Particle nucleation and coarsening in aluminum alloys

A literature study

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Contents

This presentation will be about:

- Alloys
- Diffusion
- Particle nucleation and coarsening
- Elastic deformations
- Conclusions
- Future work

Alloys

Alloys can be characterized by

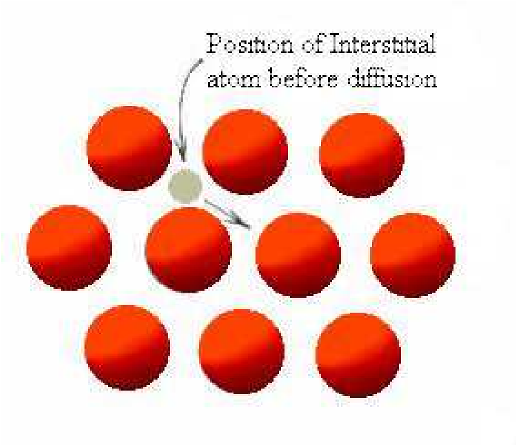
- the solvent metal, such as
  - Aluminum
  - Lead
  - Iron
- the number of elements
- by the apparent number of elements

By apparent number

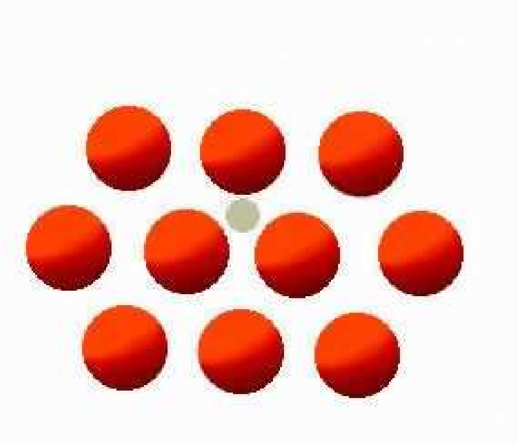
Binary	Ternary	Quaternary	Complex
			Quasi-Binary
		Quasi-Binary	
	Quasi-Binary		Quasi-Ternary
		Quasi-Ternary	
			Quasi-Quaternary

Diffusion

- Interstitial

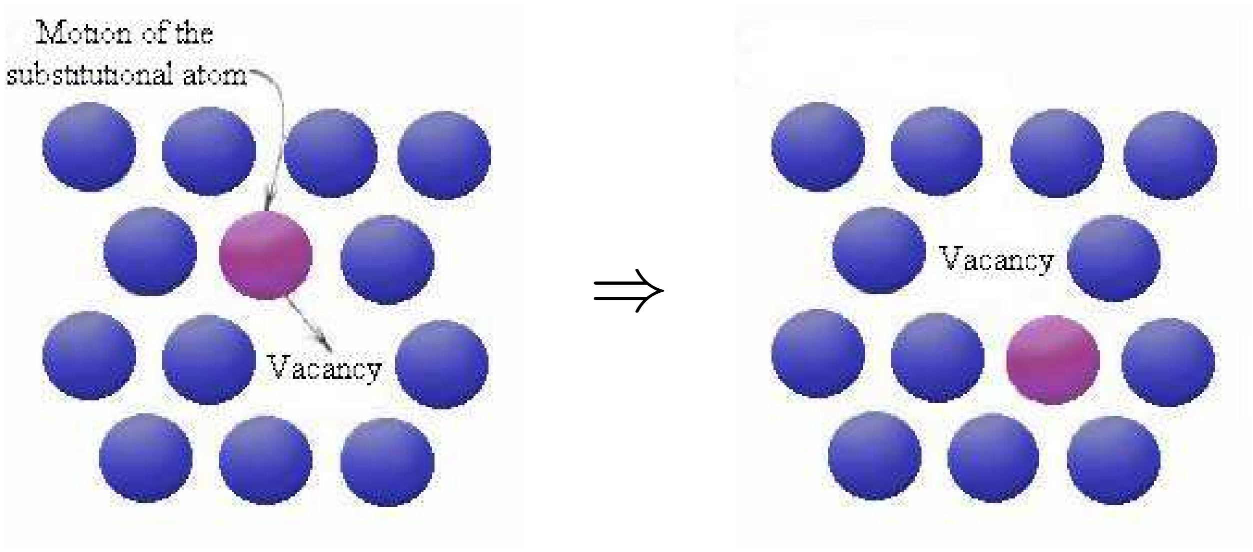


$\Rightarrow$



Diffusion

- Interstitial
- Substitutional



Nucleation of particles

Directly influenced by

- Mean concentration $\bar{C}$
- Equilibrium concentration C_e
- Temperature T
- Activation energy for diffusion Q_d

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Directly influenced by

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- Temperature T
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Formula:

$$j(t) = j_0 \exp\left(-\left(\frac{A_0}{RT}\right)^3 \left(\frac{1}{\ln(\bar{C}/C_e)}\right)^2\right) \exp\left(-\frac{Q_d}{RT}\right)$$

Growth of particles

Directly influenced by

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

Growth of particles

Directly influenced by

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

Formula:

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

Critical particles

Particles with no growth:

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

Critical particles

Particles with no growth:

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

or equivalent:

$$r^*(t) = \frac{2\sigma V_m}{RT}\left(\ln\left(\frac{\bar{C}}{c_e}\right)\right)^{-1}$$

Number of particles

Directly influenced by

- Growth rate v
- Nucleation rate j
- Critical radius r^*

Number of particles

Directly influenced by

- Growth rate v
- Nucleation rate j
- Critical radius r^*

Continuity equation:

$$\frac{\partial N}{\partial t} = -\frac{\partial N v}{\partial r} + S$$

Source term

Influenced by

- Critical radius r^*
- Nucleation rate j

Source term

Influenced by

- Critical radius r^*
- Nucleation rate j

Definition

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

Relations

Define ϕ by

$$\phi(r,t) = \frac{N(r,t)}{\Delta r}$$

Relations

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Then the particle volume fraction equals

$$f(t) = \int_0^\infty \frac{4}{3}\pi r^3 \phi(r,t)\,\mathrm{d}r$$

Relations

Define ϕ by

$$\phi(r,t) = \frac{N(r,t)}{\Delta r}$$

Then the particle volume fraction equals

$$f(t) = \int_0^\infty \frac{4}{3}\pi r^3 \phi(r,t)\,\mathrm{d}r$$

and the mean concentration

$$\bar{C}(t) = \frac{C_0 - C_p f(t)}{1 - f(t)}$$

Simulation

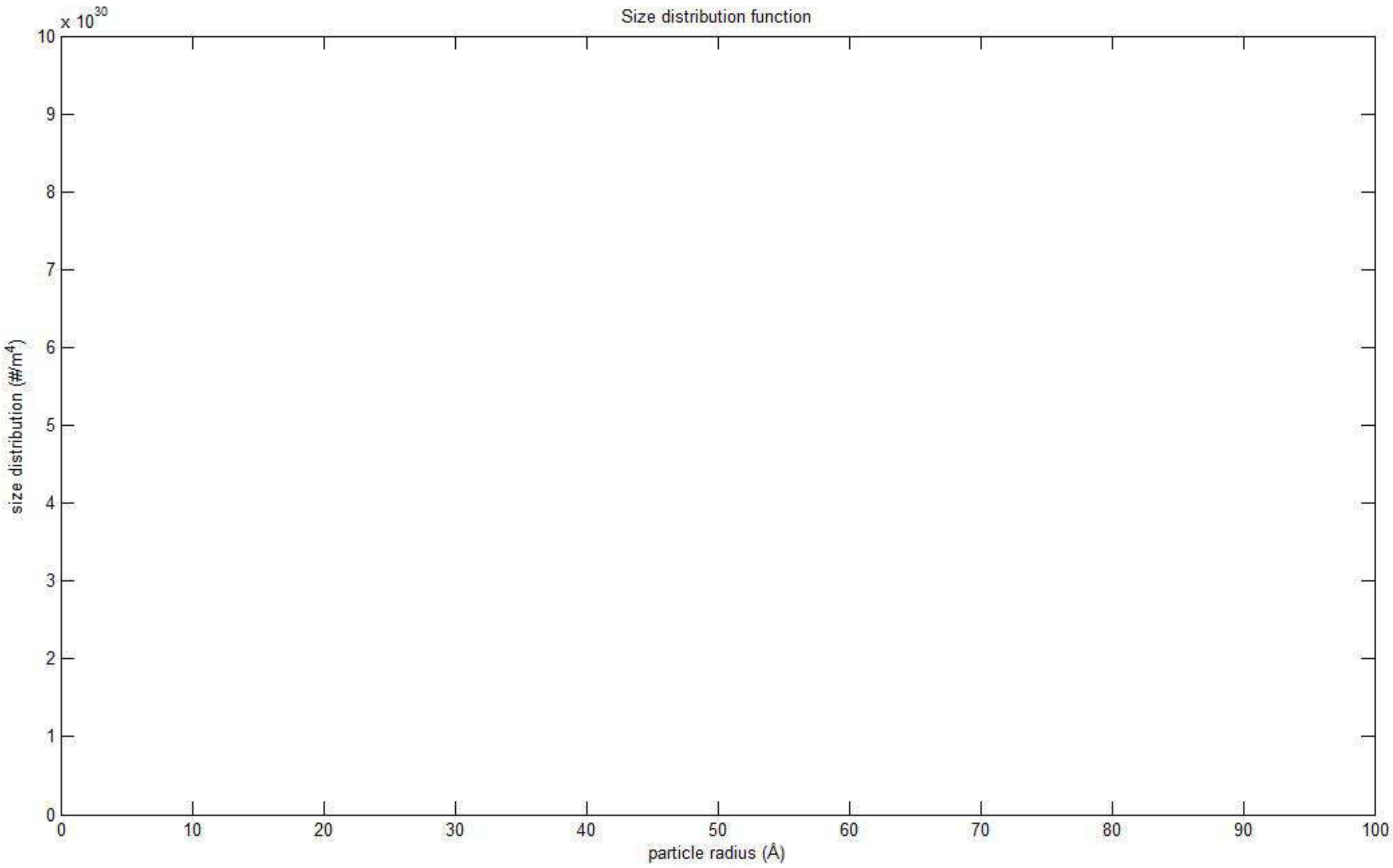
Material: Aluminum alloy AA 6082

- 0.9 wt$\%$ Silicon
- 0.6 wt$\%$ Magnesium

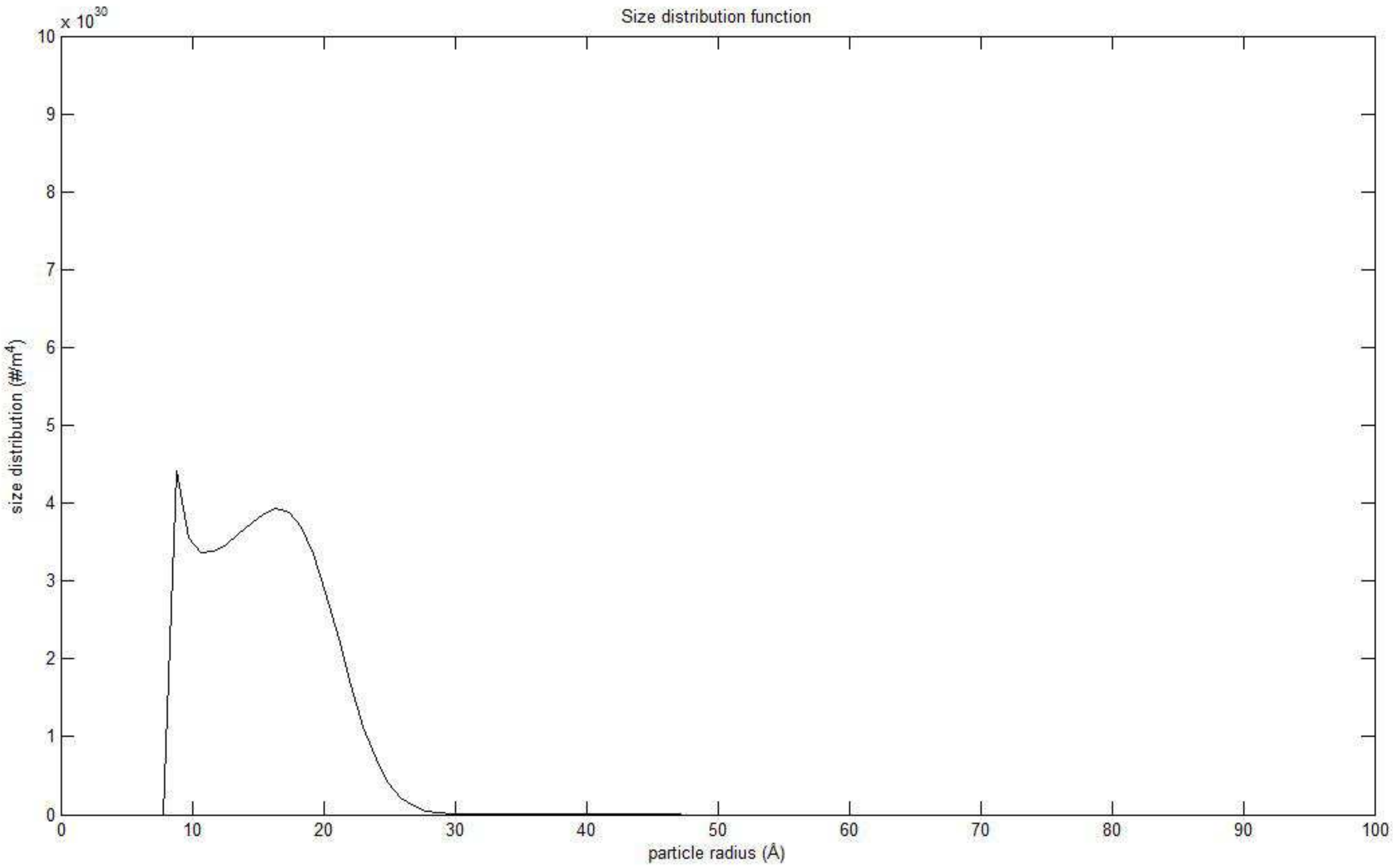
Temperature: 180° C

Initial condition: No particles

Distribution function ϕ



Distribution function ϕ



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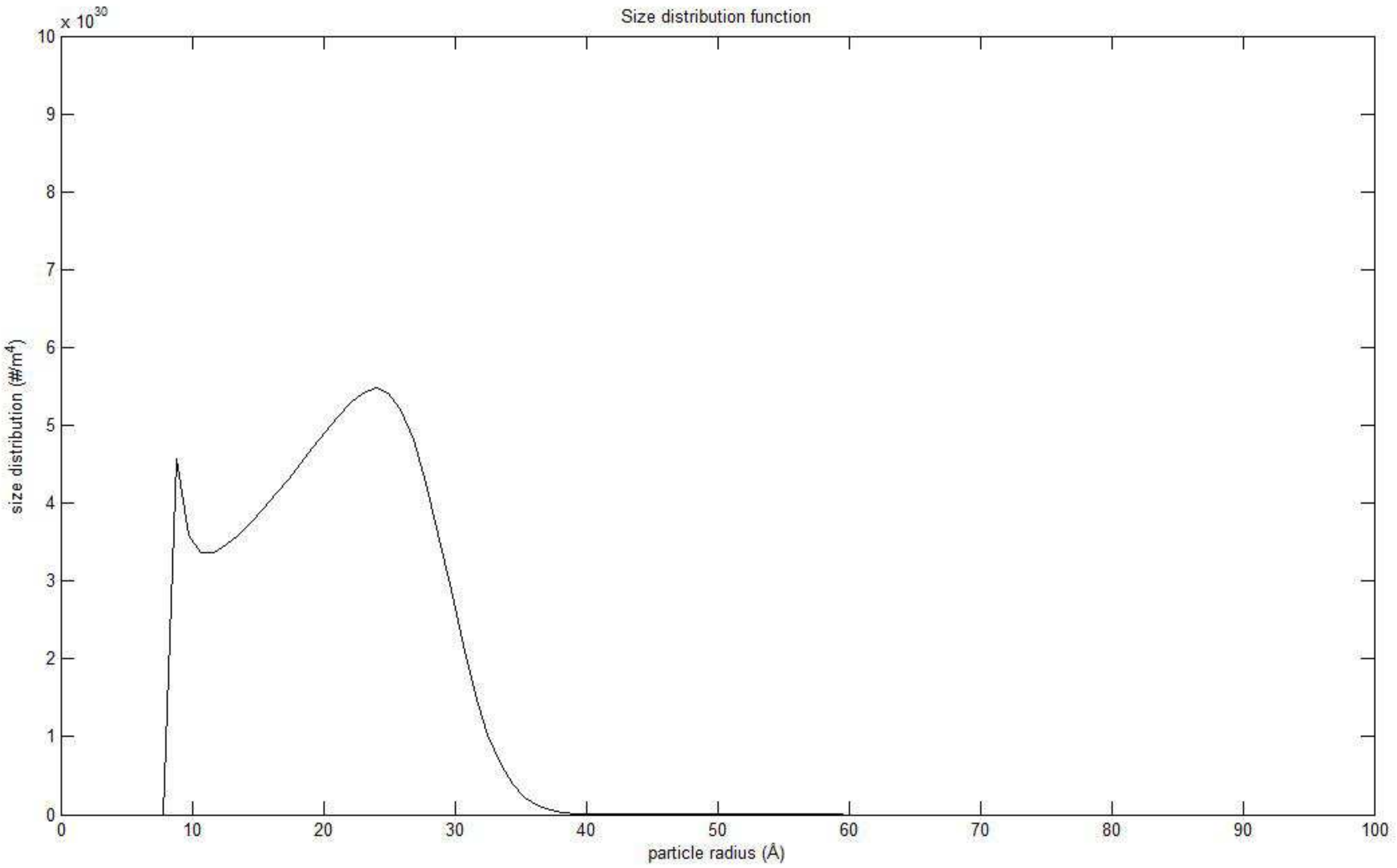

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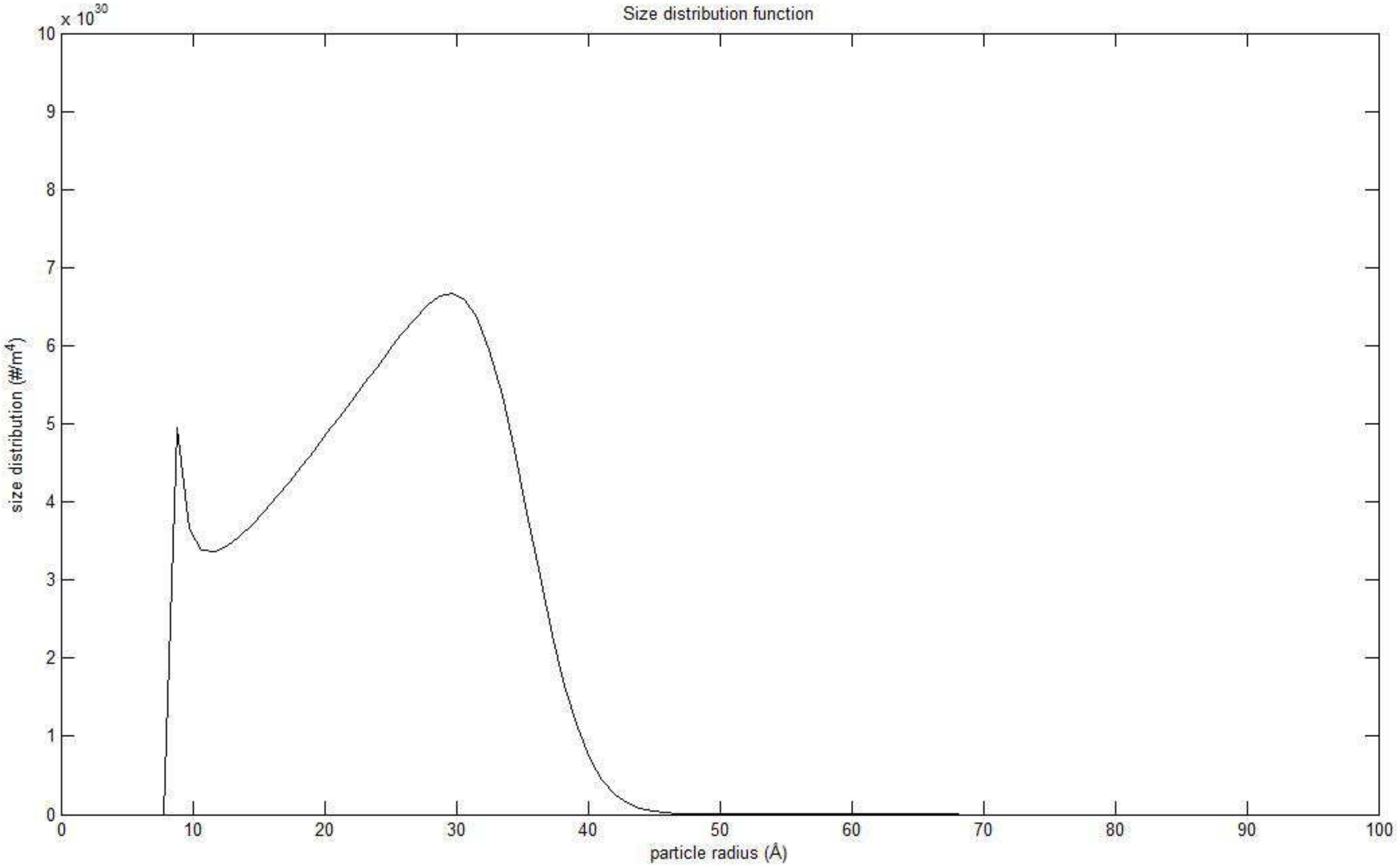

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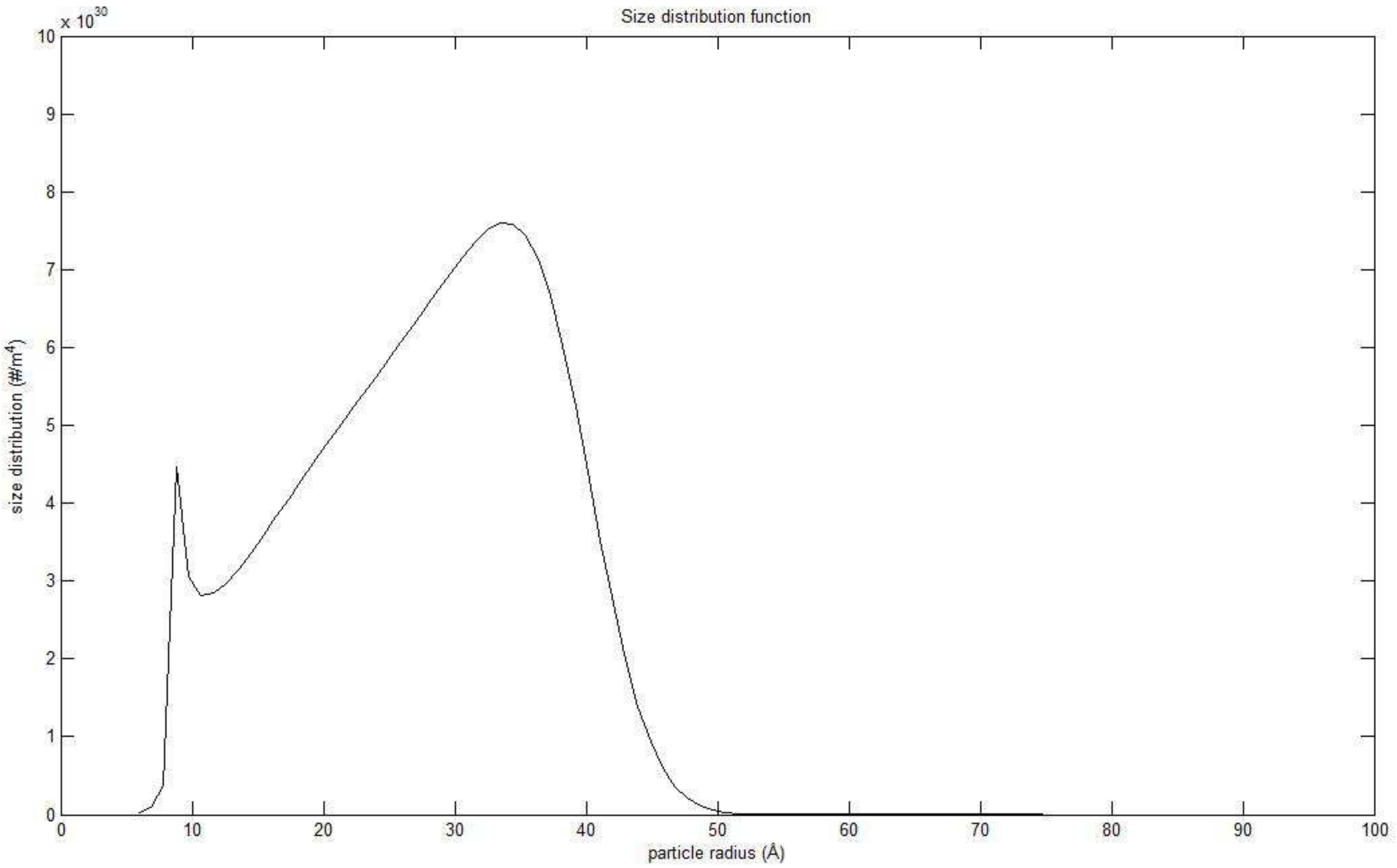

