Modeling of soot restructuring

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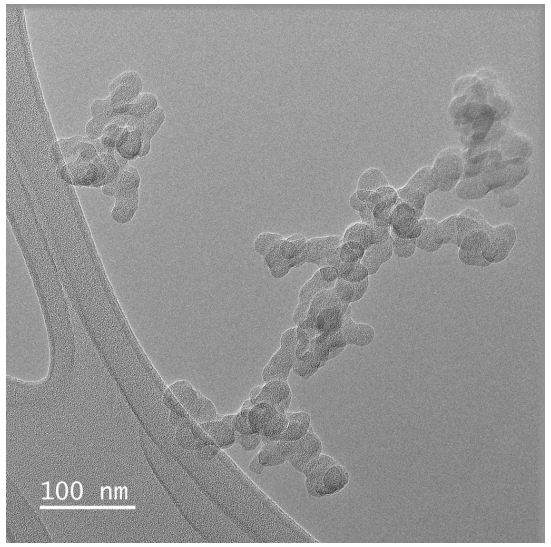
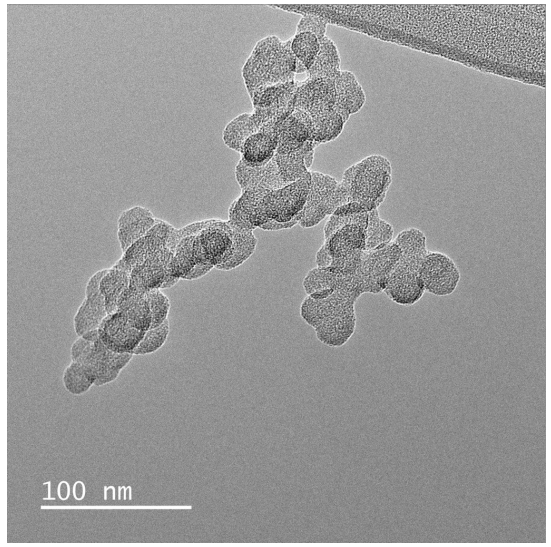
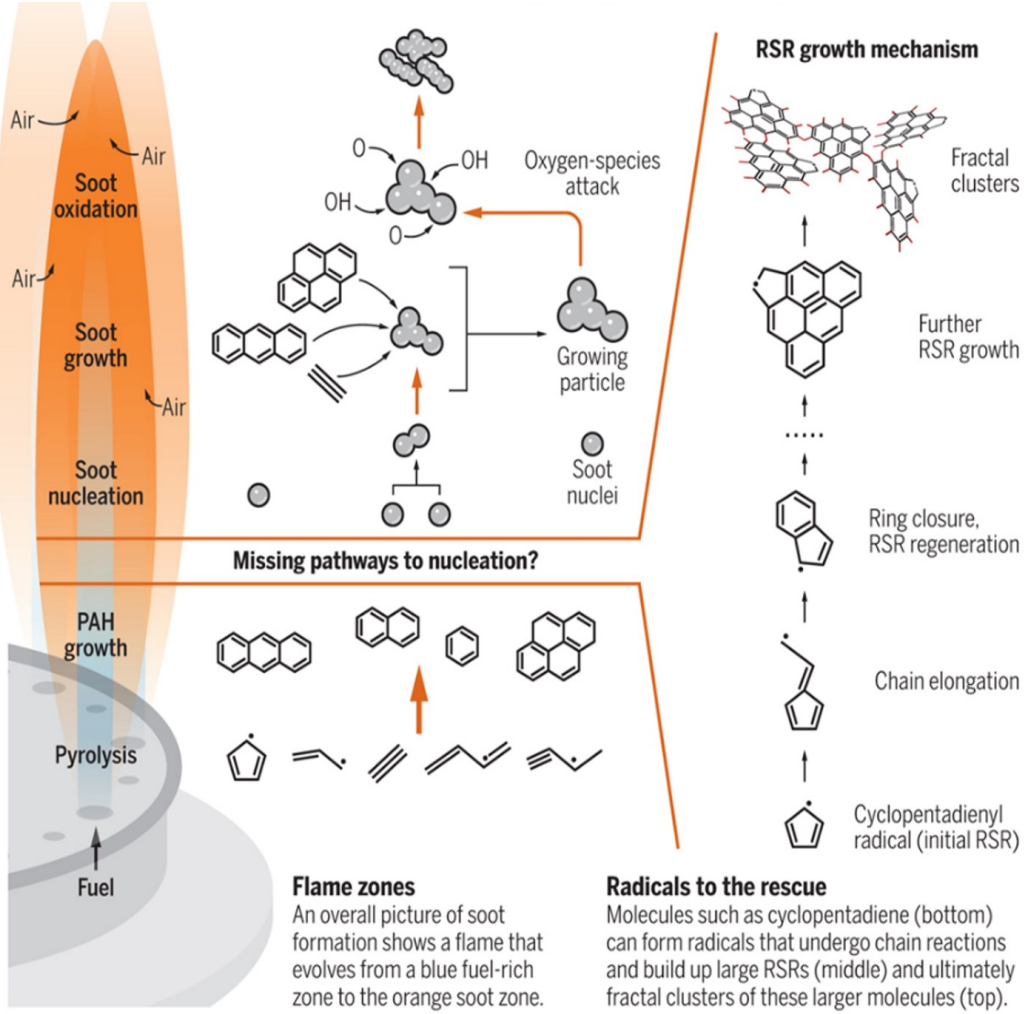
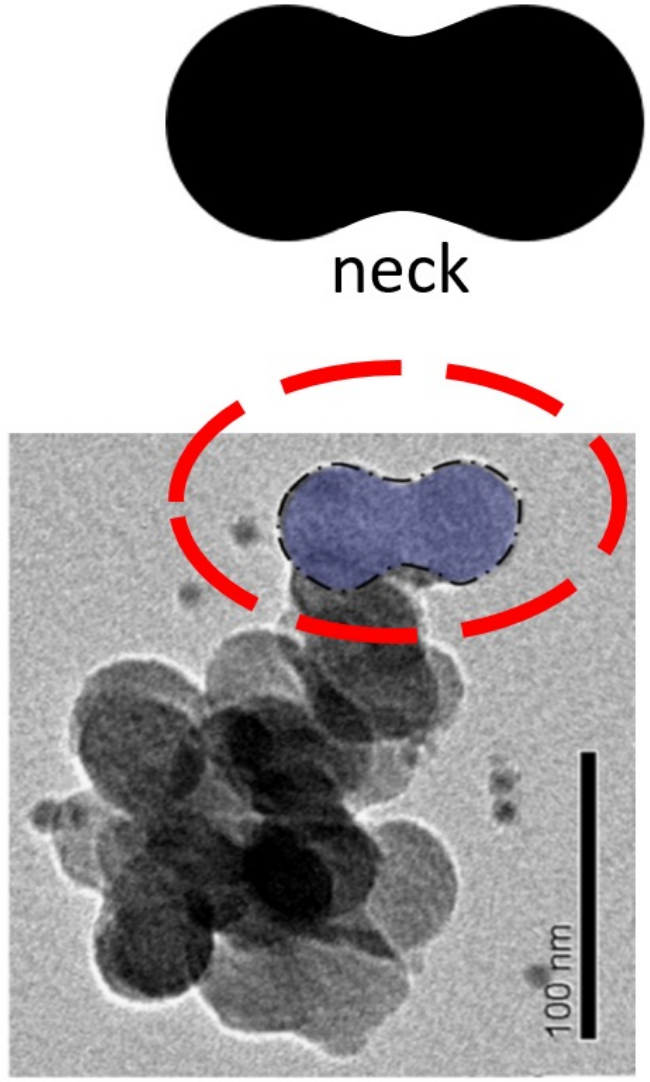




