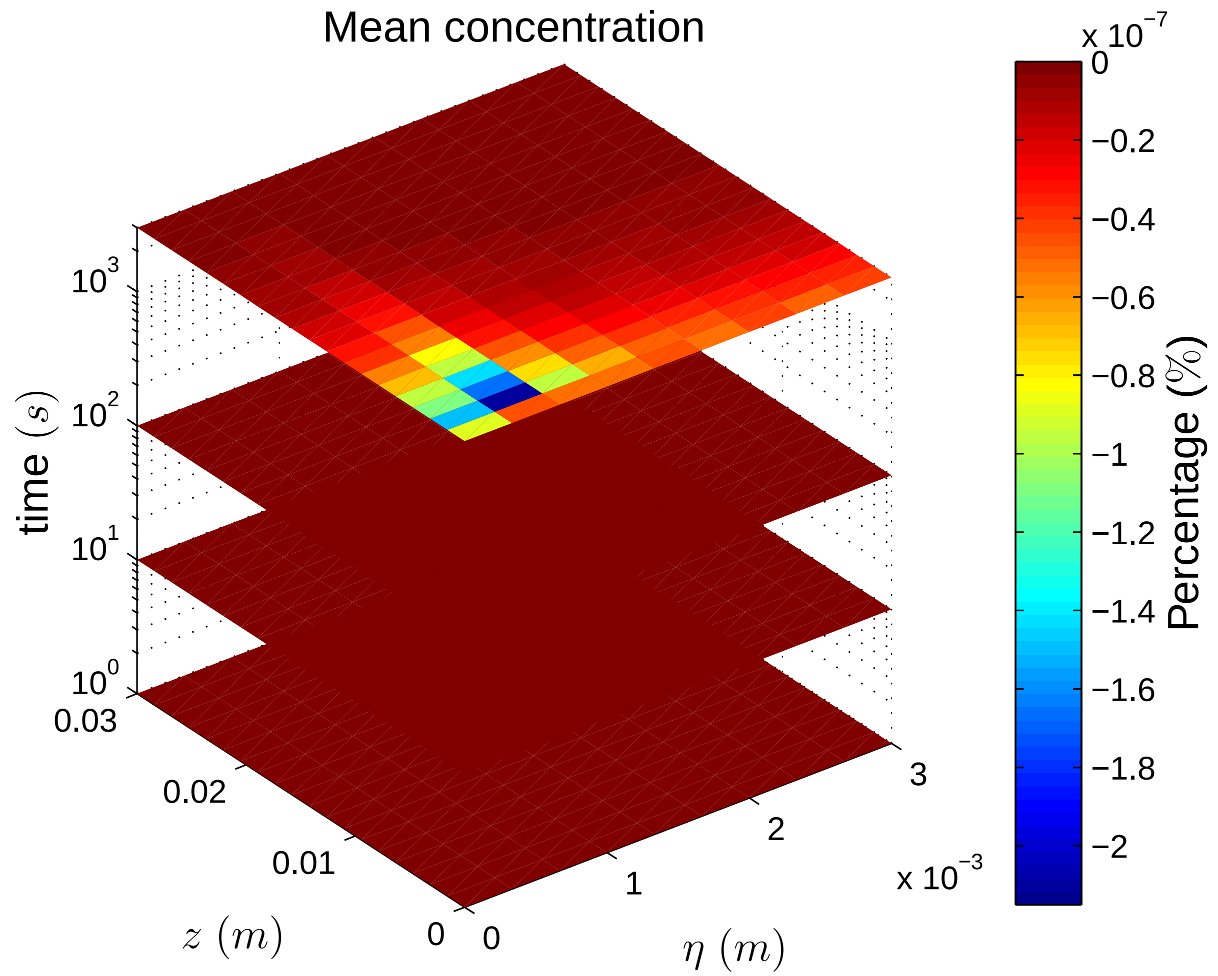
Nucleation results: Nucleation rate



Nucleation results: Number density



Nucleation results: Concentration



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Reflection

Are the results anomalies during simulation?

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Increase force to test for similar behavior.

$$F = 6 \times 10^9 \frac{N}{m^2}$$

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Increase force to test for similar behavior.