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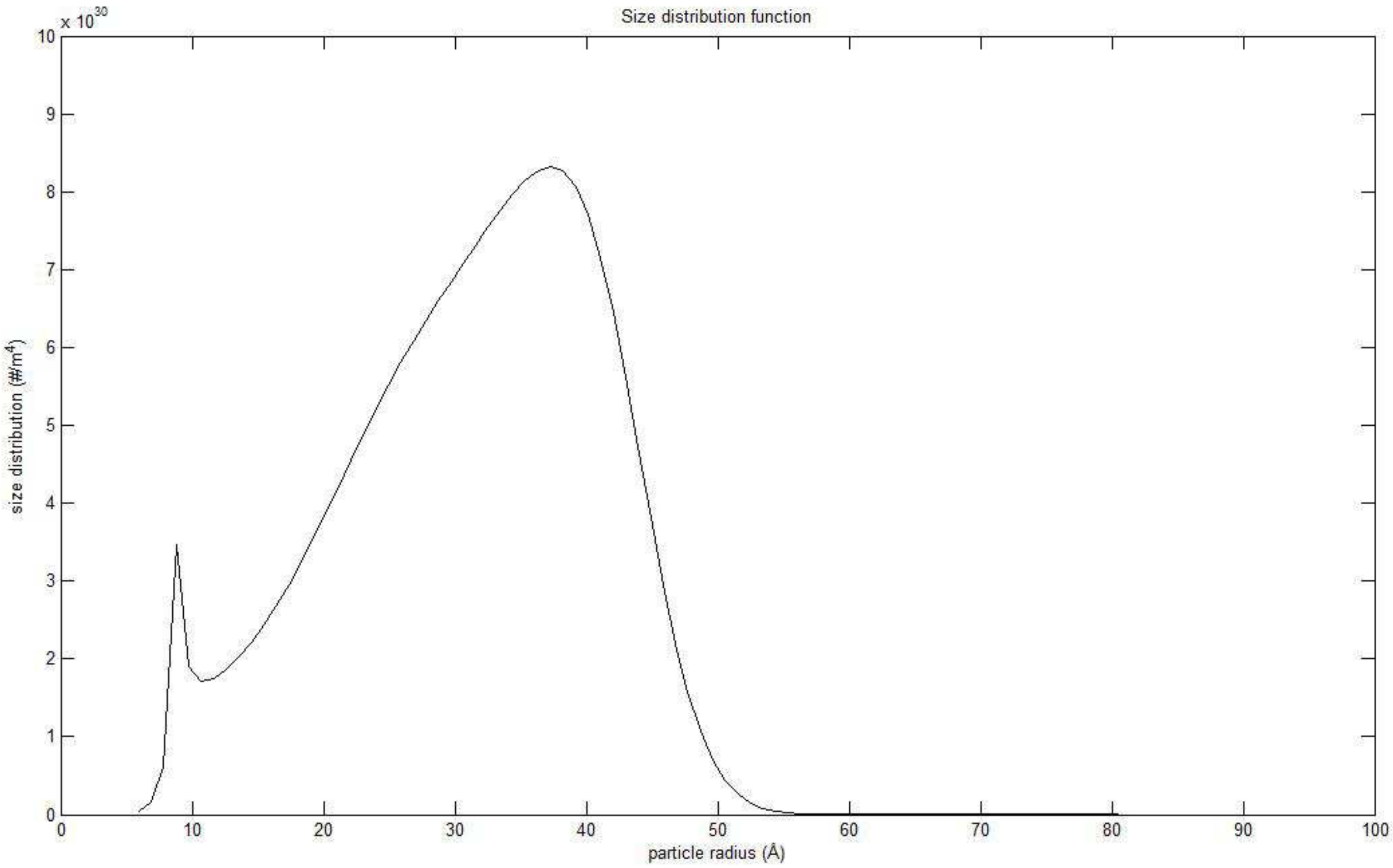

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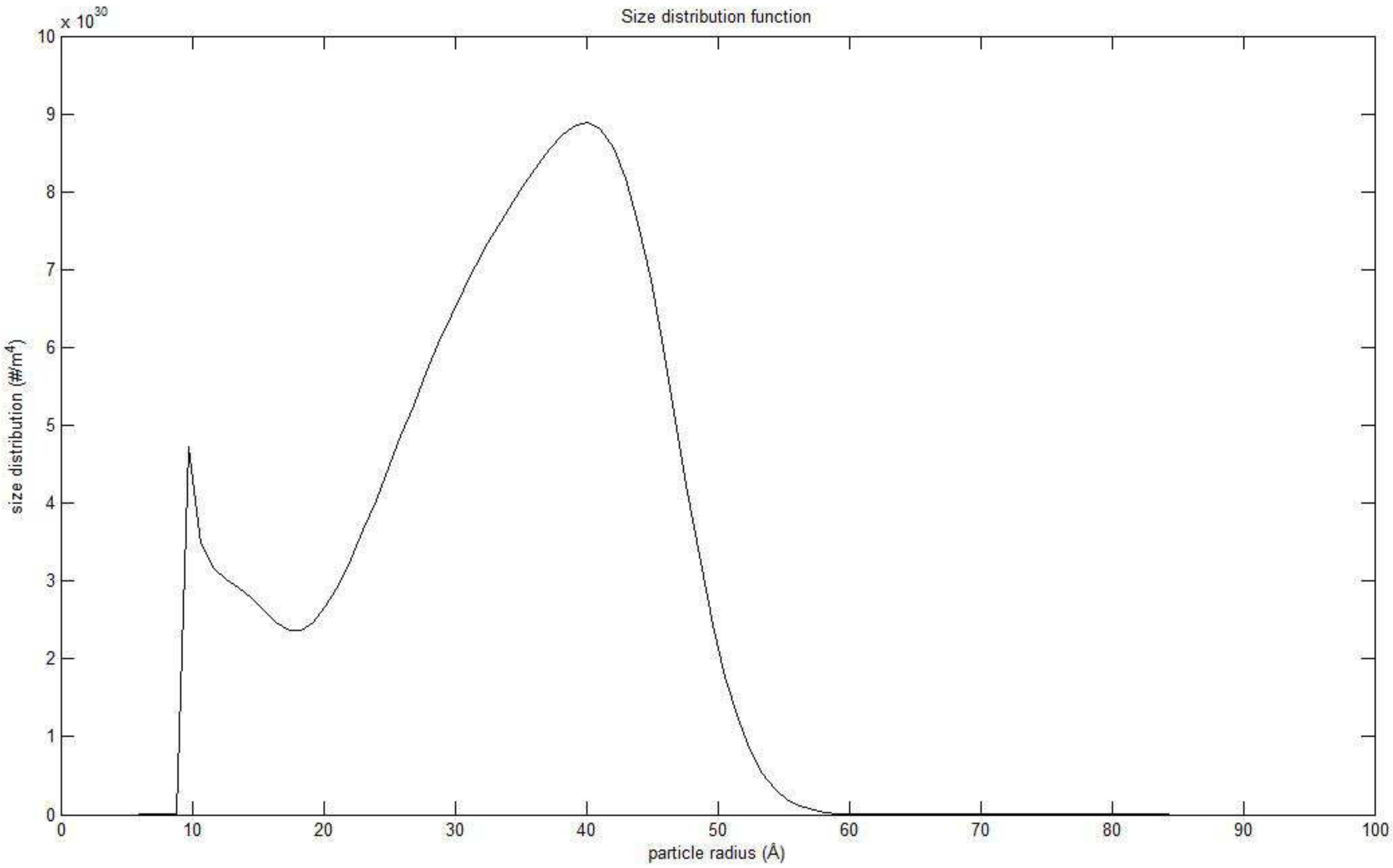

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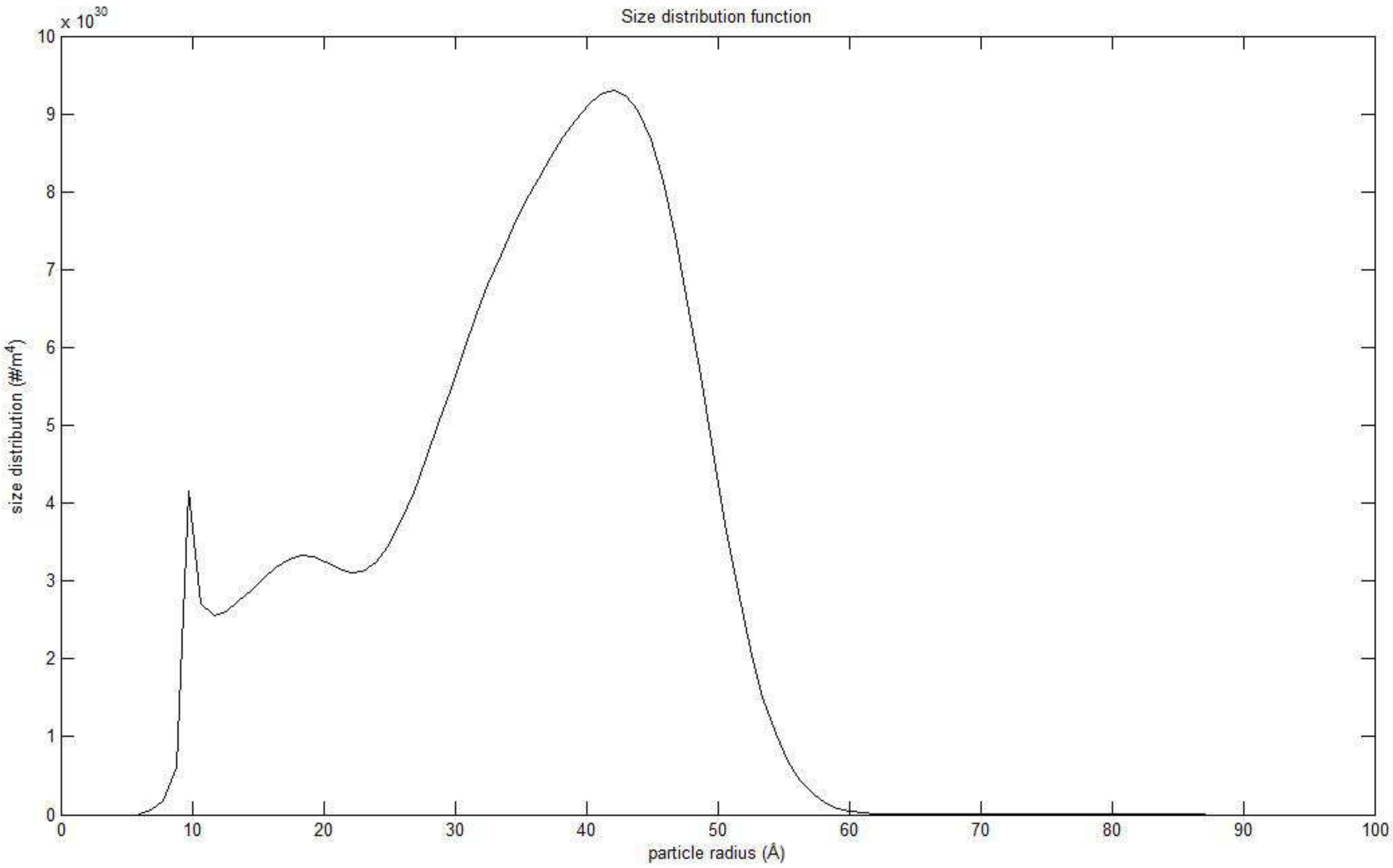

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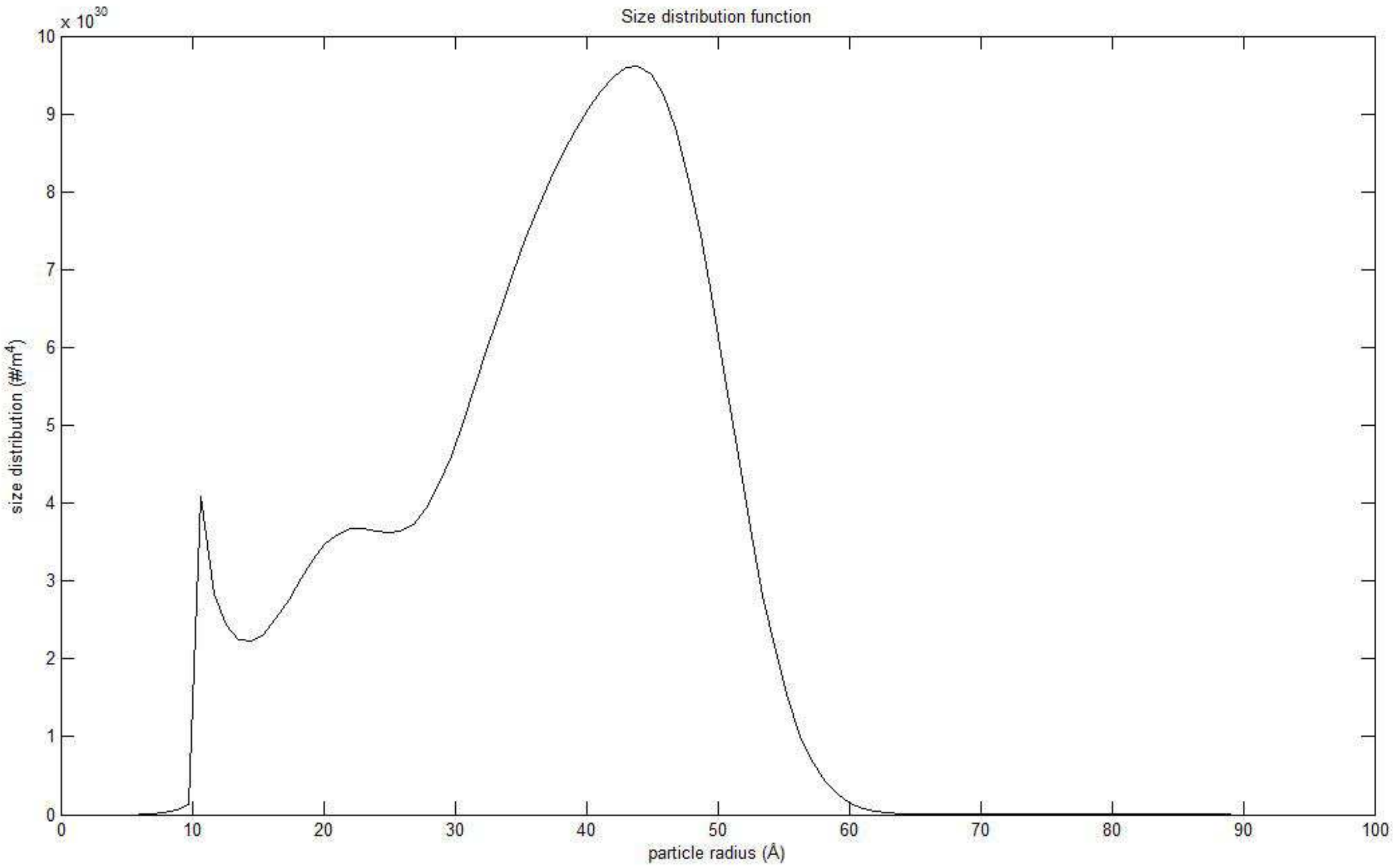

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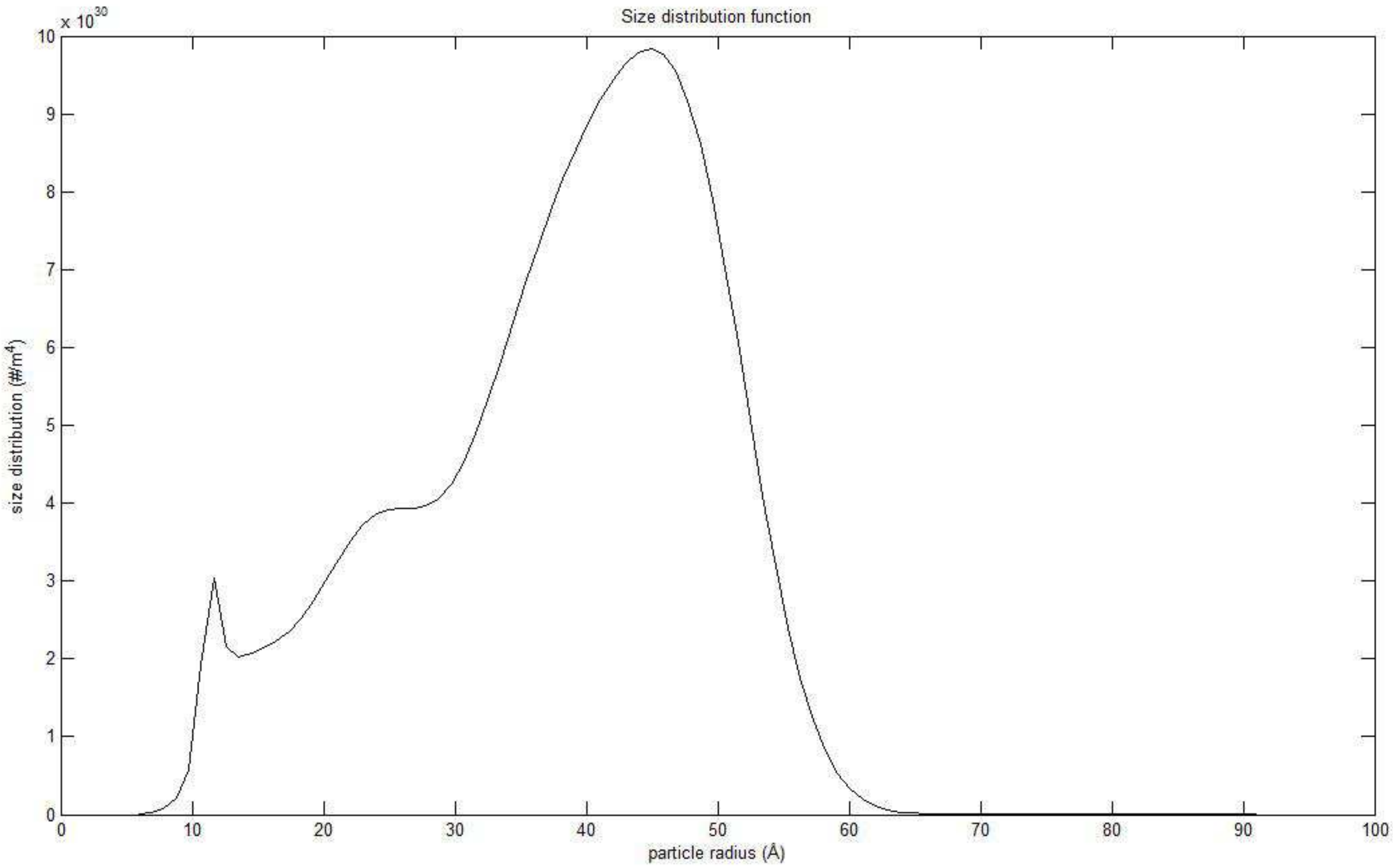

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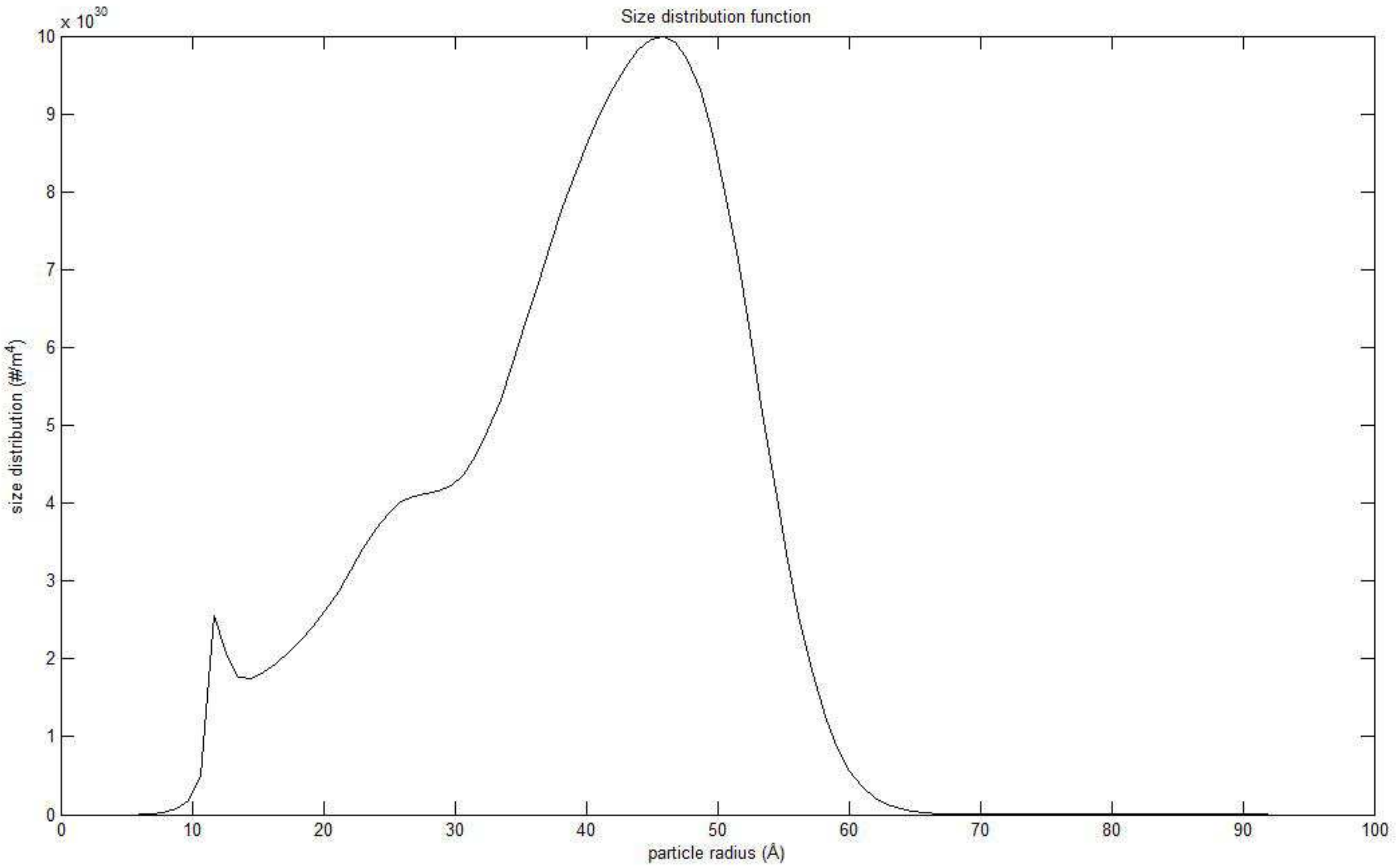