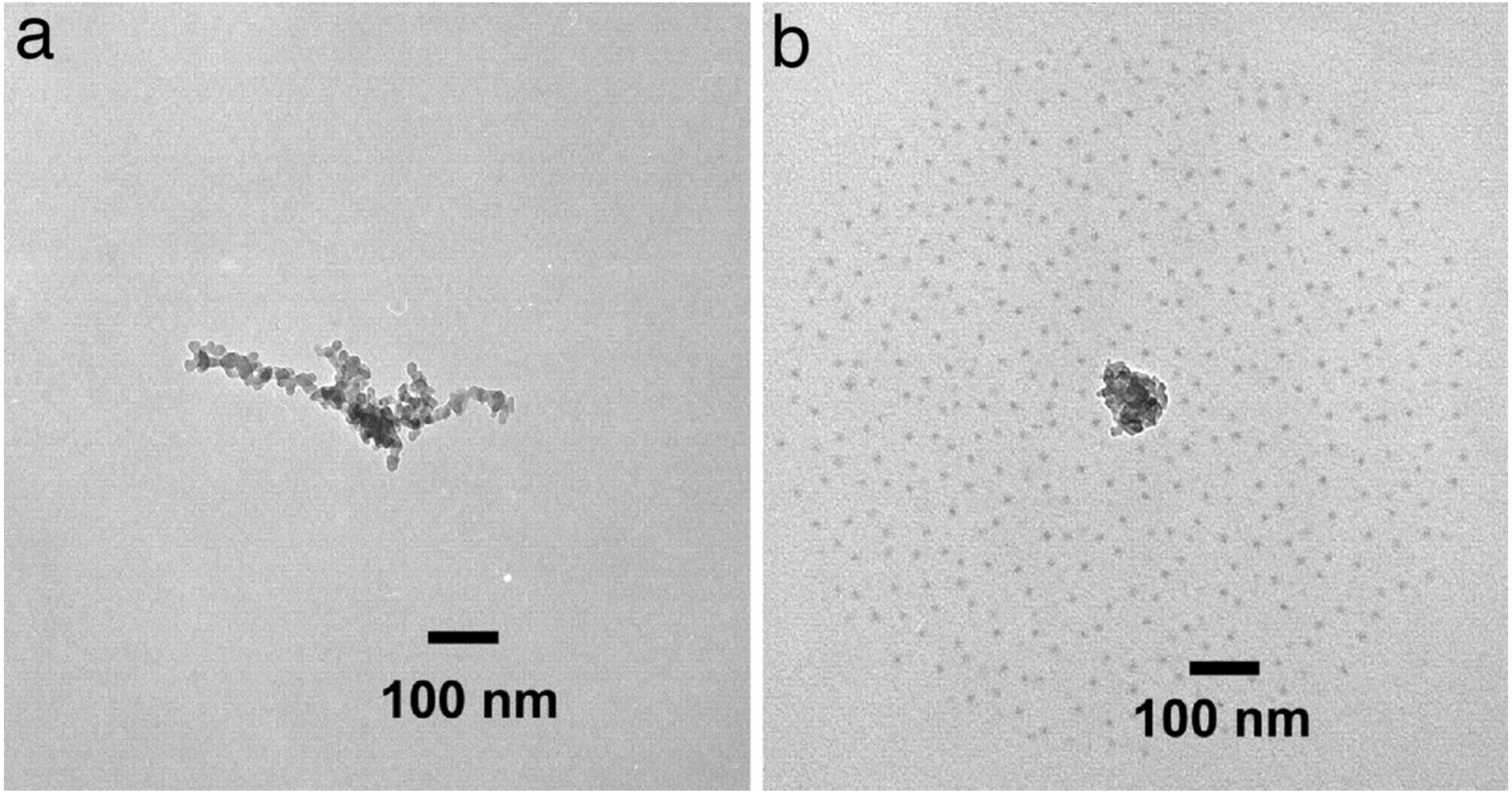
Soot formation and climate impact



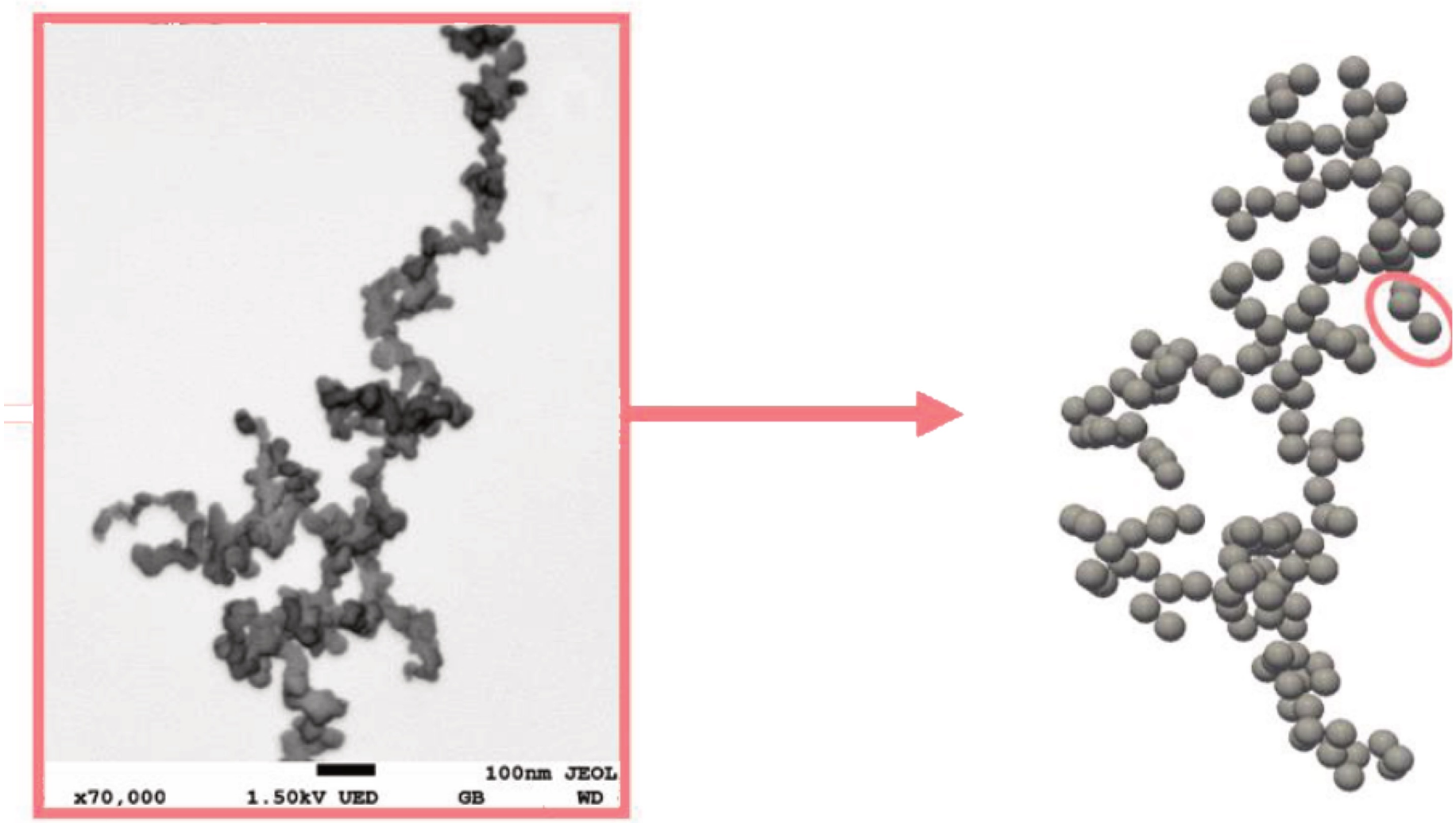
Thomson, M., & Mitra, T. (2018). A radical approach to soot formation. Science, 361(6406), 978-979.