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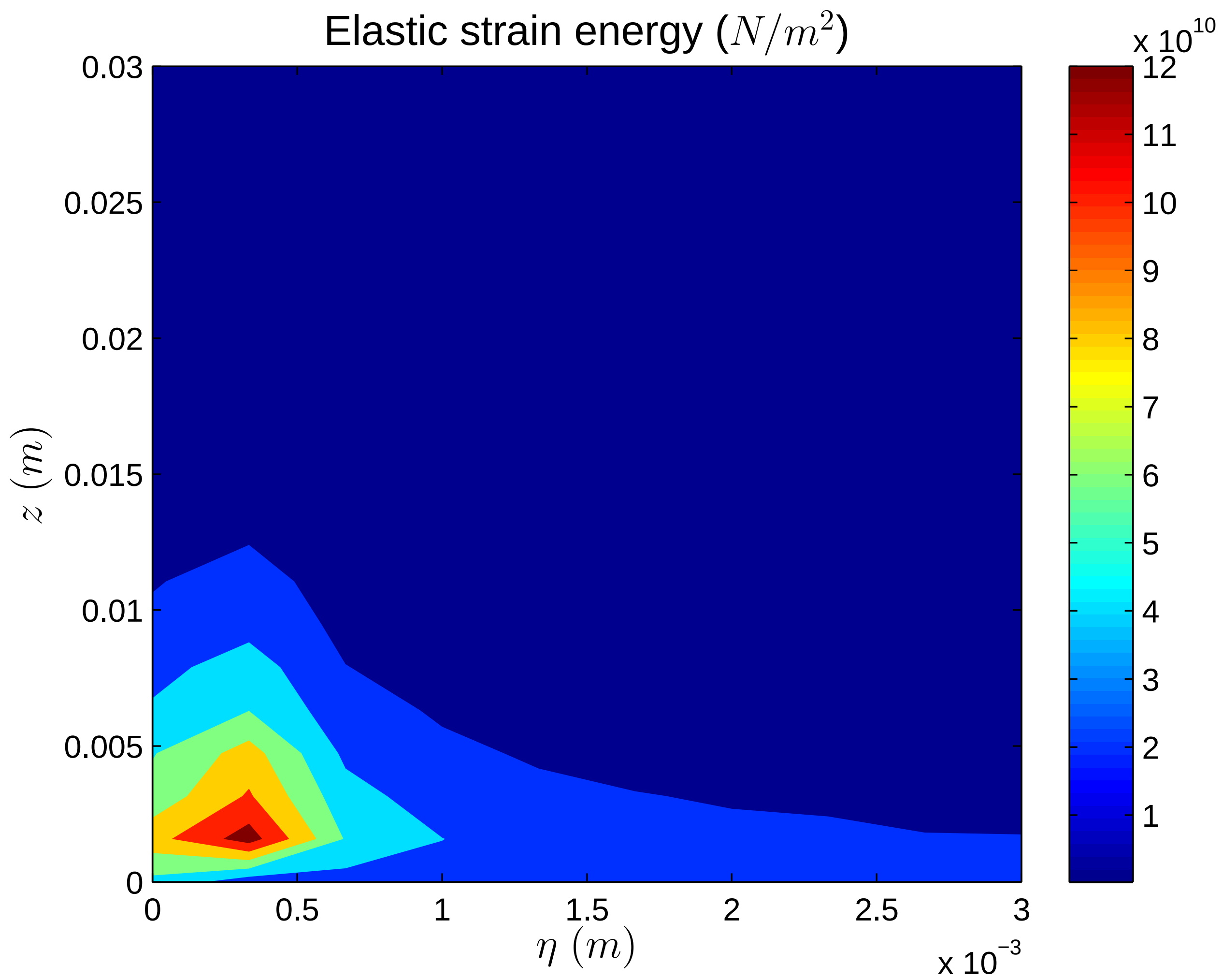
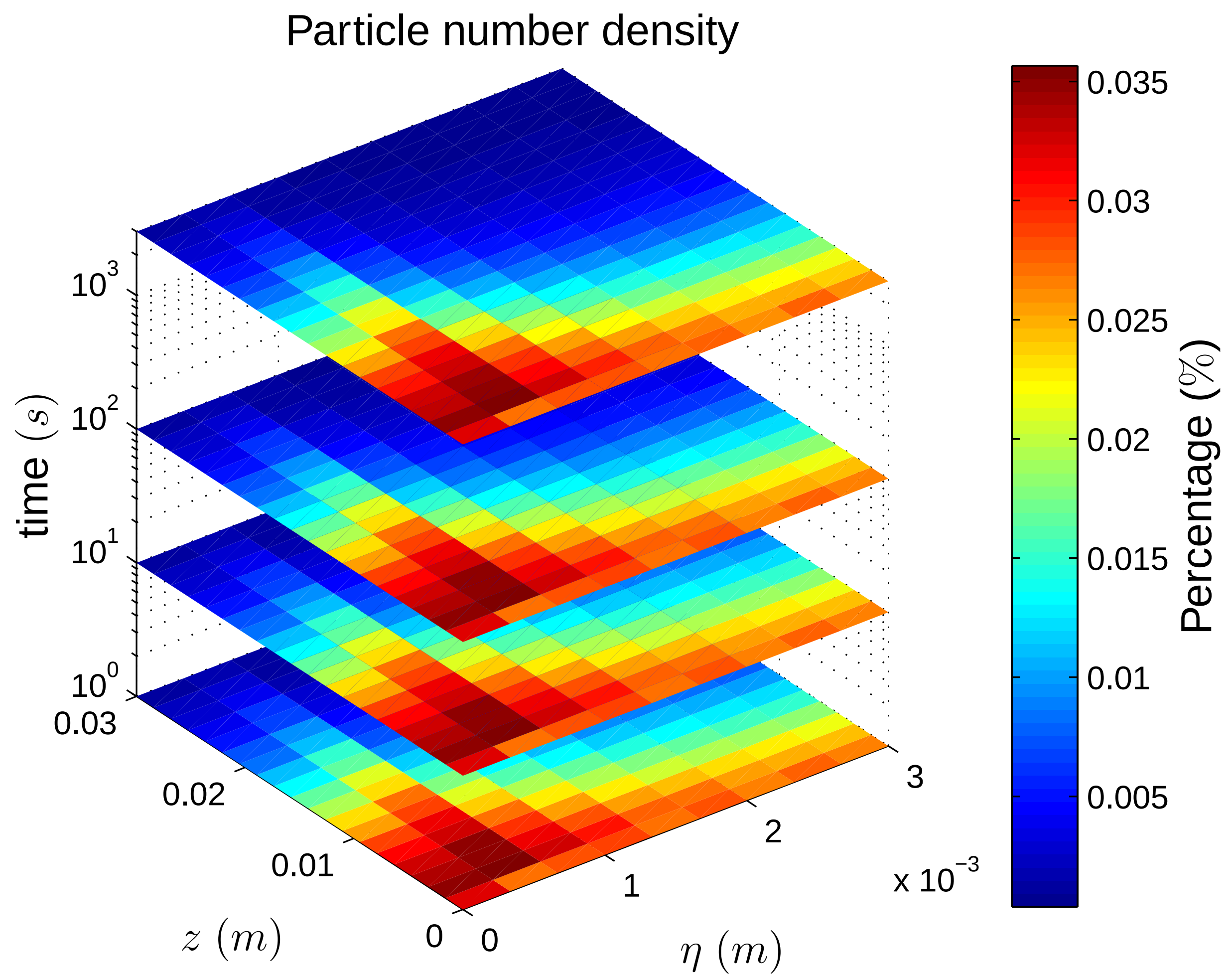
Physically no longer elasticity

New elastic stain energy



Nucleation results: Number density



Conclusions

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- Two separate nucleation models combined
- Formulated model for elastic deformations
- Coupling between nucleation and deformations
- Simulations show influence of deformations on nucleation

Recommended future work

- Extension to multiple particle configurations

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- Adaption to other alloys

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- Including homogeneous nucleation
- Including grain prediction models

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