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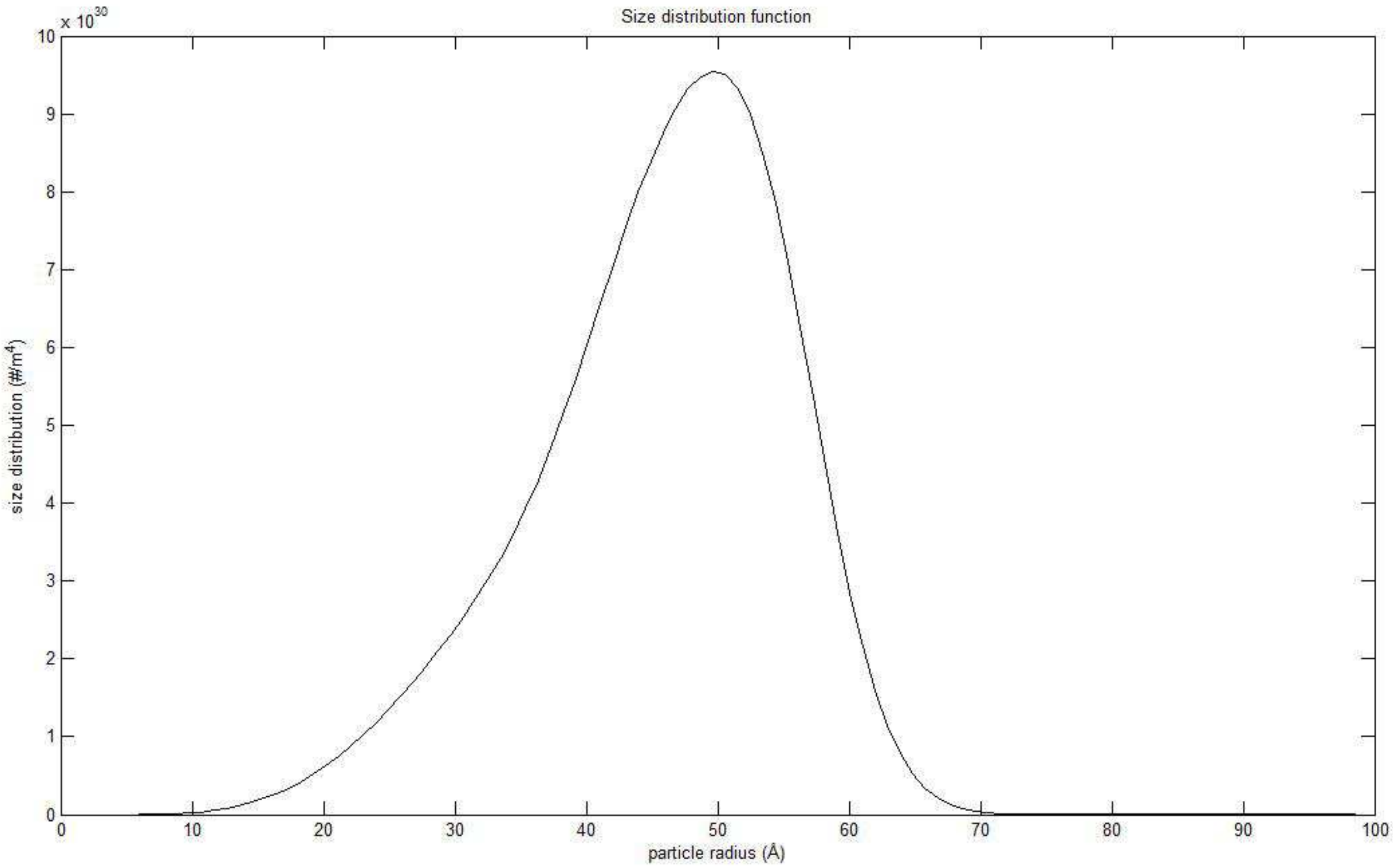

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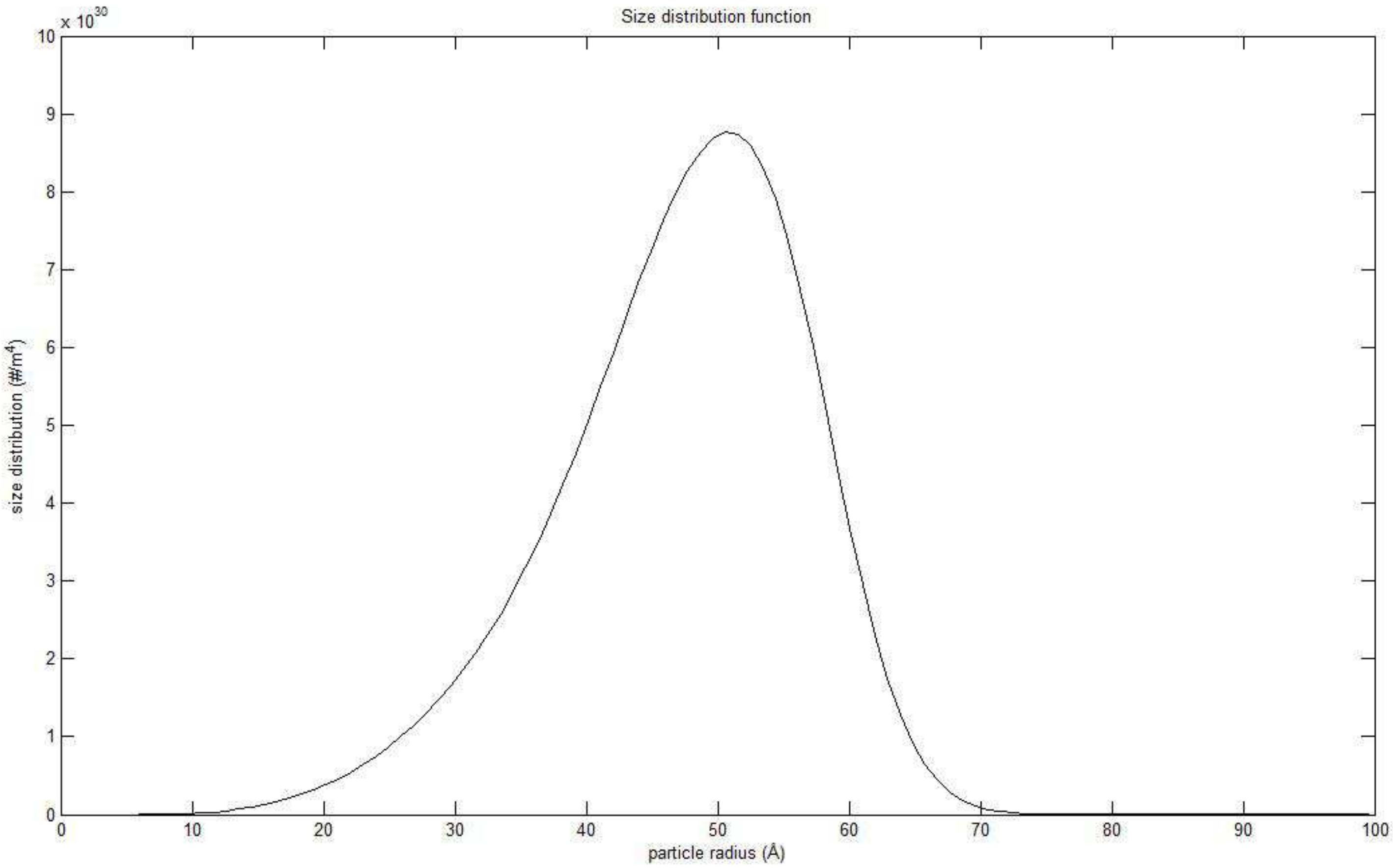

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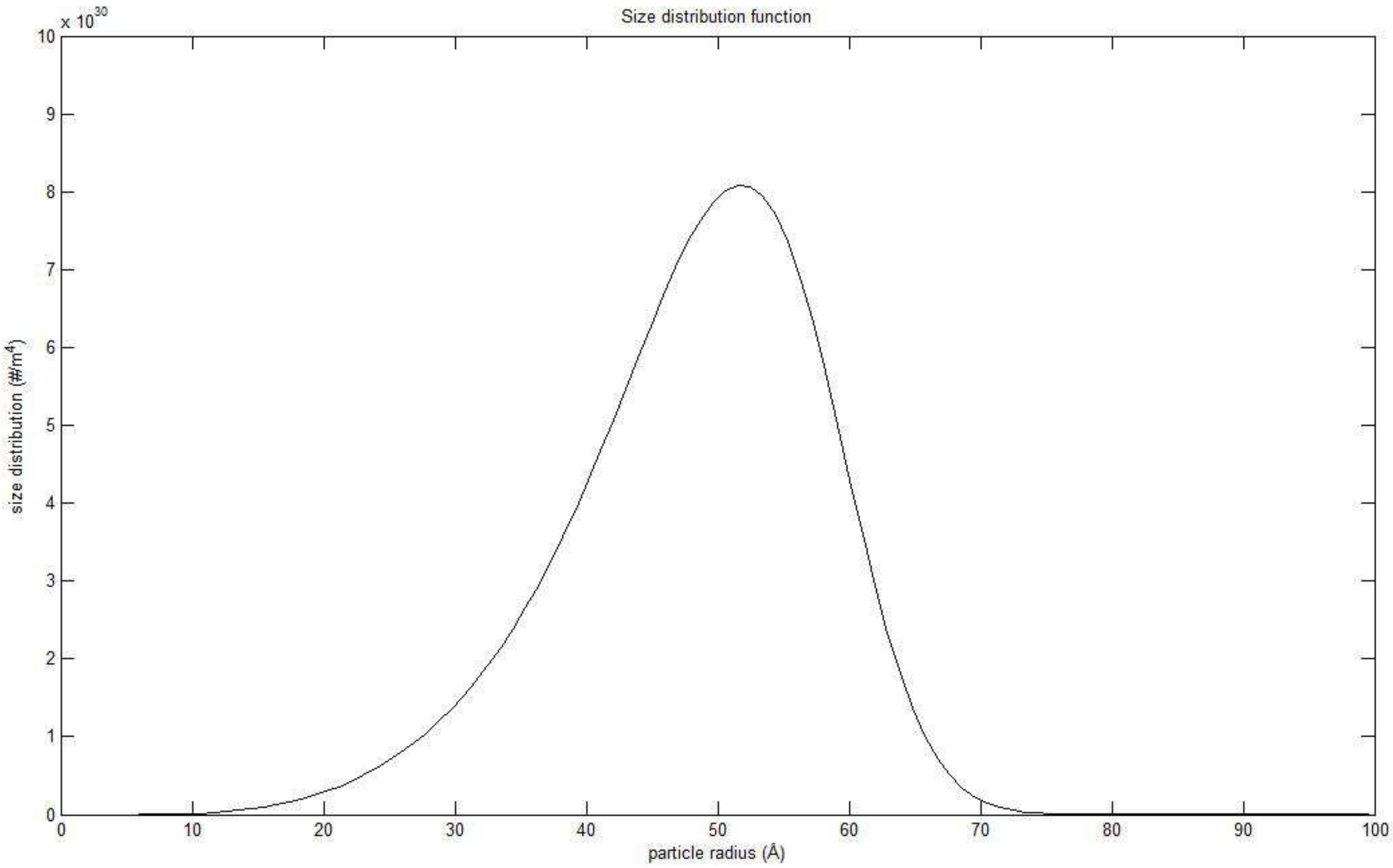

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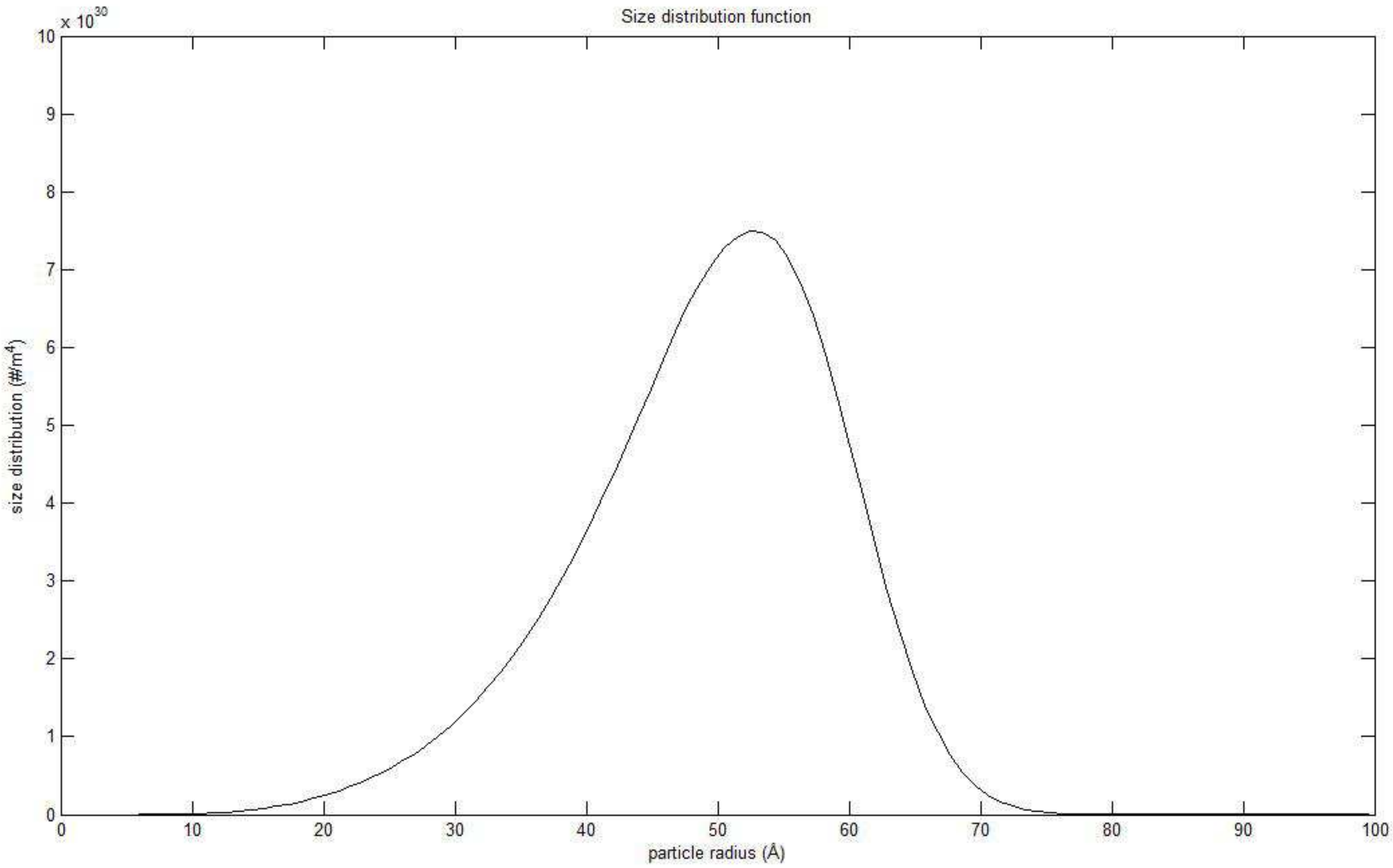

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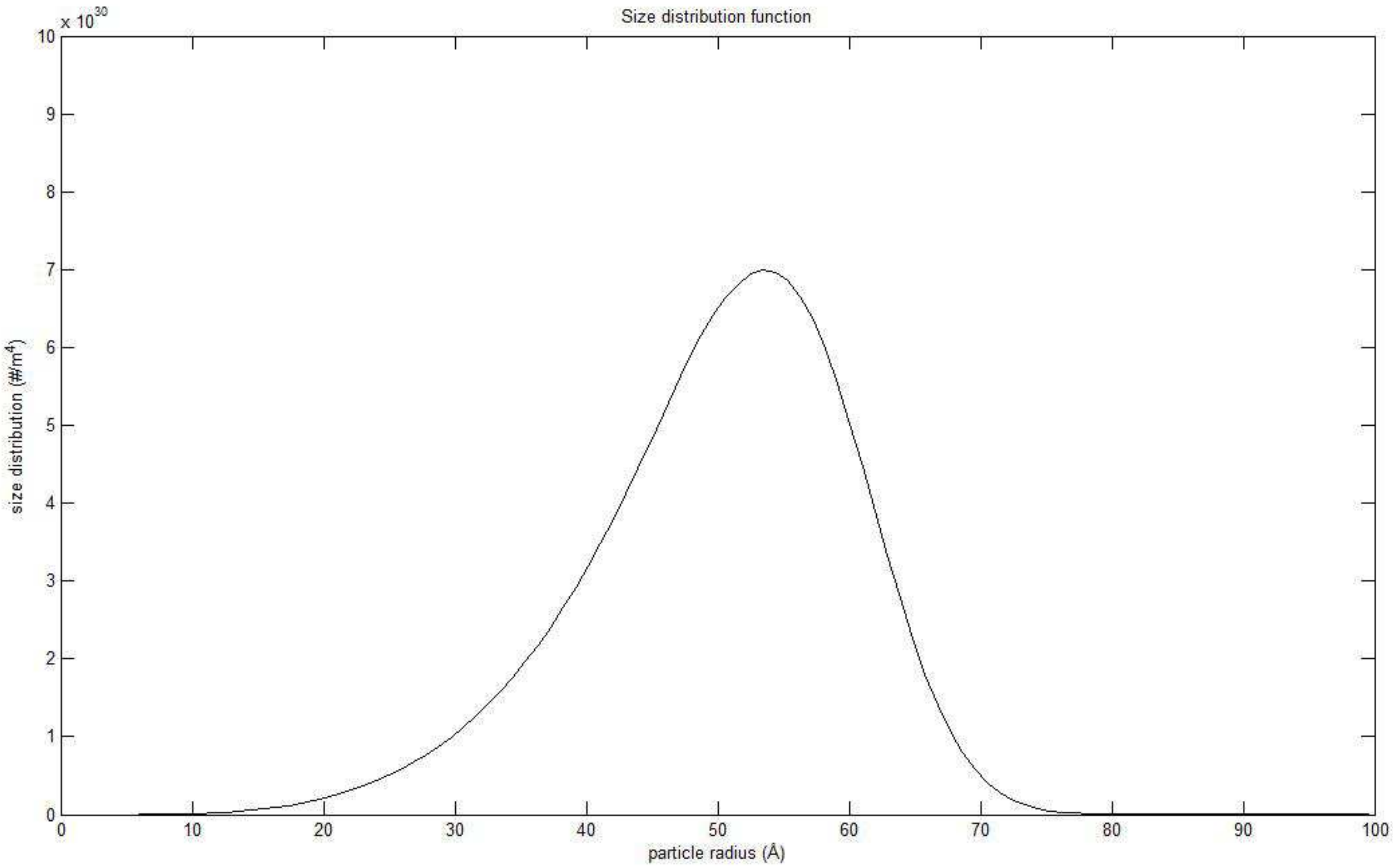

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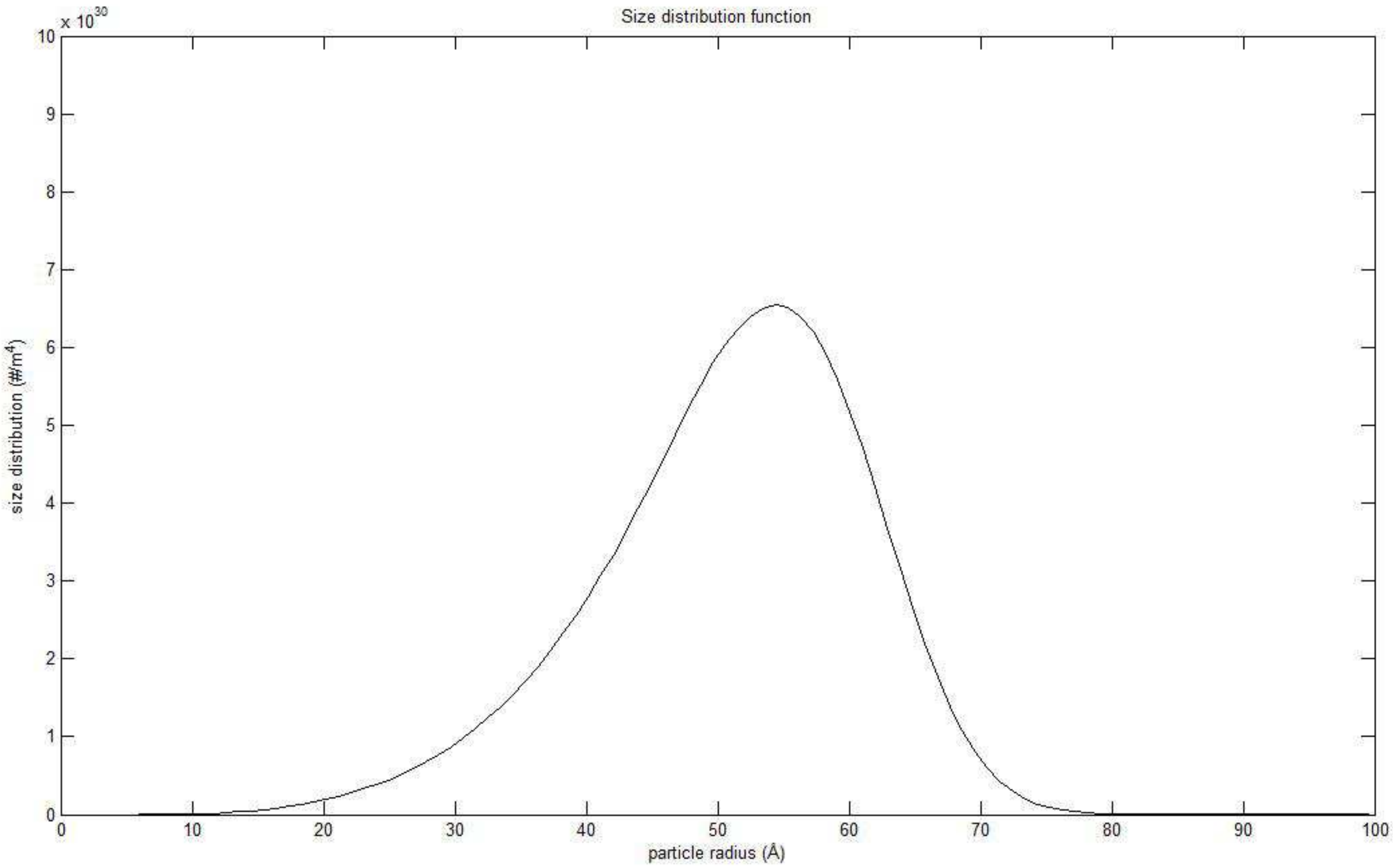

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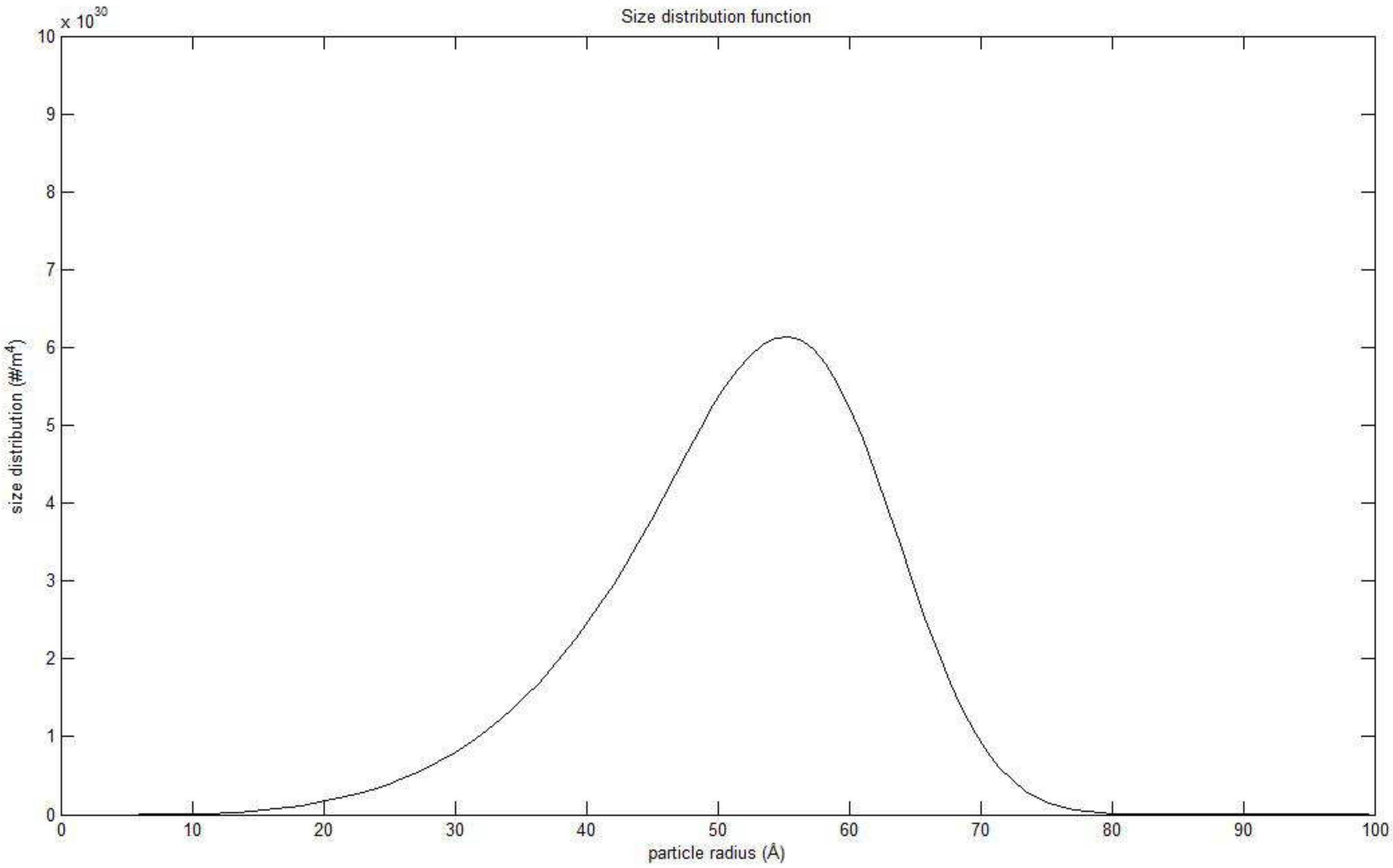