Morphological changes of soot in the atmosphere



Representation of soot in a simulation



Discrete element method

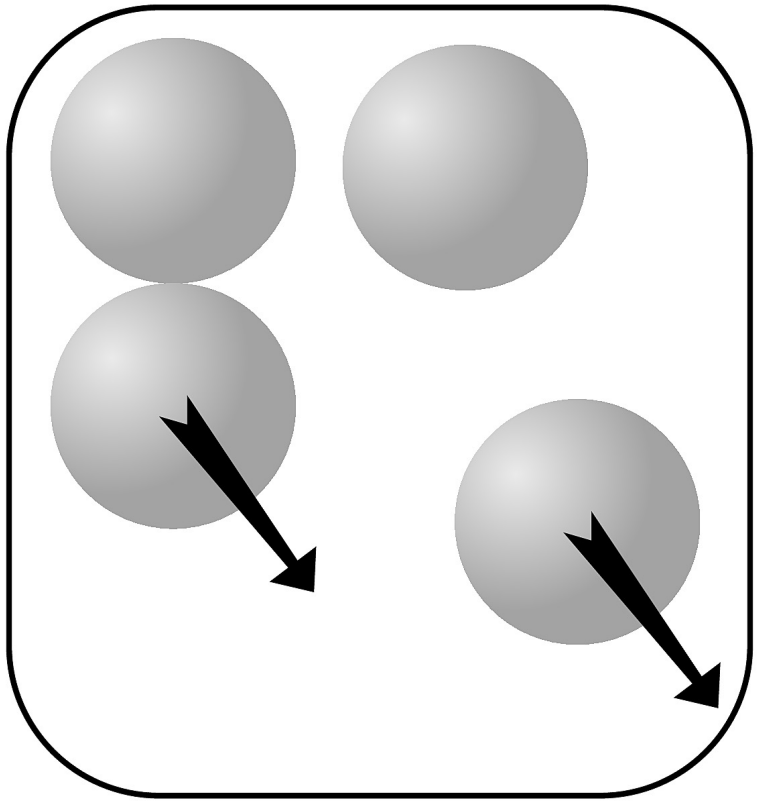
- In a system of N particles, acceleration of particle i:

$$\mathbf{a}_i = \frac{1}{m}\left[\mathbf{f}_{i,\mathrm{u}} + \sum_{j=1}^{N} \mathbf{f}_{ij,\mathrm{b}}\right]$$

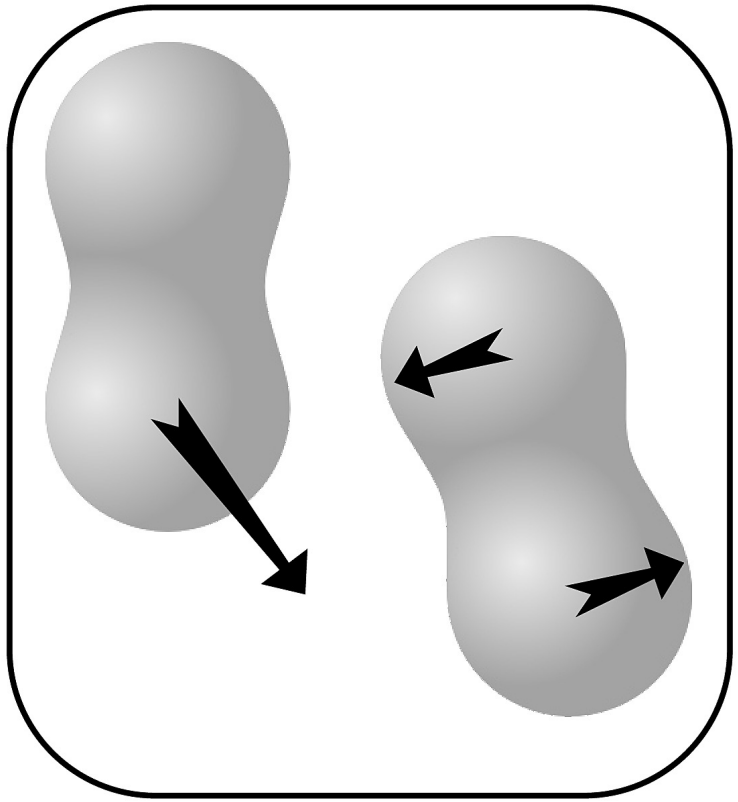
- Also, inter-particle friction can result in rotation:

$$\boldsymbol{\alpha}_i = \frac{1}{I}\left[\sum_{j=1}^{N} \boldsymbol{\tau}_{ij}\right]$$

Types of contacts that need to be represented

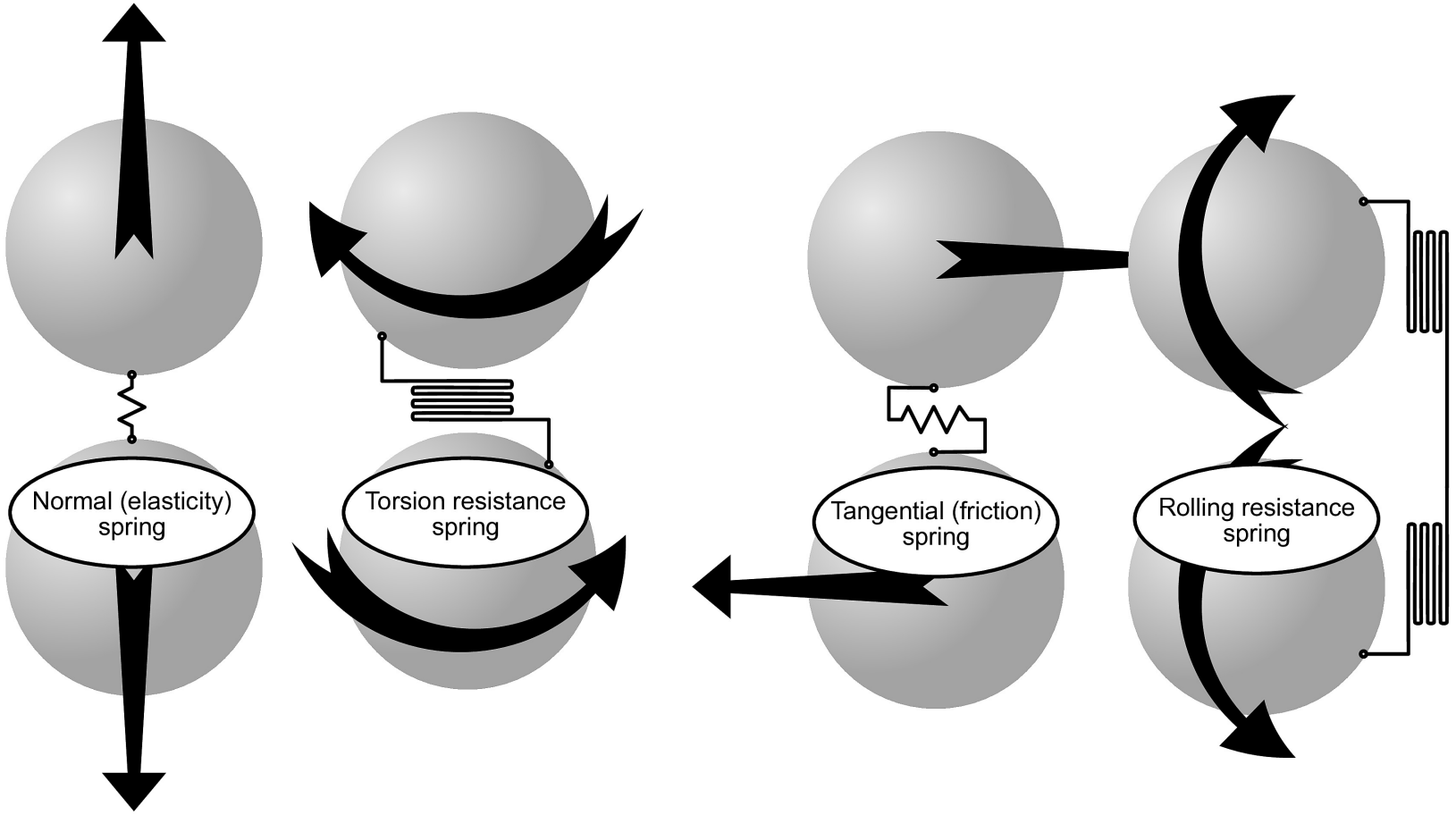


Non-bonded contact under tension



Bonded contact under tension

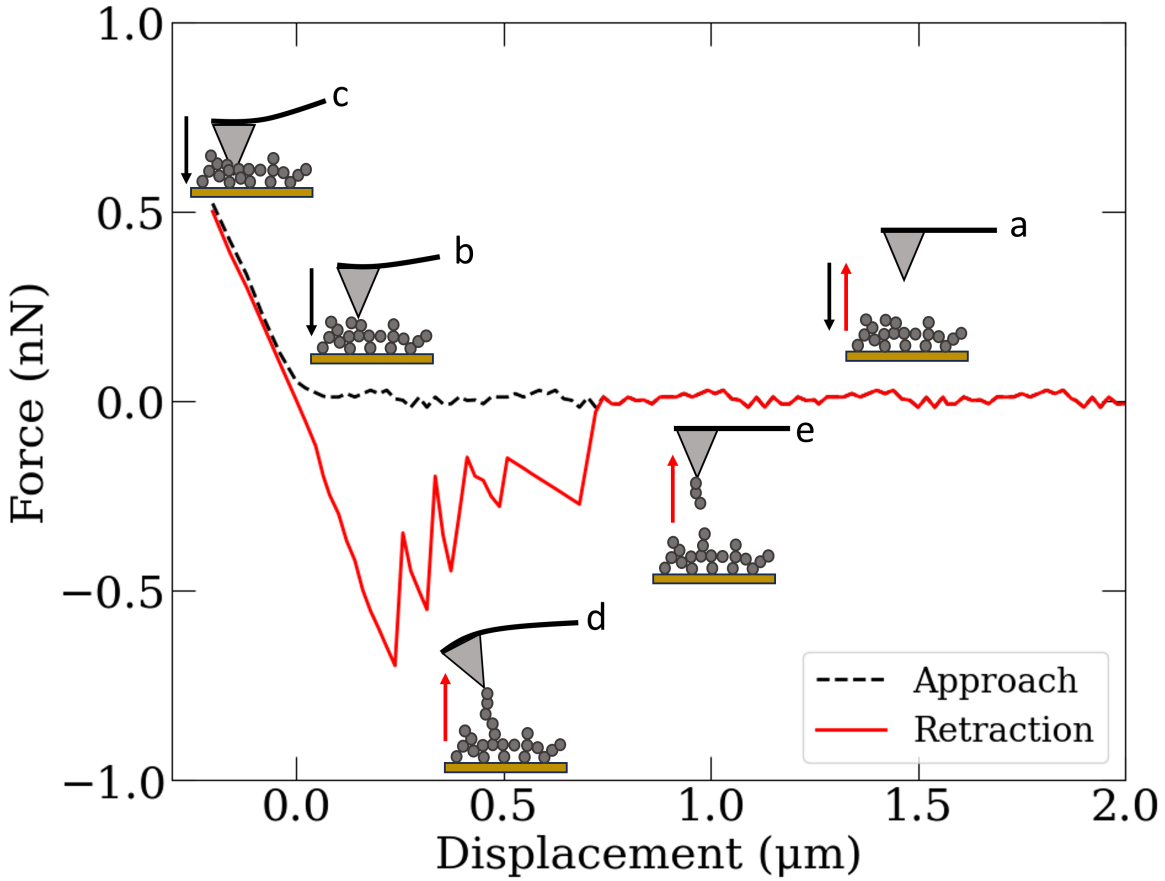
Degrees of freedom in a pair of particles