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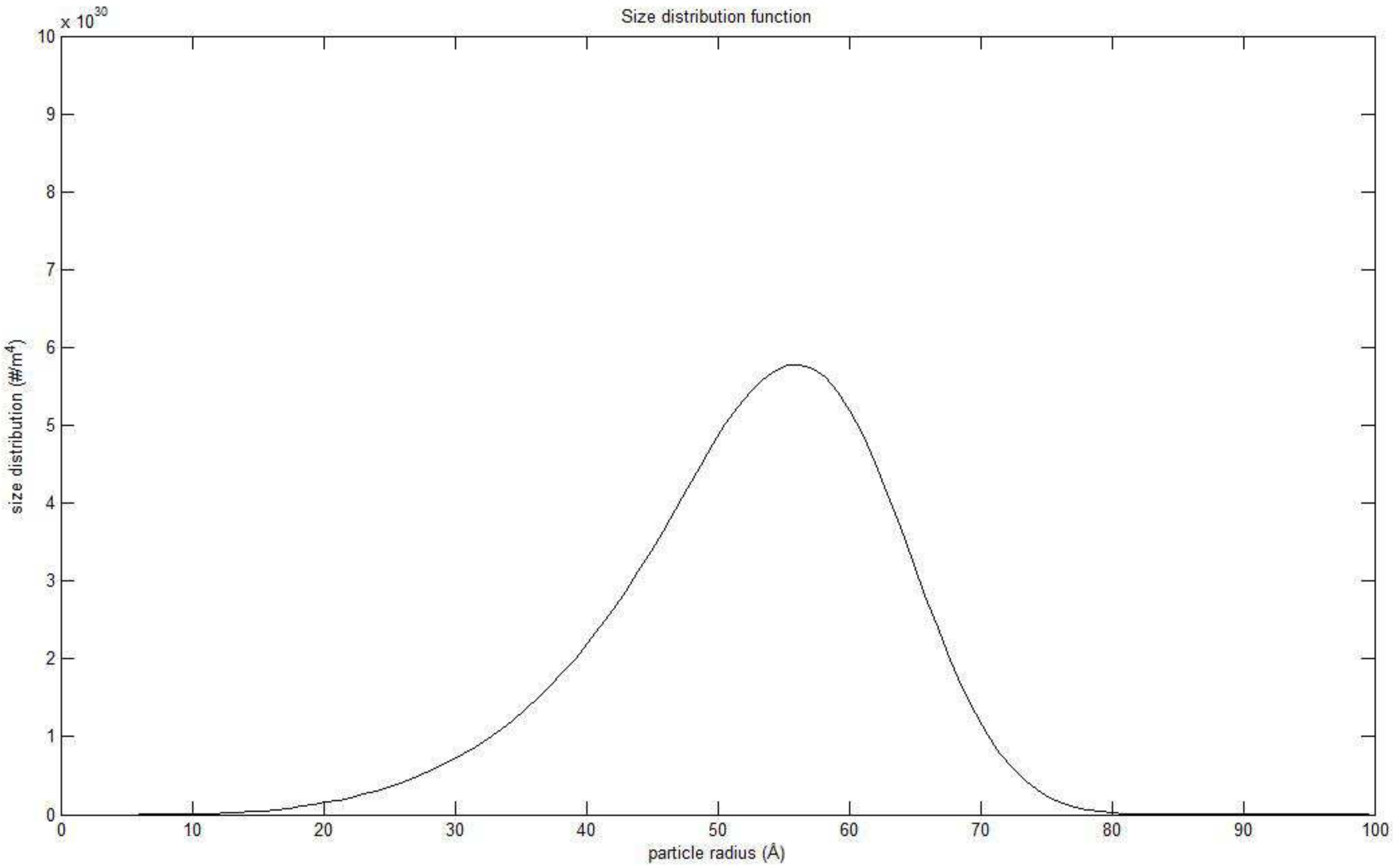

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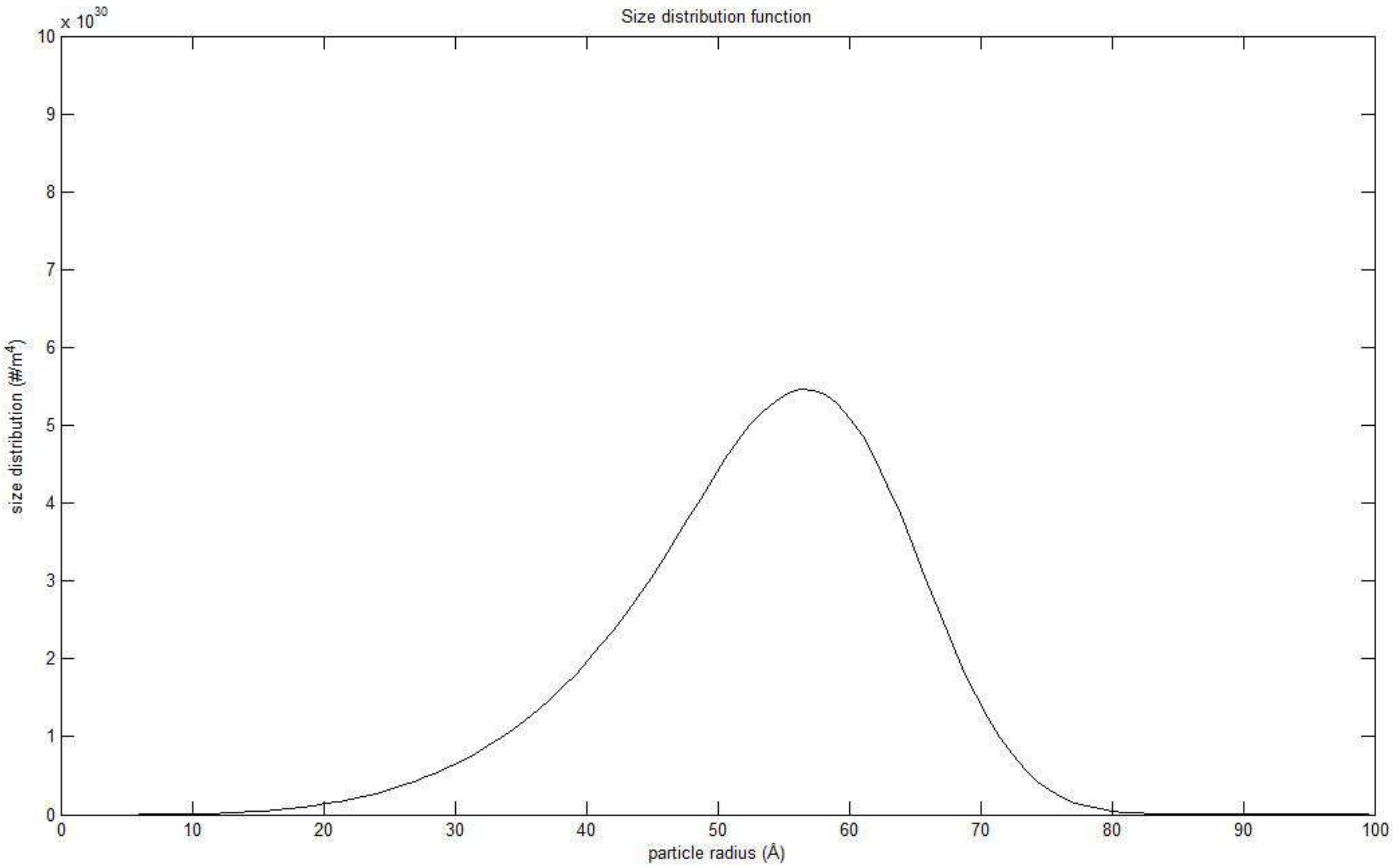

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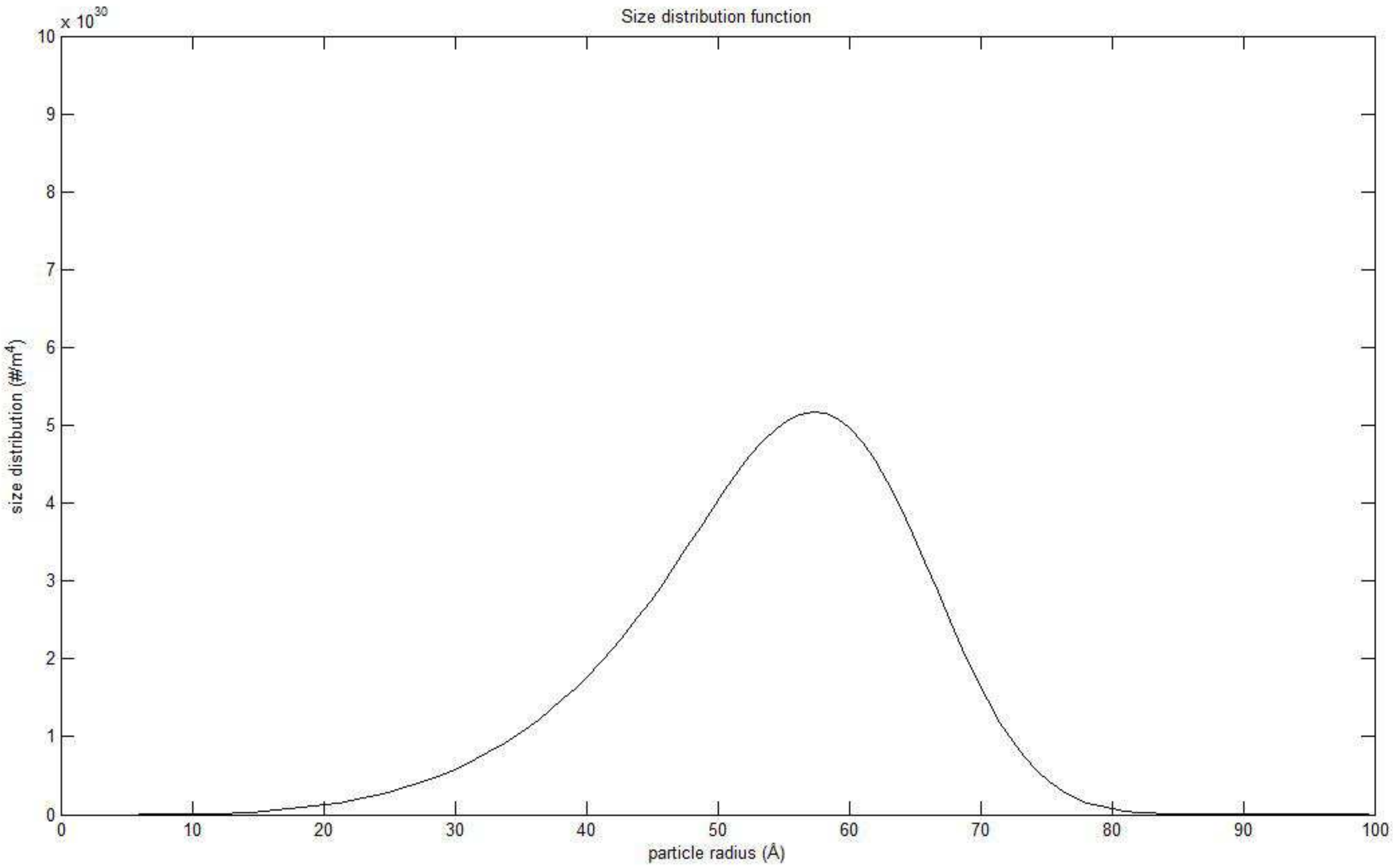

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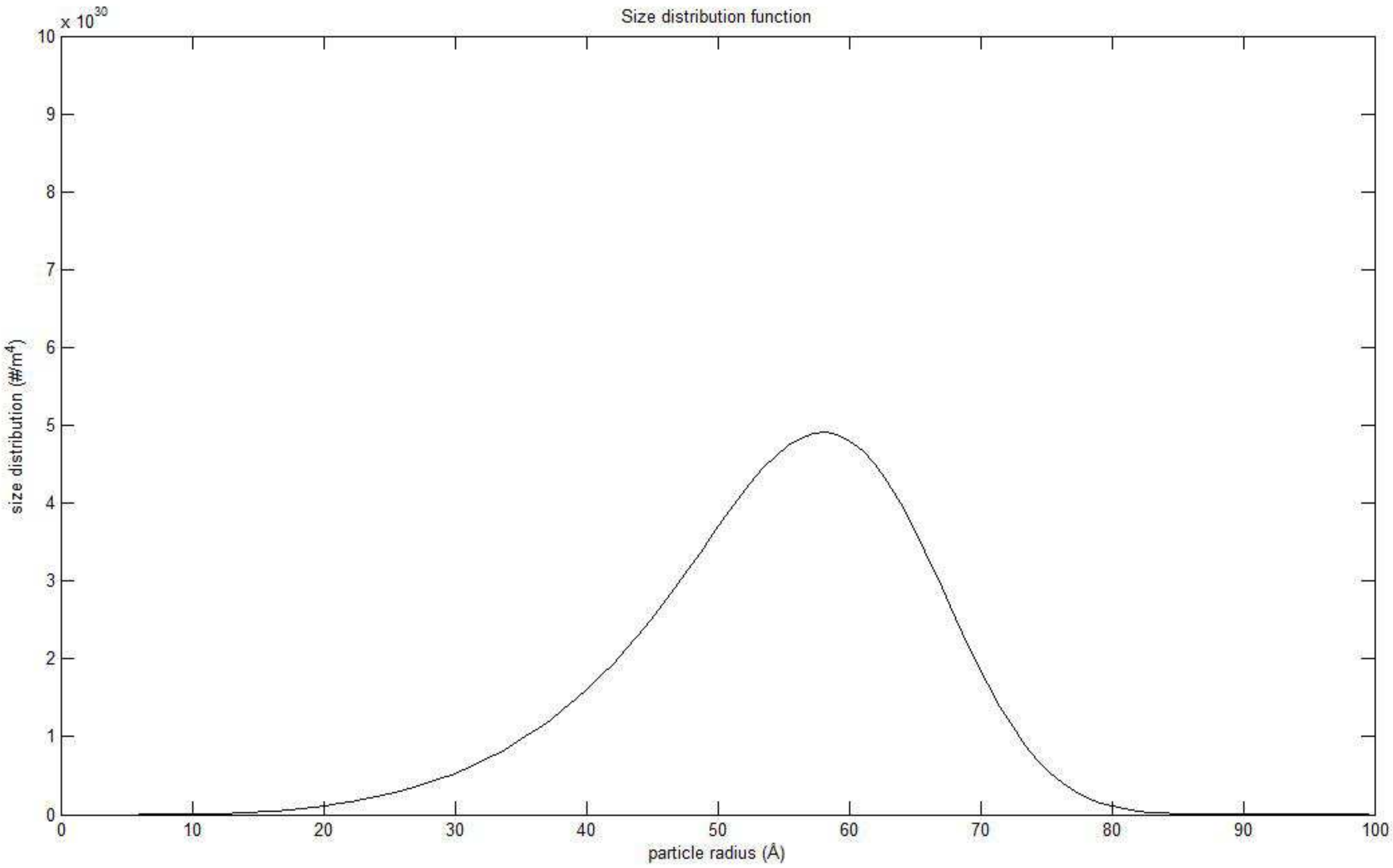

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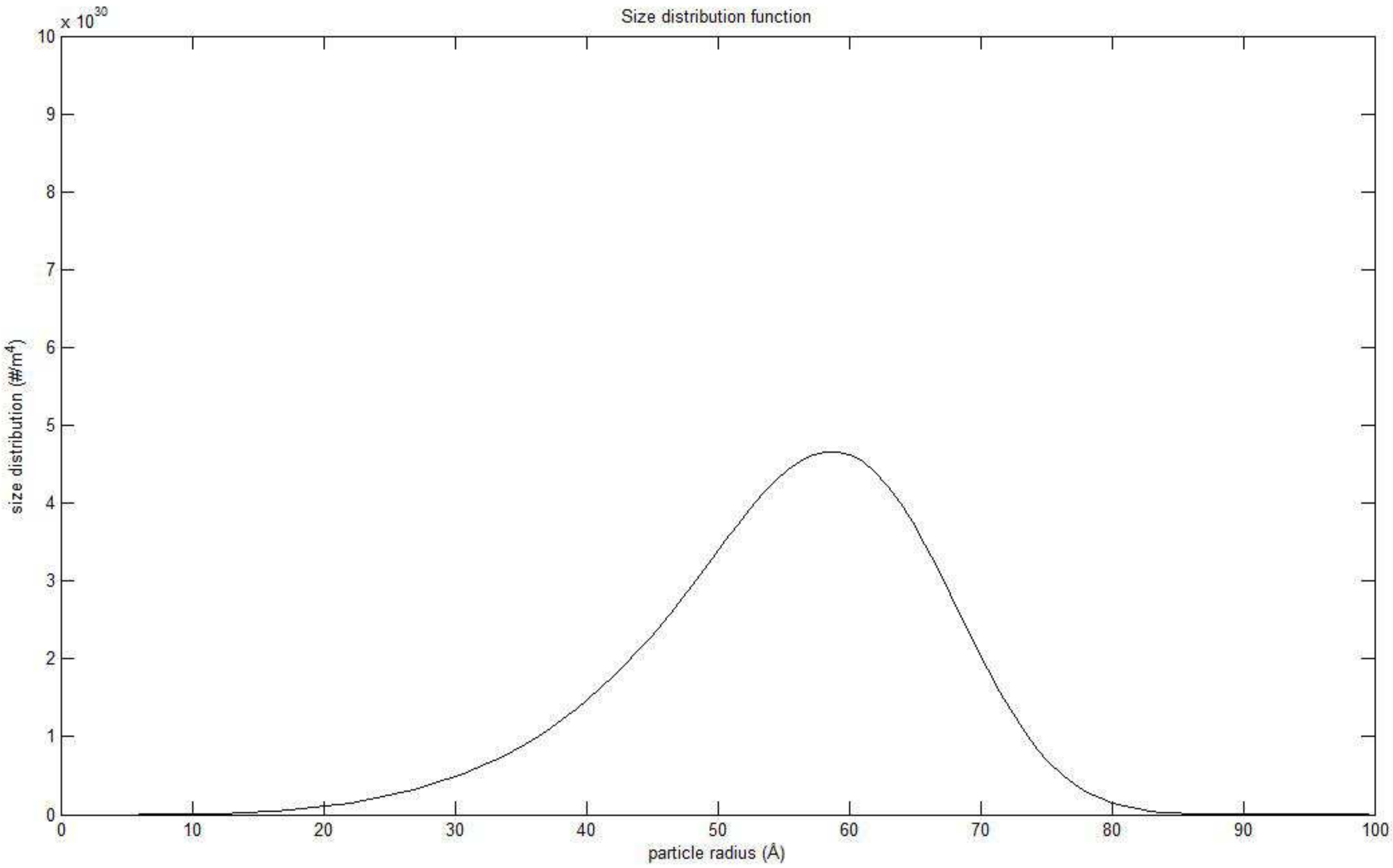

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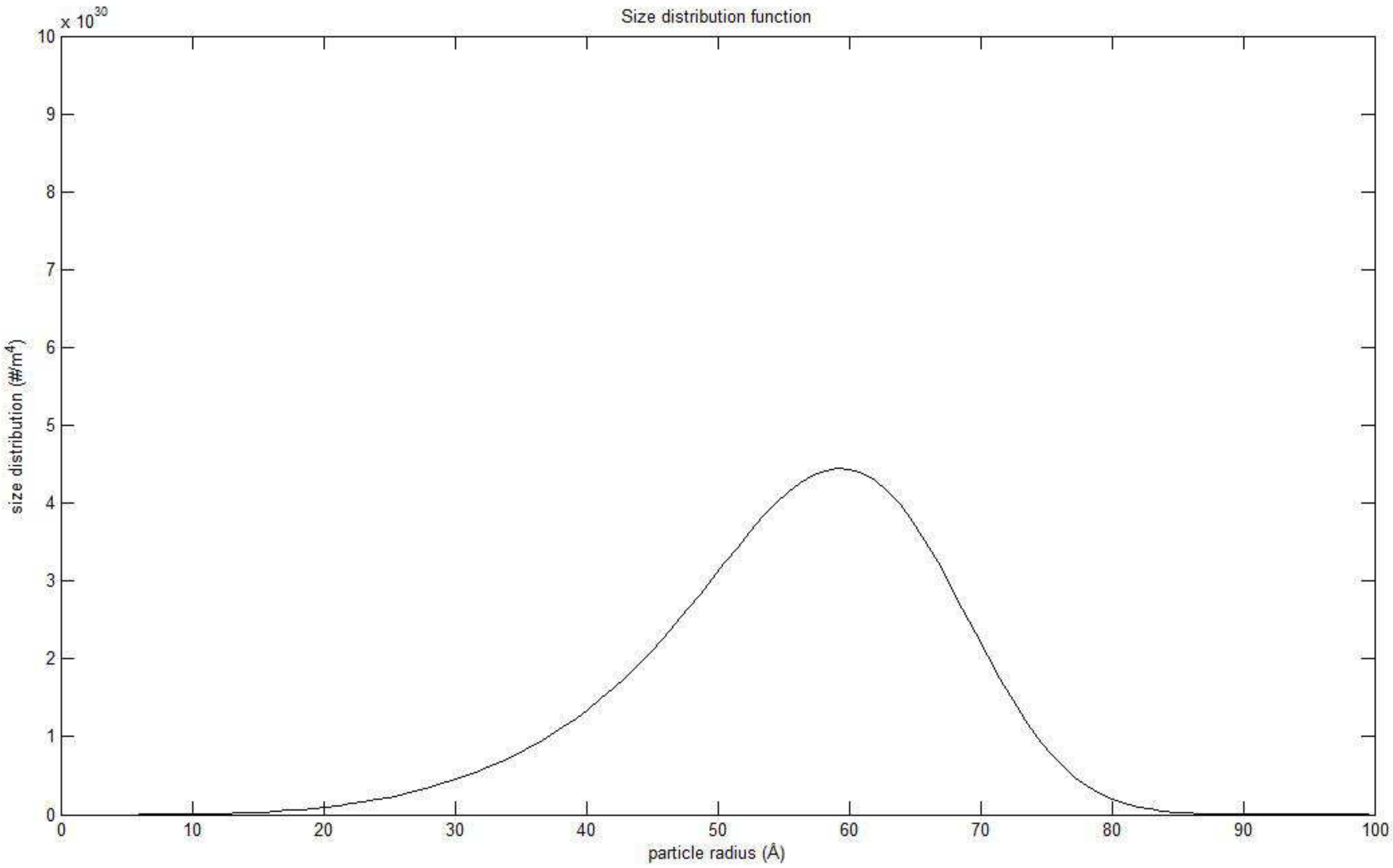

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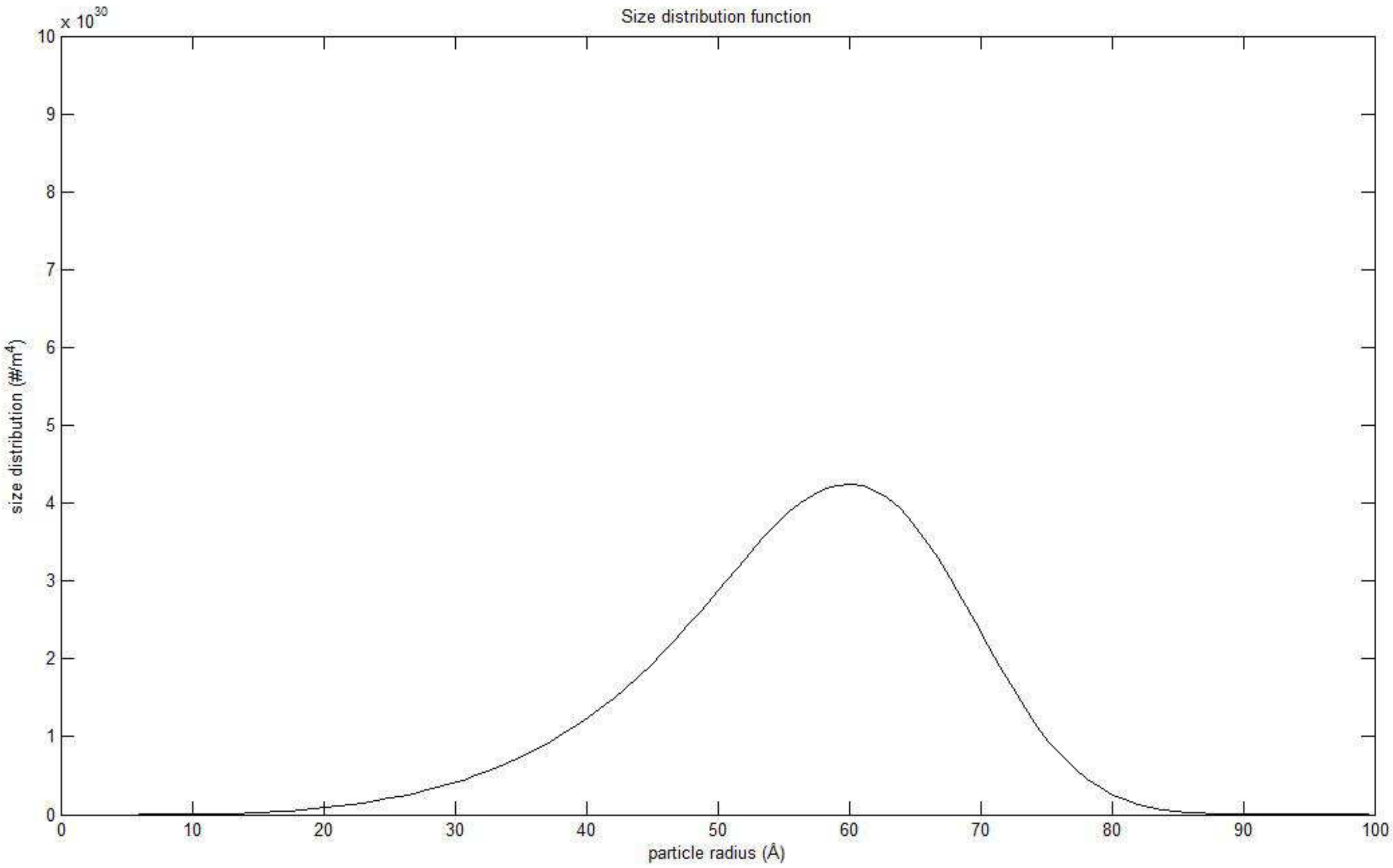

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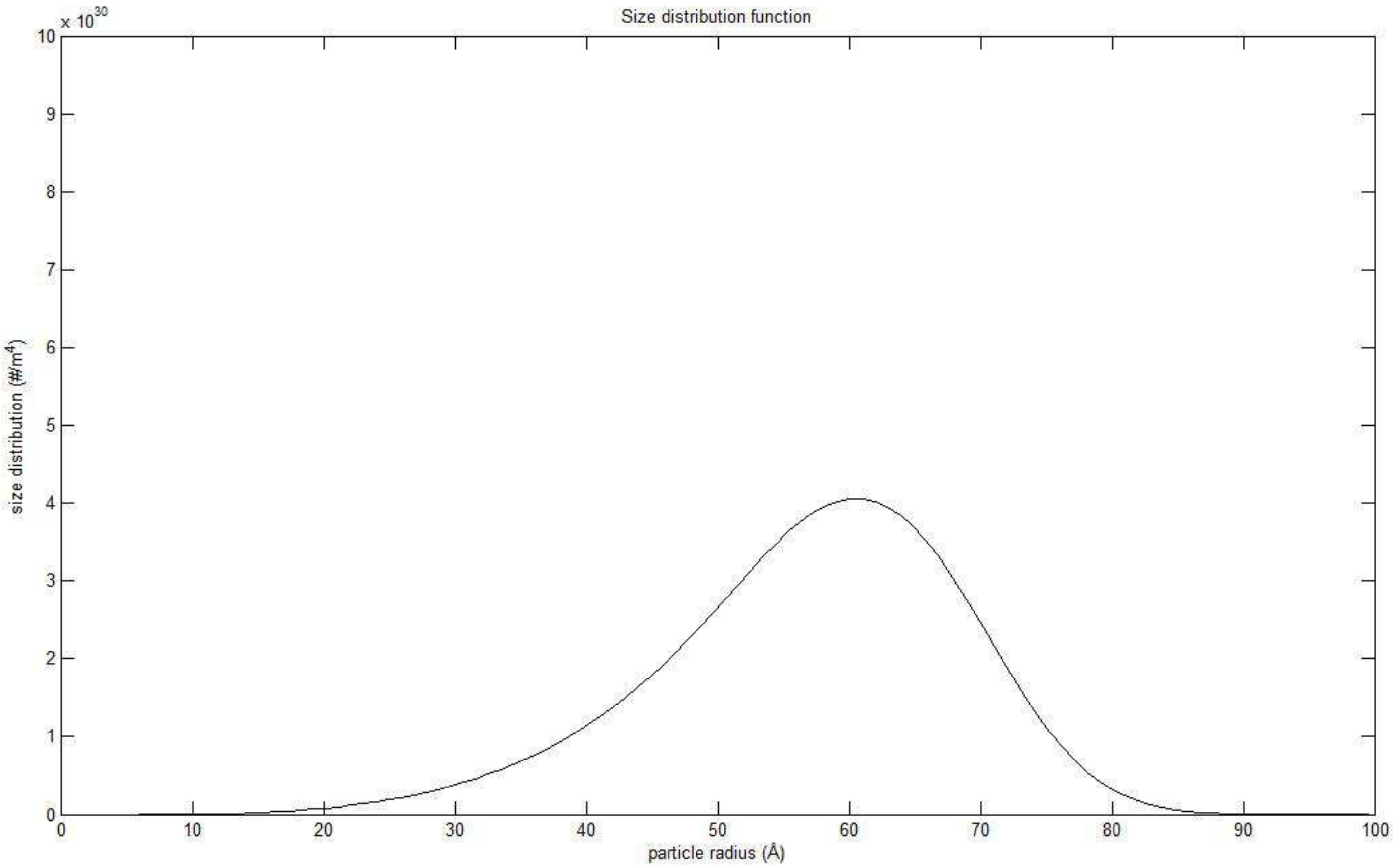

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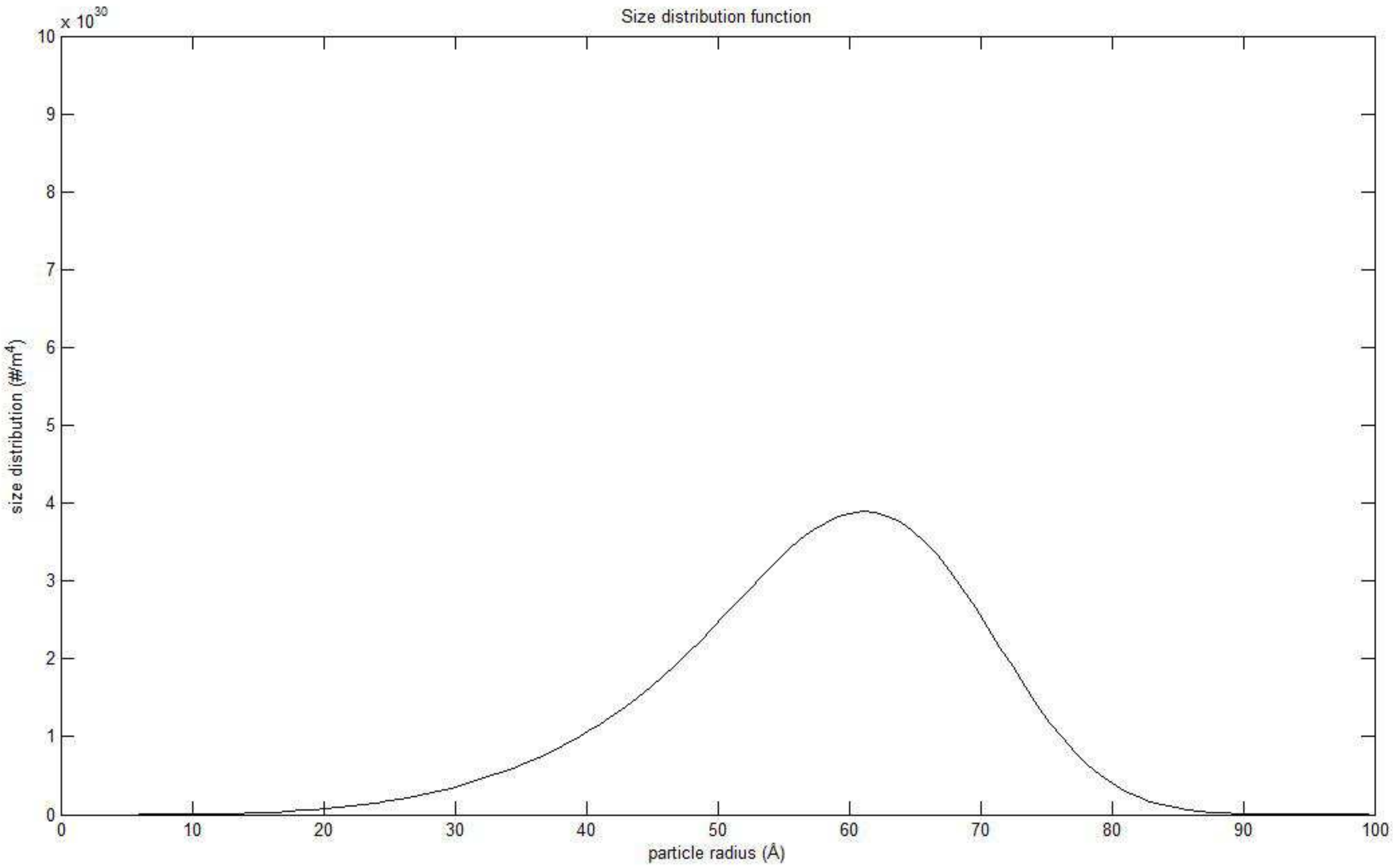

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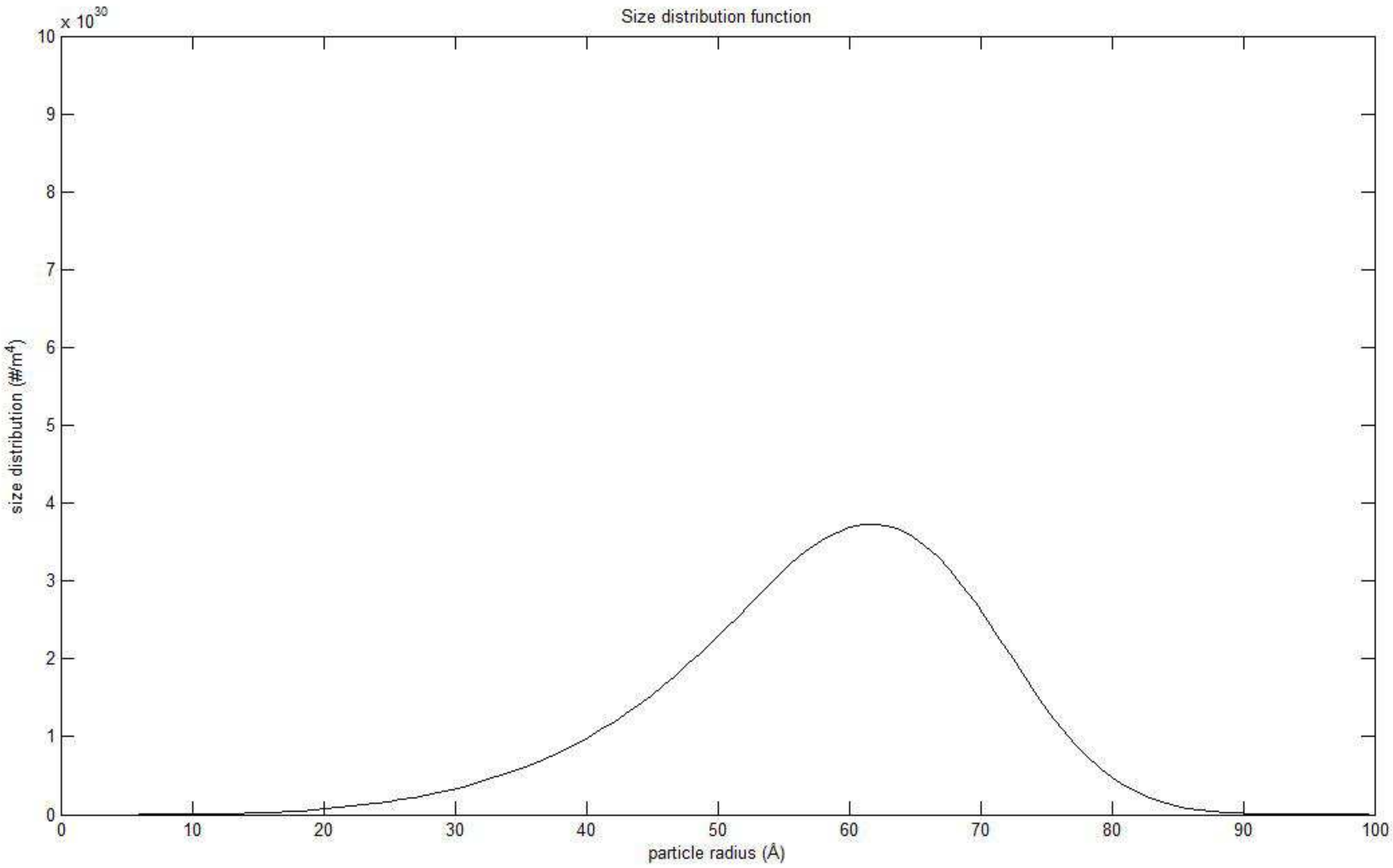

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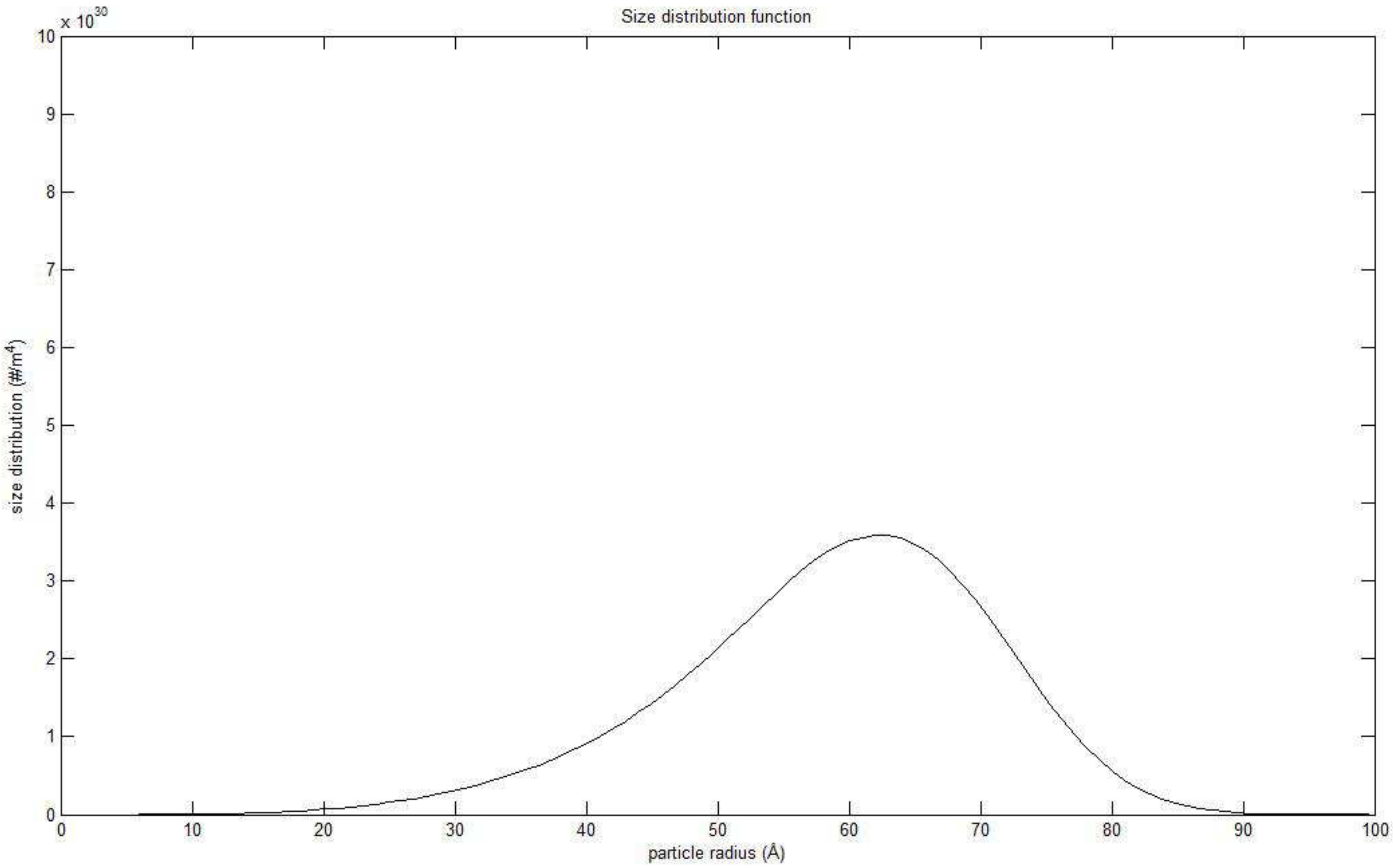

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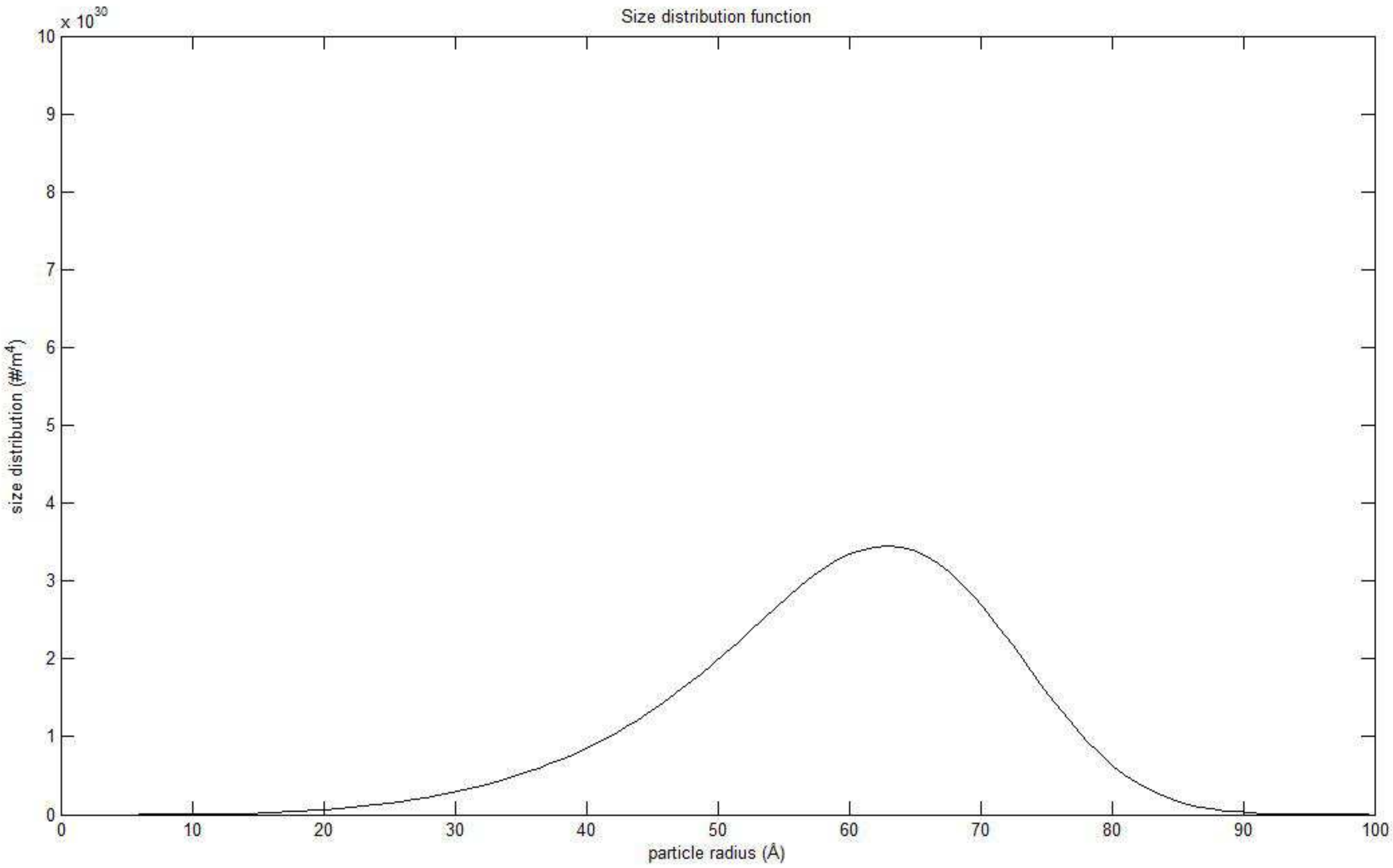

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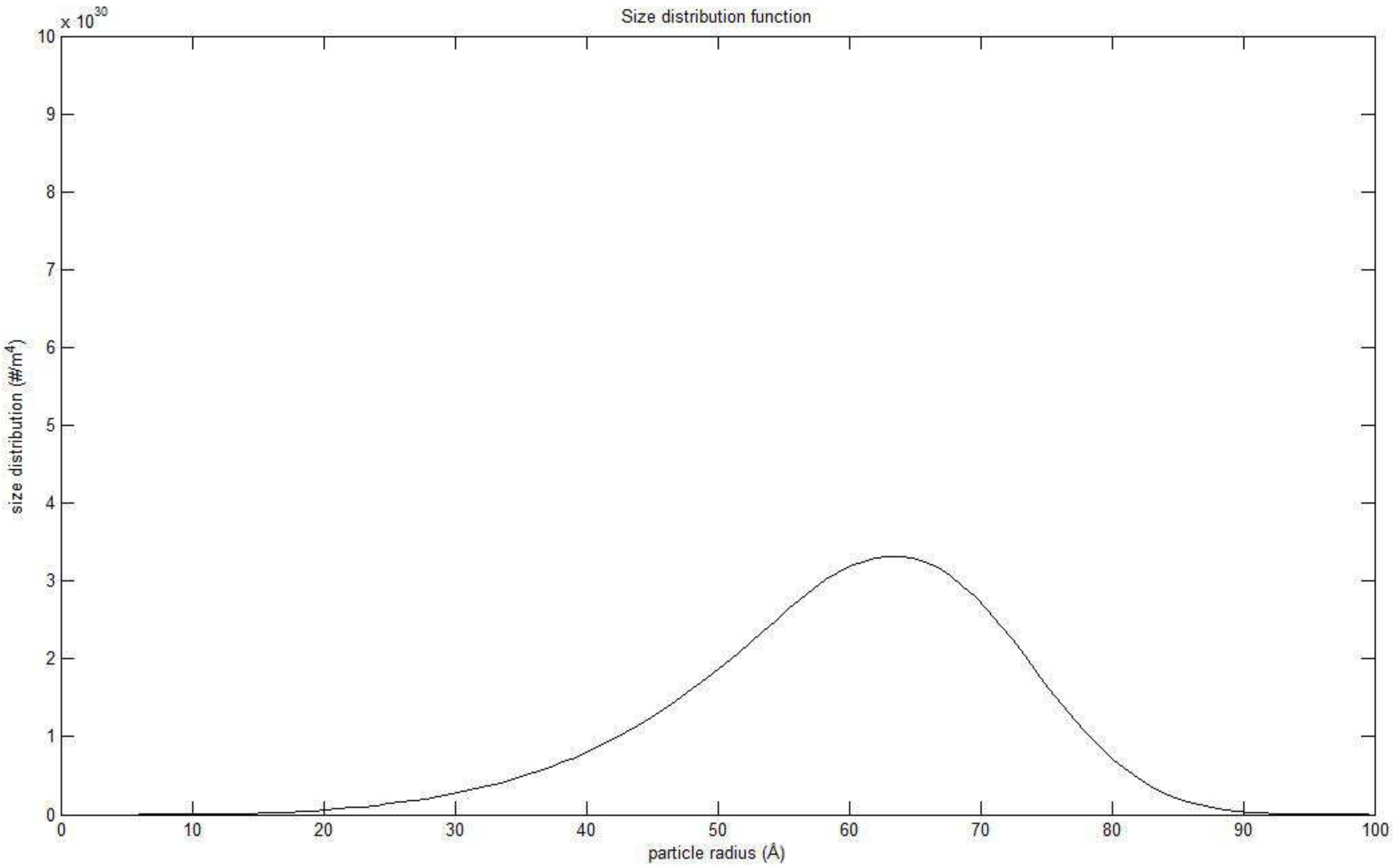

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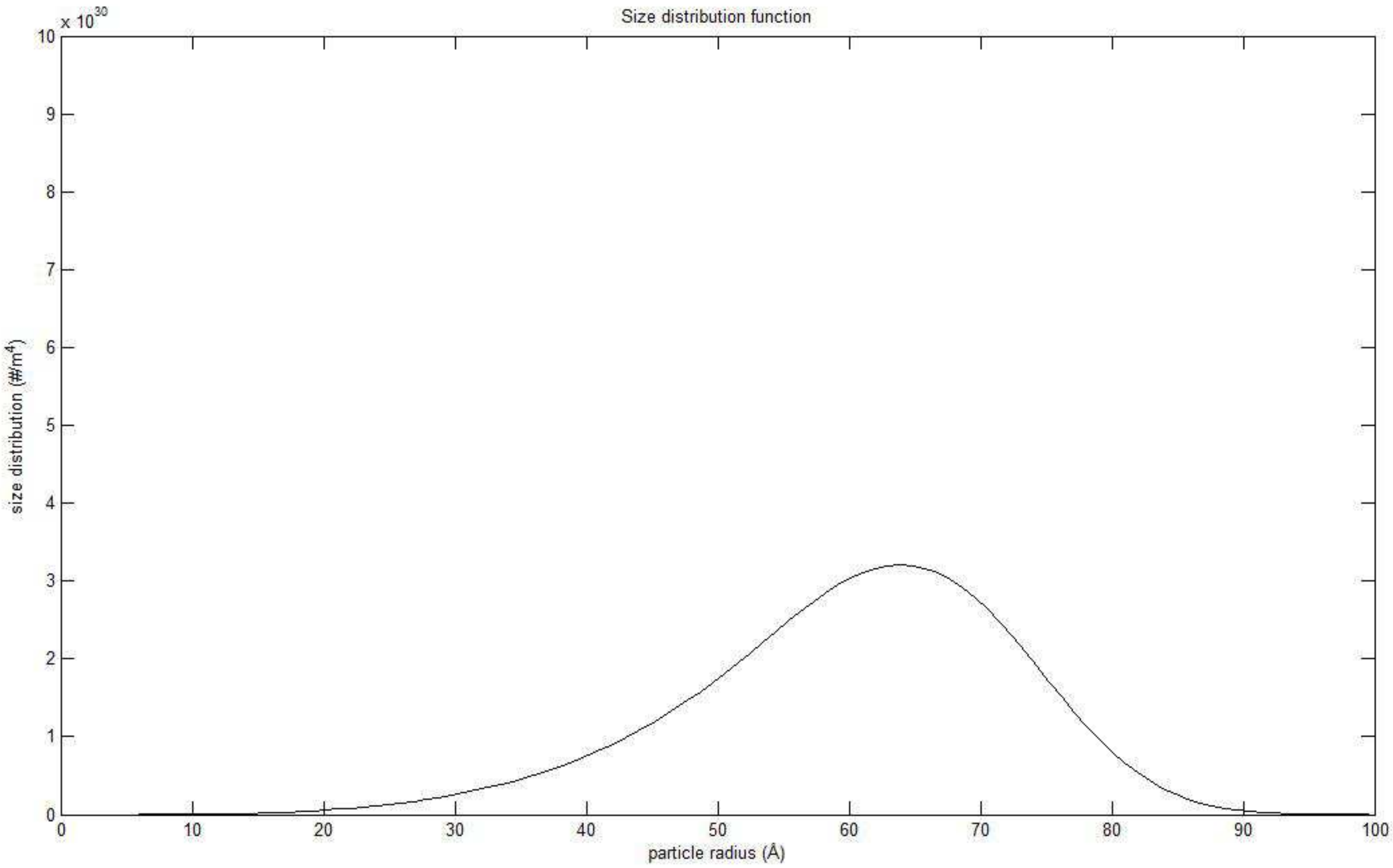

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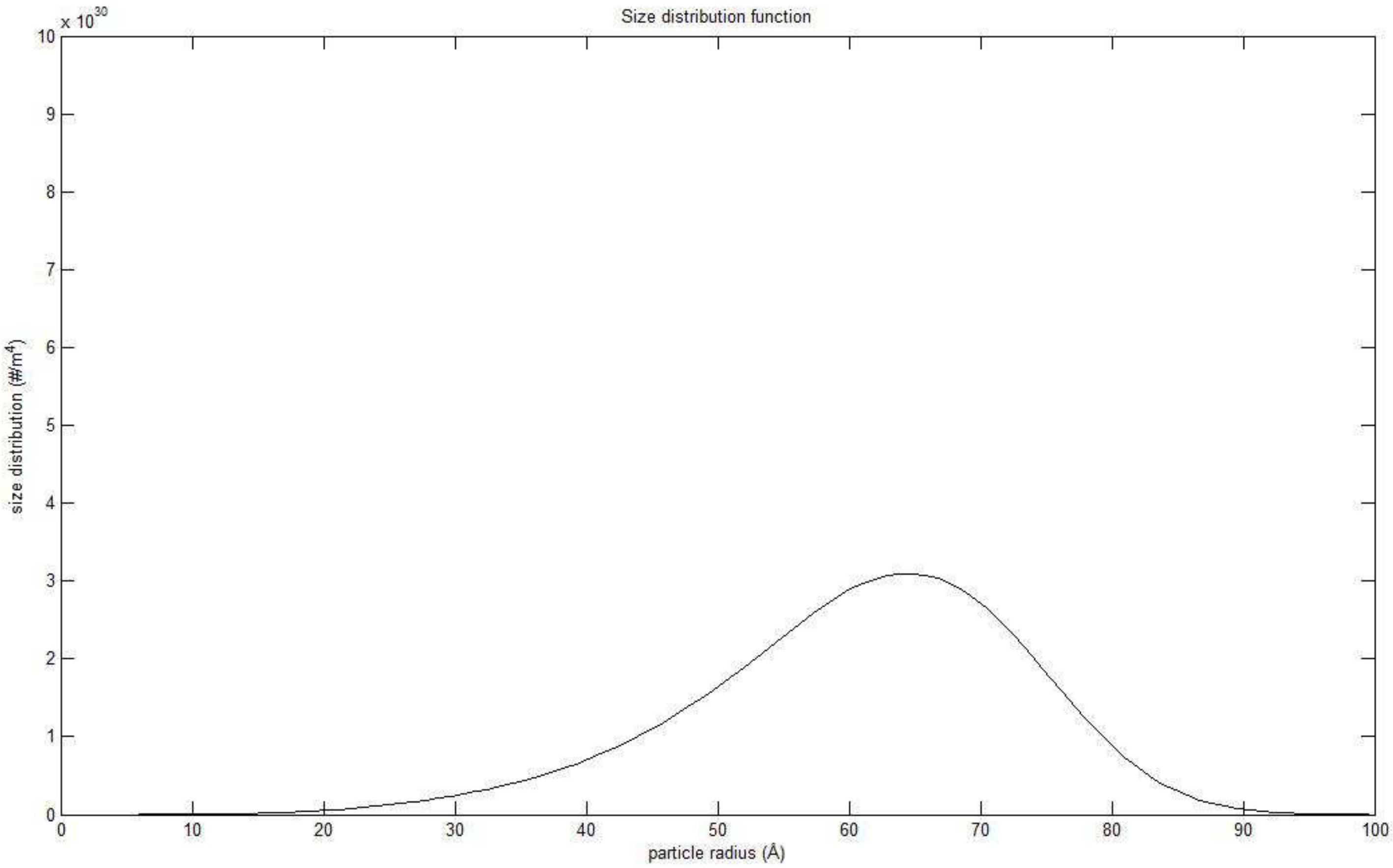

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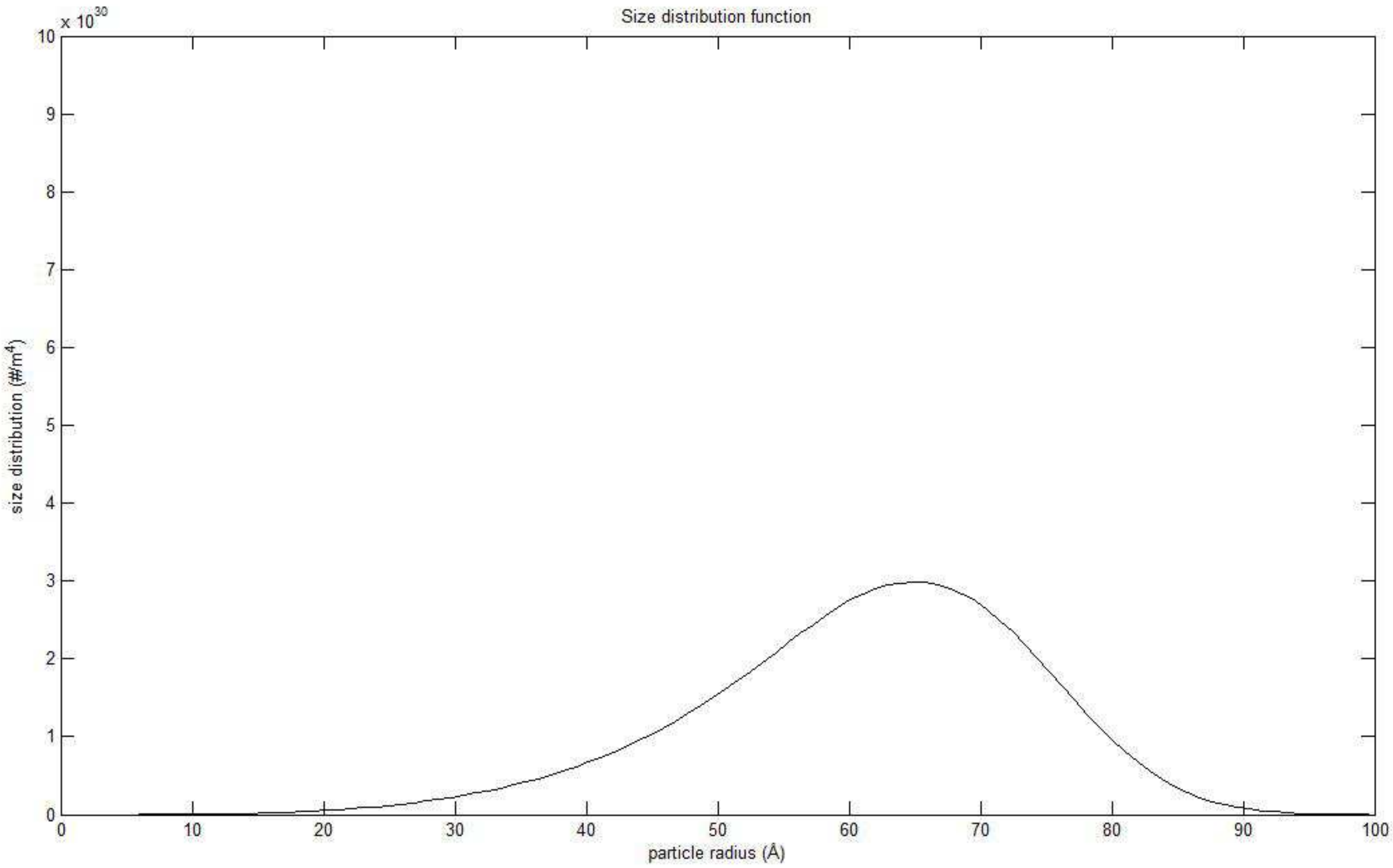

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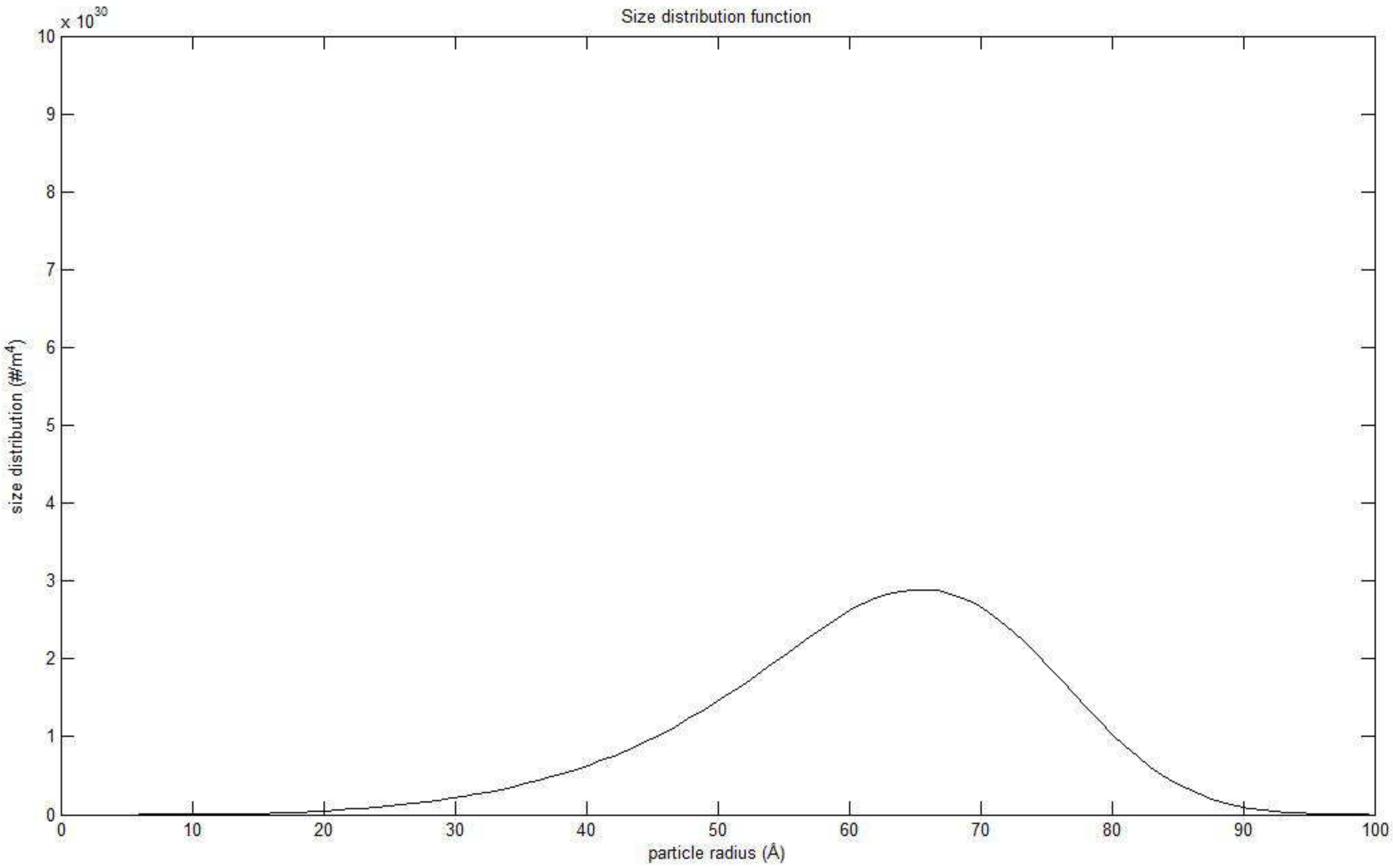

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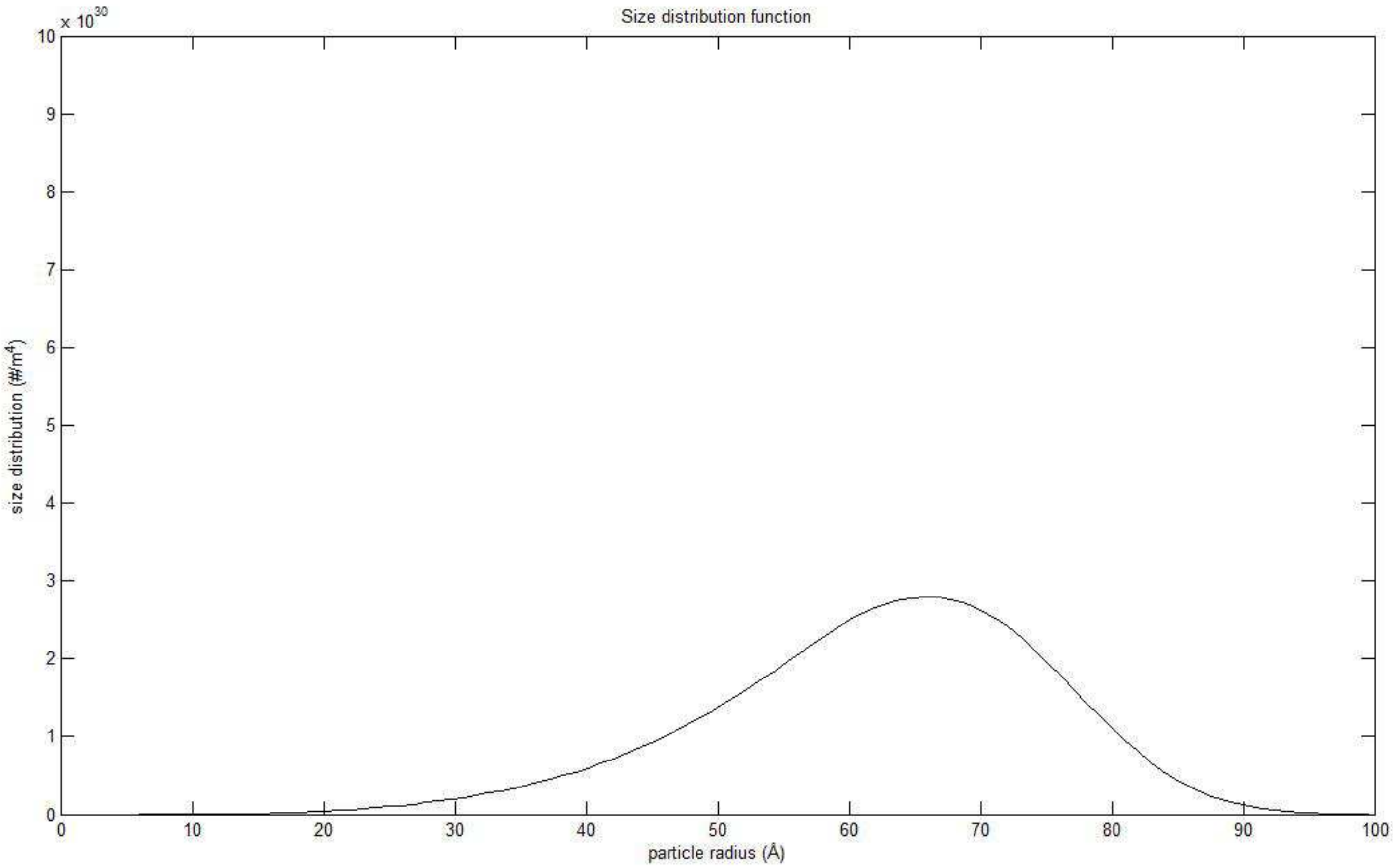

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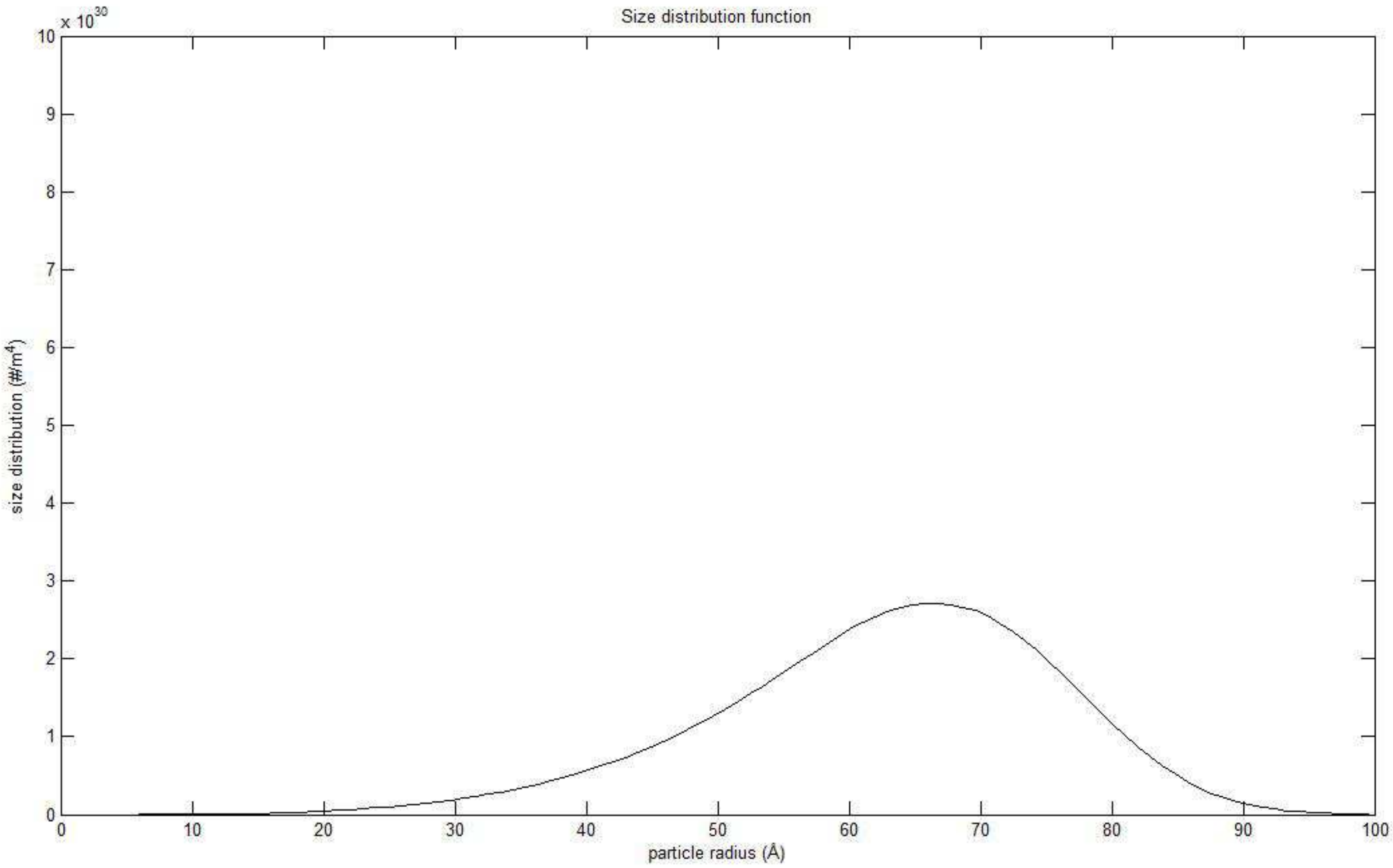

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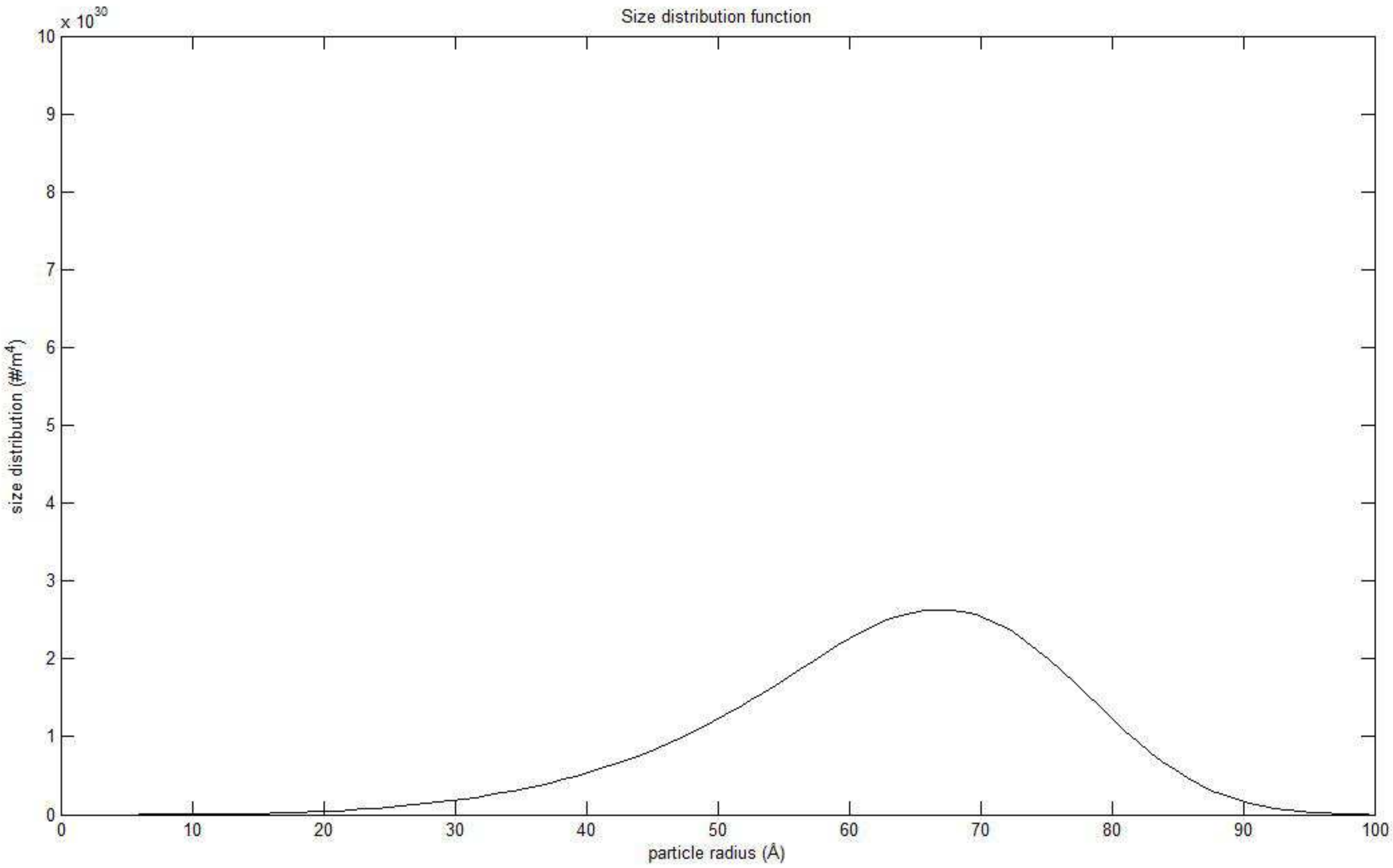

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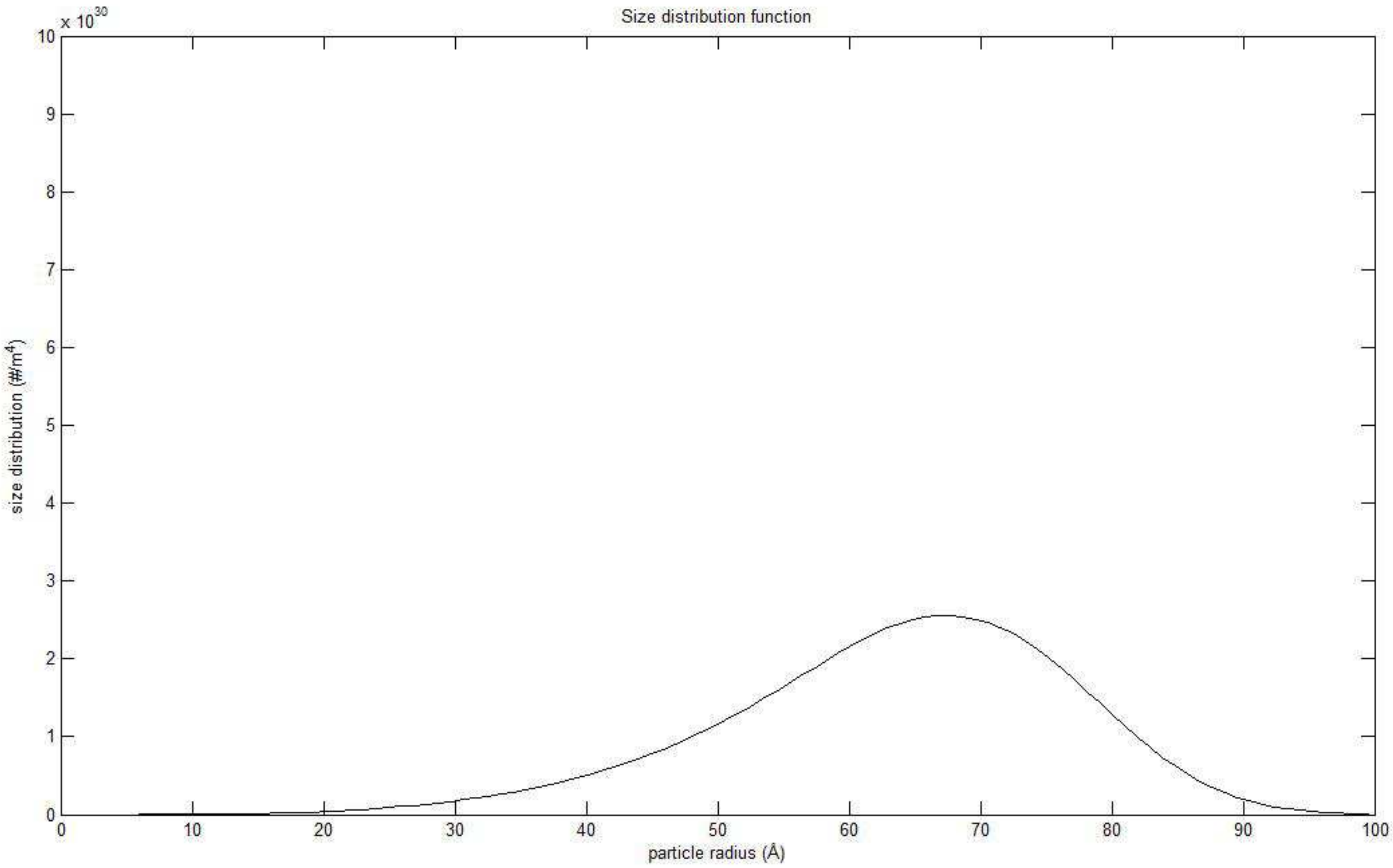

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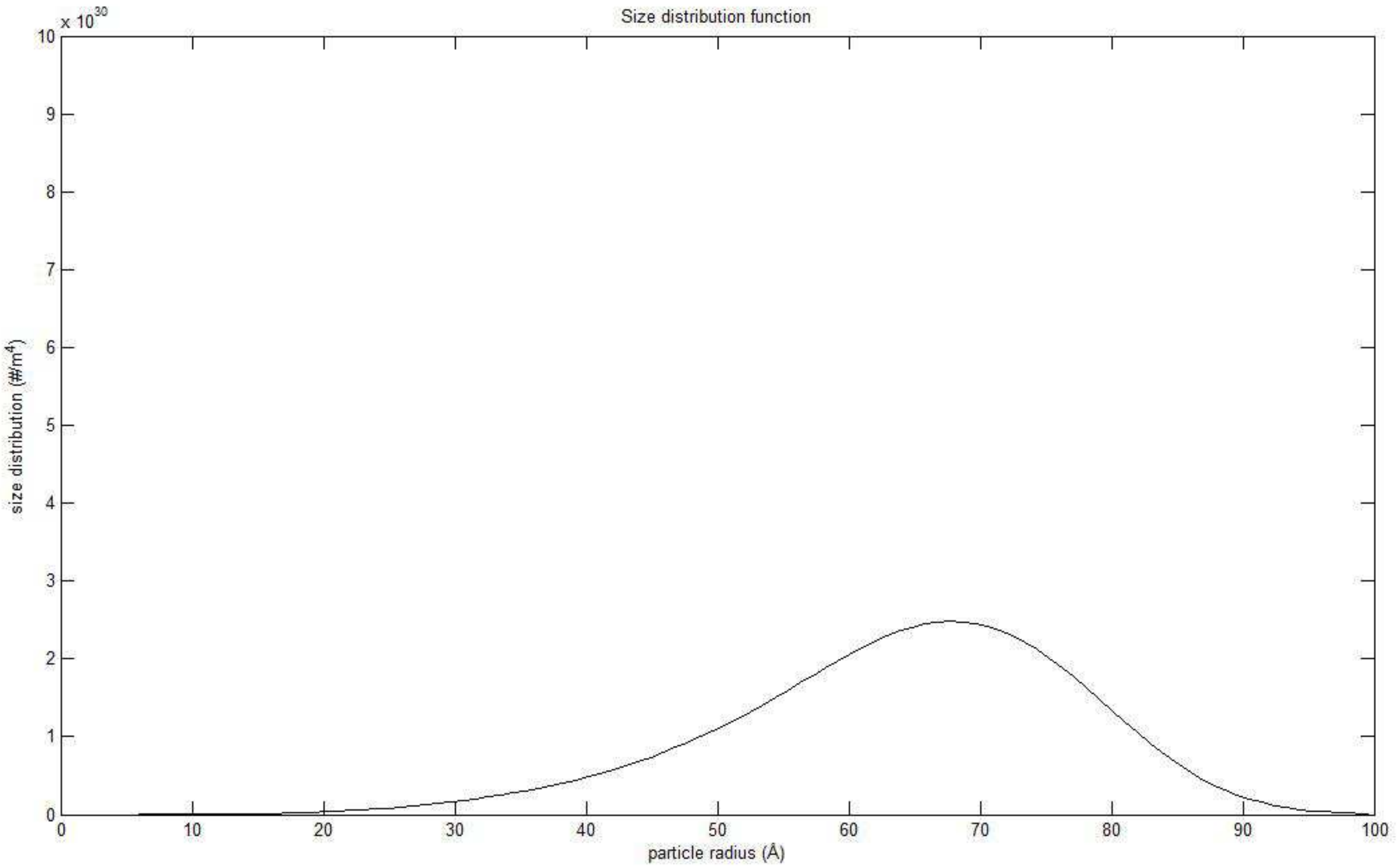

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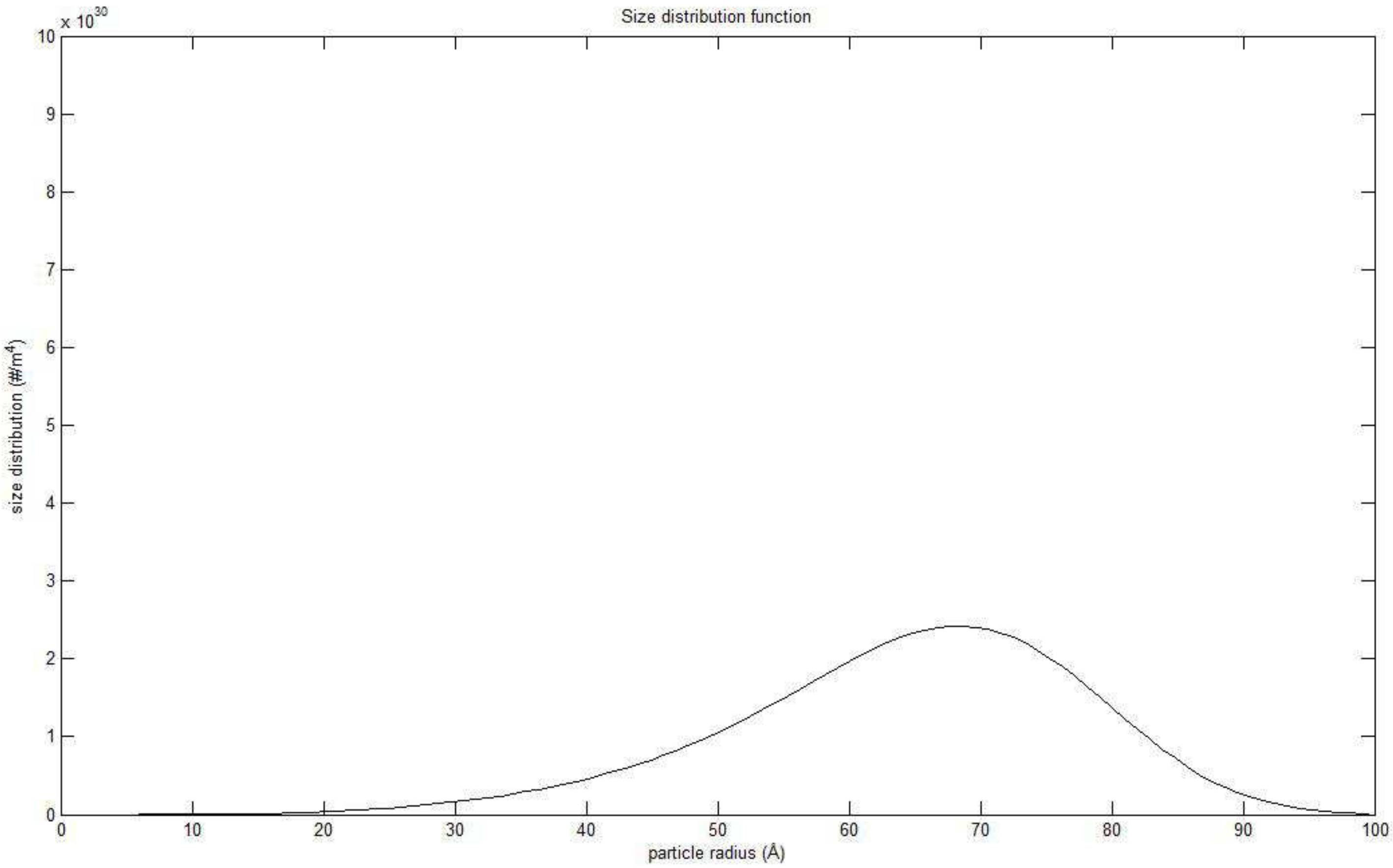
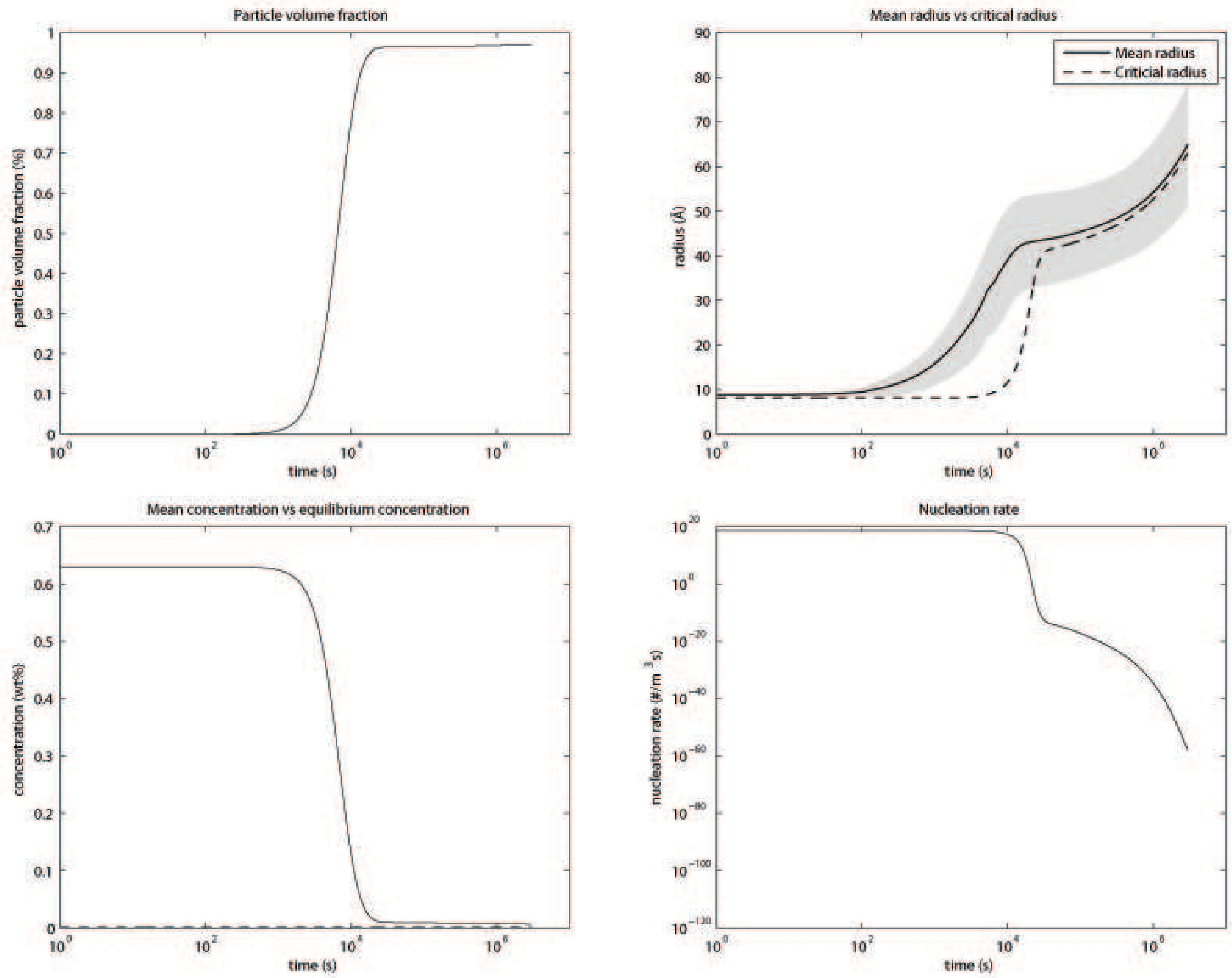


Derived quantities



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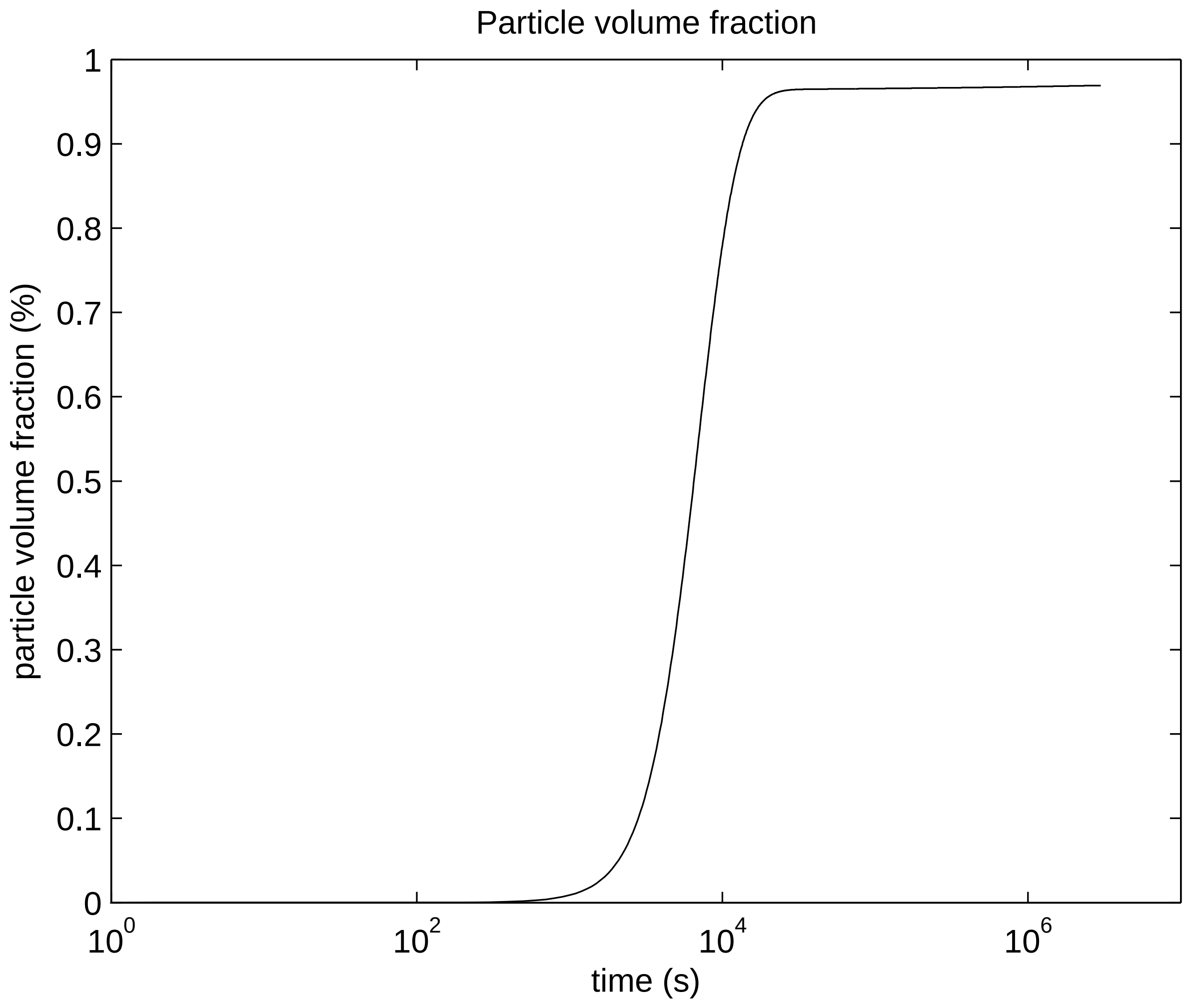

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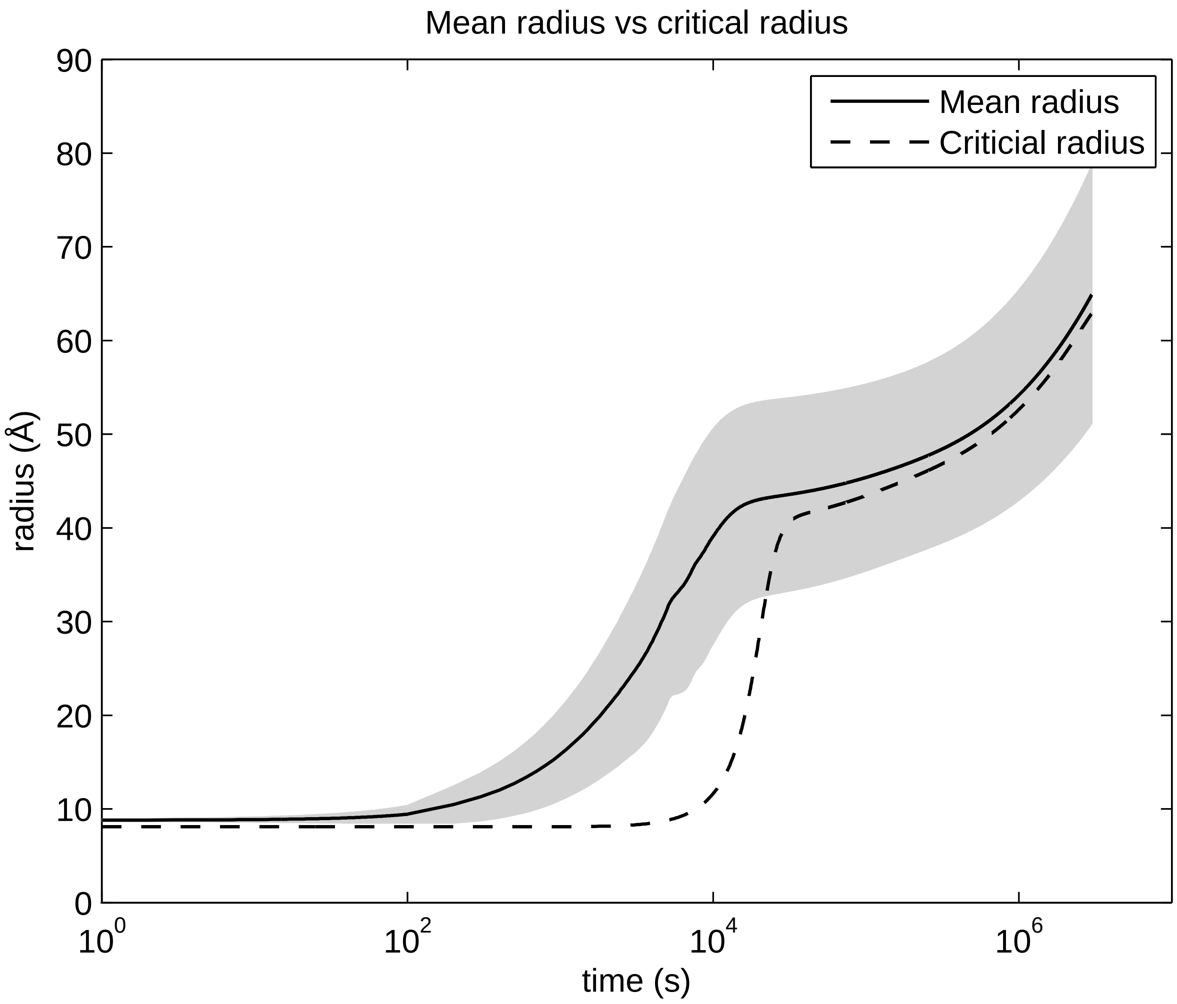

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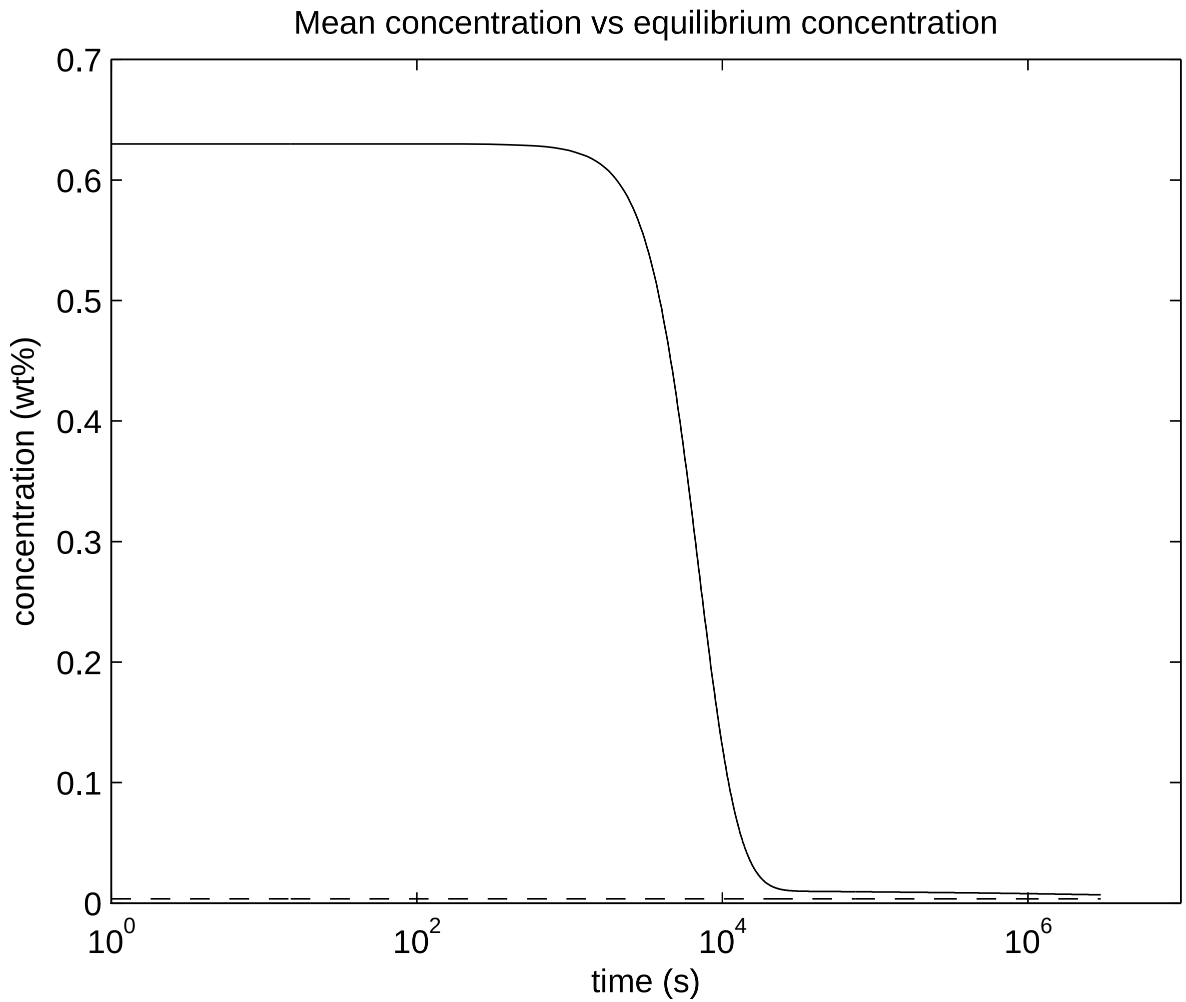

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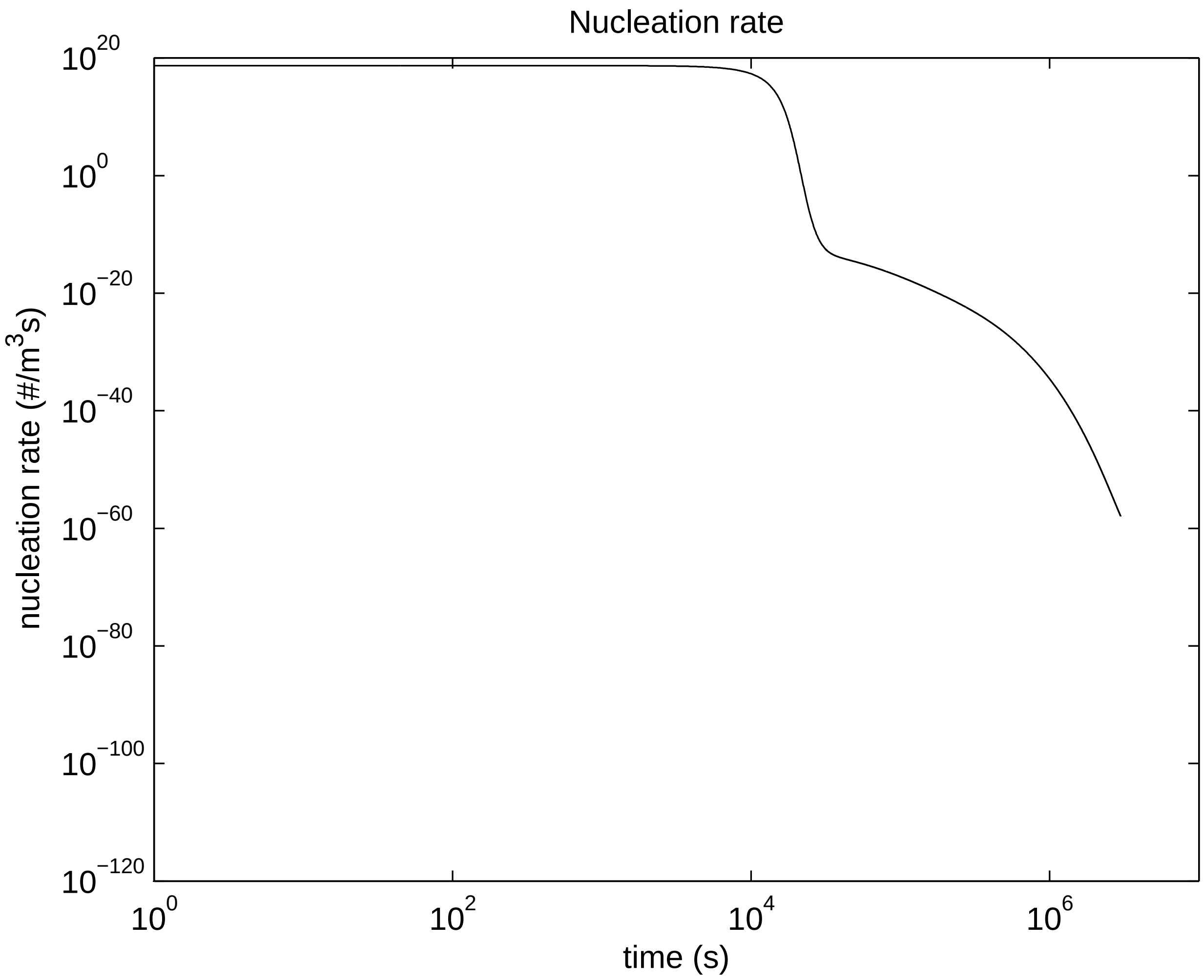


Time integration

Three methods:

- θ-method

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

Time integration

Three methods:

- θ-method
- First DIRK-method

$$\vec{N}^{n+1} = \vec{N}^{n} + \frac{\Delta t}{2} A^{n} \left(\vec{N}^{n1} + \vec{N}^{n2} \right) + \Delta t \vec{S}^{n}$$

$$\vec{N}^{n1} = \vec{N}^{n} + \Delta t \gamma \left(A^{n} \vec{N}^{n1} + \vec{S}^{n} \right)$$

$$\vec{N}^{n2} = \vec{N}^{n} + \Delta t A^{n} \left((1-2\gamma) \vec{N}^{n1} + \gamma \vec{N}^{n2} \right) + \Delta t (1-\gamma) \vec{S}^{n}$$

Time integration

Three methods:

- θ-method
- First DIRK-method
- Second DIRK-method

$$\vec{N}^{n+1} = \vec{N}^{n} + \Delta t A^{n}\left(b_1\vec{N}^{n} + b_2\vec{N}^{n2} + \gamma\vec{N}^{n3}\right) + \Delta t\vec{S}^{n}$$

$$\vec{N}^{n2} = \vec{N}^{n} + \Delta t\gamma A^{n}\left(\vec{N}^{n} + \vec{N}^{n2}\right) + 2\Delta t\gamma\vec{S}^{n}$$

$$\vec{N}^{n3} = \vec{N}^{n} + \Delta t A^{n}\left(b_1\vec{N}^{n} + b_2\vec{N}^{n2} + \gamma\vec{N}^{n3}\right) + \Delta t\vec{S}^{n}$$

Time integration

	Operation			
Method	Vector addition	Matrix addition	Matrix multiplication	Matrix inversion
θ-method	1	2	1	1
DIRK-1	6	2	2	2
DIRK-2	9	2	3	2

Time integration

Results:

- θ-method large differences

  Second order for $\theta = 1/2$

Time integration

Results:

- θ-method large differences
  Second order for $\theta = 1/2$
- DIRK-methods small differences
  Second order for all γ

Time integration

Results:

- θ-method large differences
  Second order for $\theta = 1/2$
- DIRK-methods small differences
  Second order for all γ
- $\theta = 1/2$- and DIRK-methods small differences

Time integration

Results:

- θ-method large differences
  Second order for $\theta = 1/2$
- DIRK-methods small differences
  Second order for all γ
- $\theta = 1/2$- and DIRK-methods small differences

Conclusion:

$\theta = 1/2$-method favorable

Recap

Results:

- Model correctly predicts nucleation and coarsening

Recap

Results:

- Model correctly predicts nucleation and coarsening
- Second order accuracy at low costs

Elastic deformation

Strain in a deformed block:

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Elastic deformation

Strain in a deformed block:

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Stress in a deformed block:

$$\sigma_{ij} = \lambda \delta_{ij} \sum_{k=1}^{3} \varepsilon_{kk} + 2\mu\varepsilon_{ij}$$

Elastic deformation

Force balance:

$$\nabla \cdot \boldsymbol{\sigma} = -\boldsymbol{b}$$

Elastic deformation

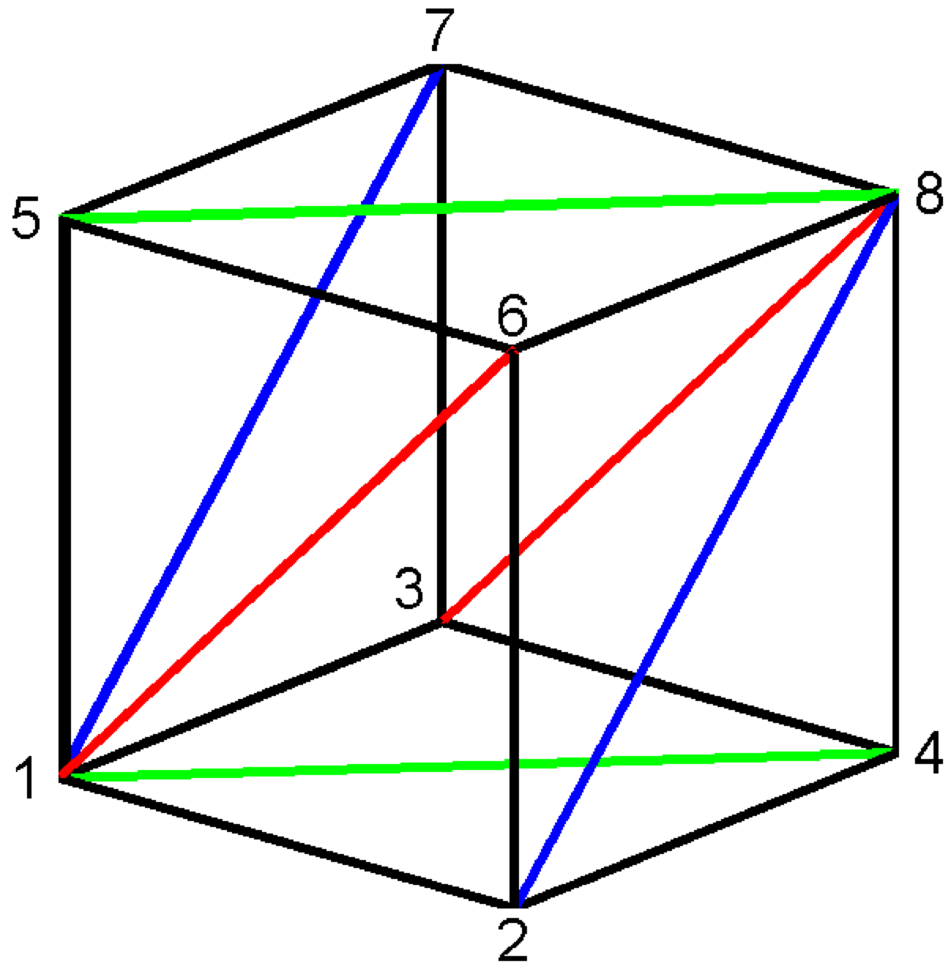
Force balance:

$$\nabla \cdot \boldsymbol{\sigma} = -\boldsymbol{b}$$

Or equivalent:

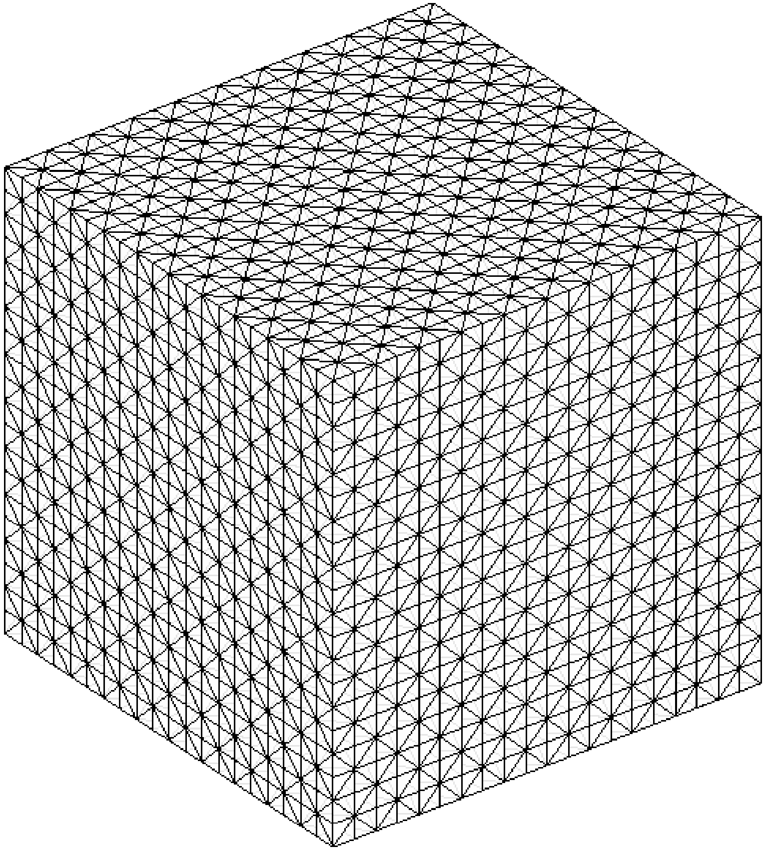
$$\begin{cases} \lambda \dfrac{\partial}{\partial x_1}(\nabla \cdot \boldsymbol{u}) + \mu \left(\nabla \cdot \left(\nabla u_1 + \dfrac{\partial \boldsymbol{u}}{\partial x_1} \right) \right) & = & -b_1 \\ \lambda \dfrac{\partial}{\partial x_2}(\nabla \cdot \boldsymbol{u}) + \mu \left(\nabla \cdot \left(\nabla u_2 + \dfrac{\partial \boldsymbol{u}}{\partial x_2} \right) \right) & = & -b_2 \\ \lambda \dfrac{\partial}{\partial x_3}(\nabla \cdot \boldsymbol{u}) + \mu \left(\nabla \cdot \left(\nabla u_3 + \dfrac{\partial \boldsymbol{u}}{\partial x_3} \right) \right) & = & -b_3 \end{cases}$$

Finite Element Mesh



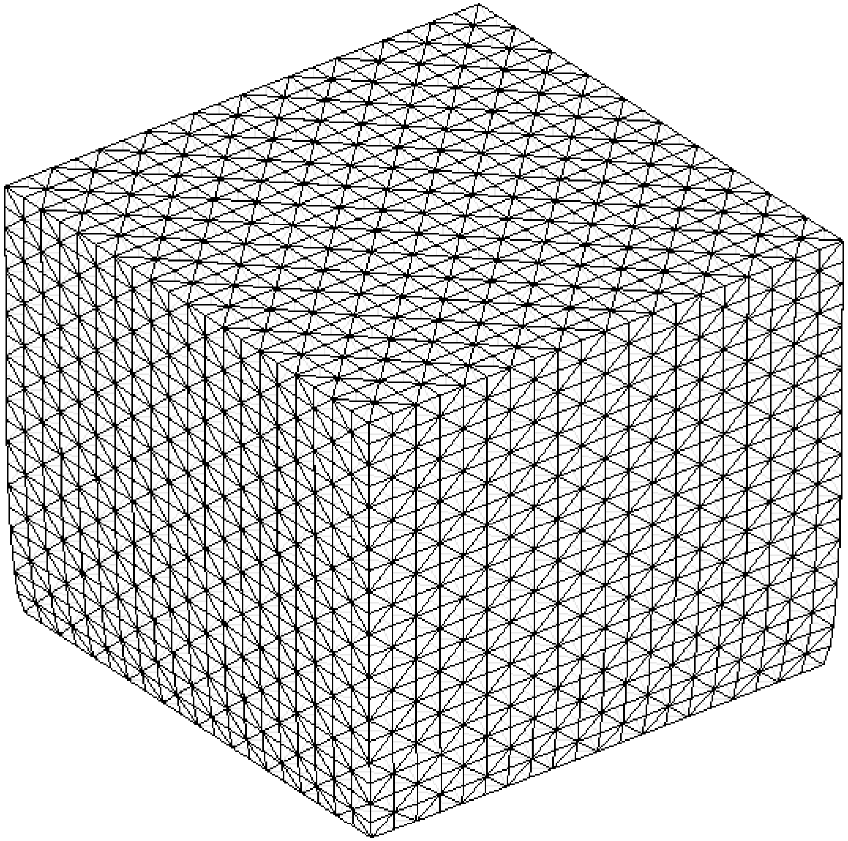
Simulation

Before deformation:



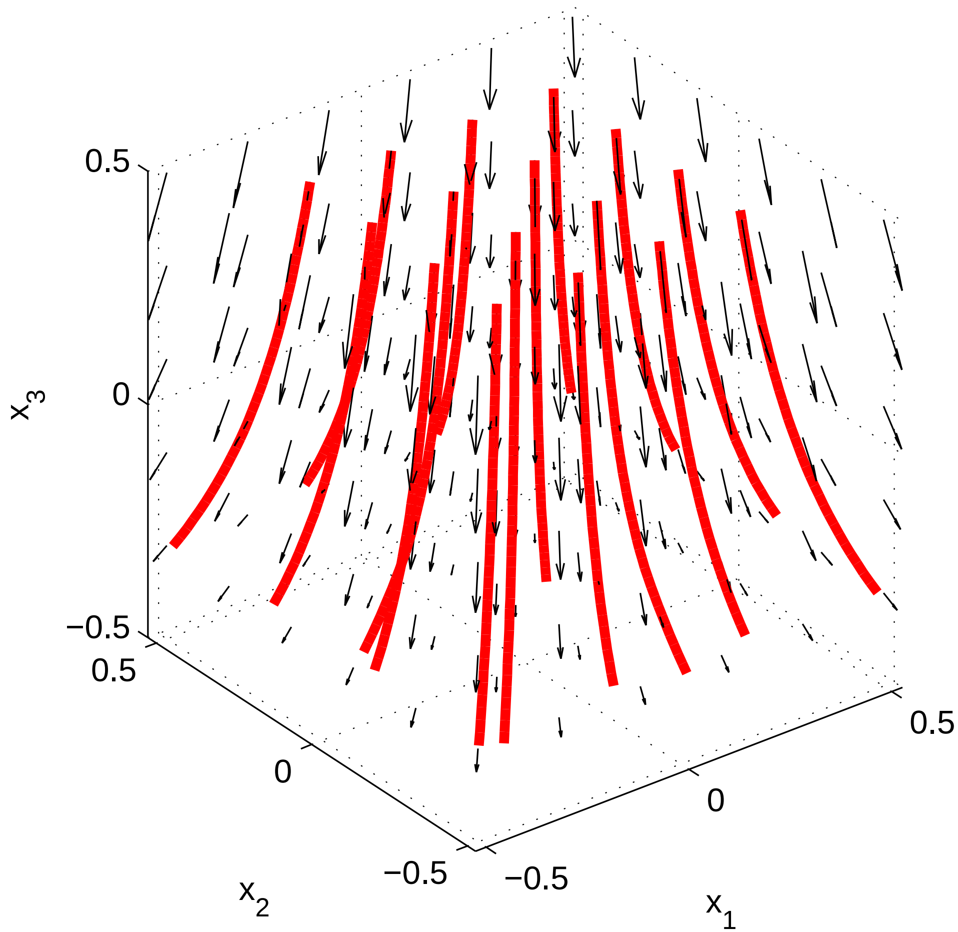
Simulation

After deformation:



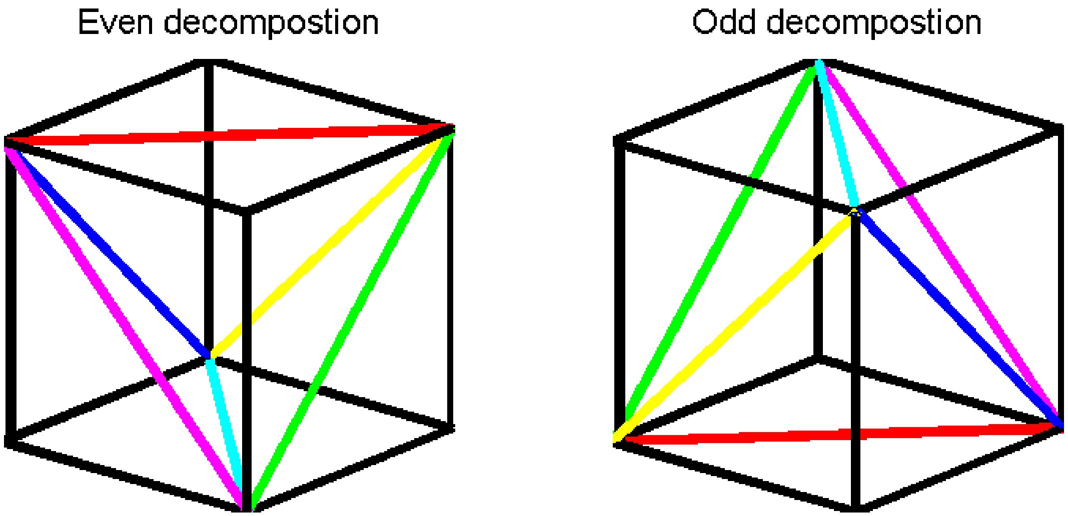
Simulation

Displacements:



Simulation

Update:



Conclusions

Conclusions:

- Realistic results with both models
- High accuracy
- Easy to derive data

Future work

- Coupling of the two models

Future work

- Coupling of the two models
- Non-elastic deformations

Future work

- Coupling of the two models
- Non-elastic deformations
- Coupling with elastic deformations

Future work

- Coupling of the two models
- Non-elastic deformations
- Coupling with elastic deformations
- Coupling of the three models

Future work

- Coupling of the two models
- Non-elastic deformations
- Coupling with elastic deformations
- Coupling of the three models
- Extension to multi-component alloys

Questions?