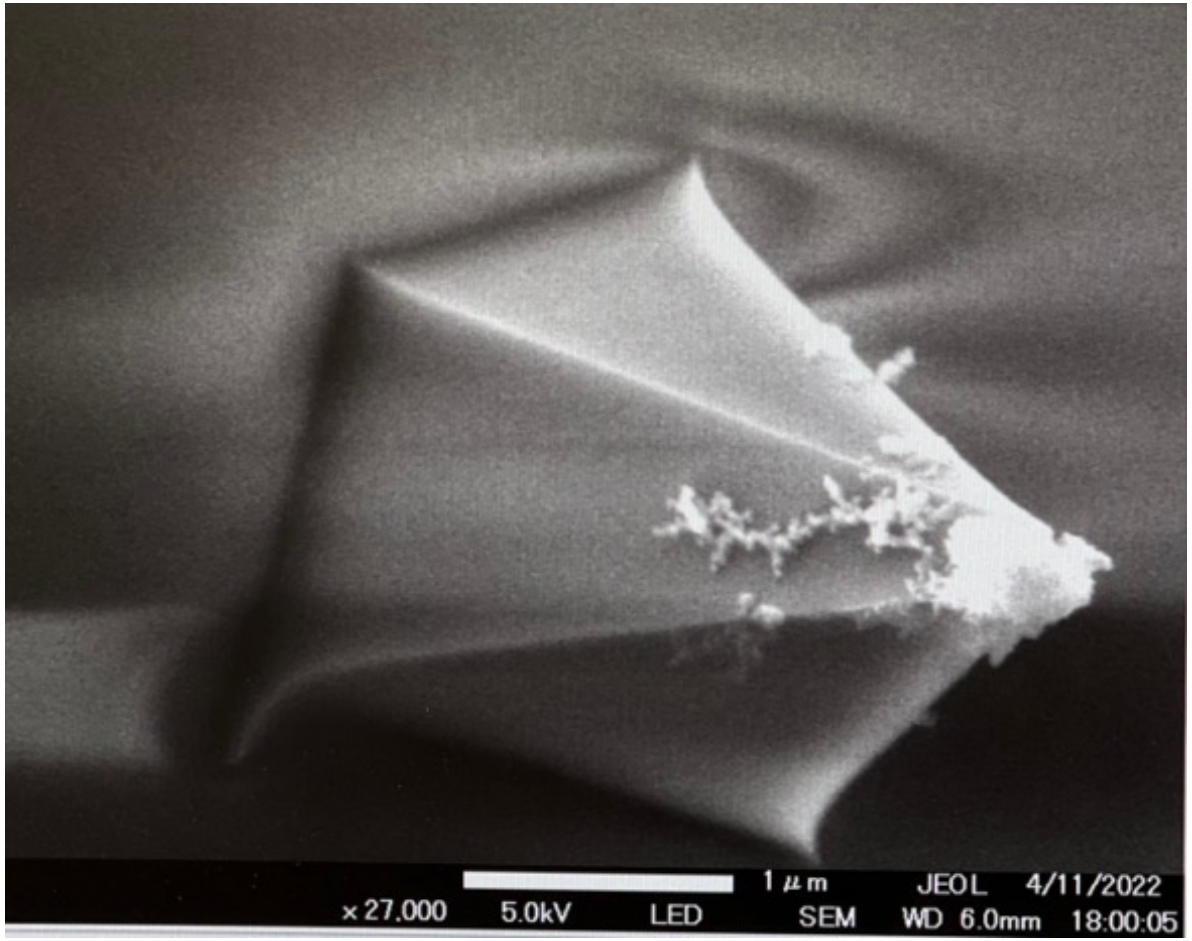


Normal degrees of freedom

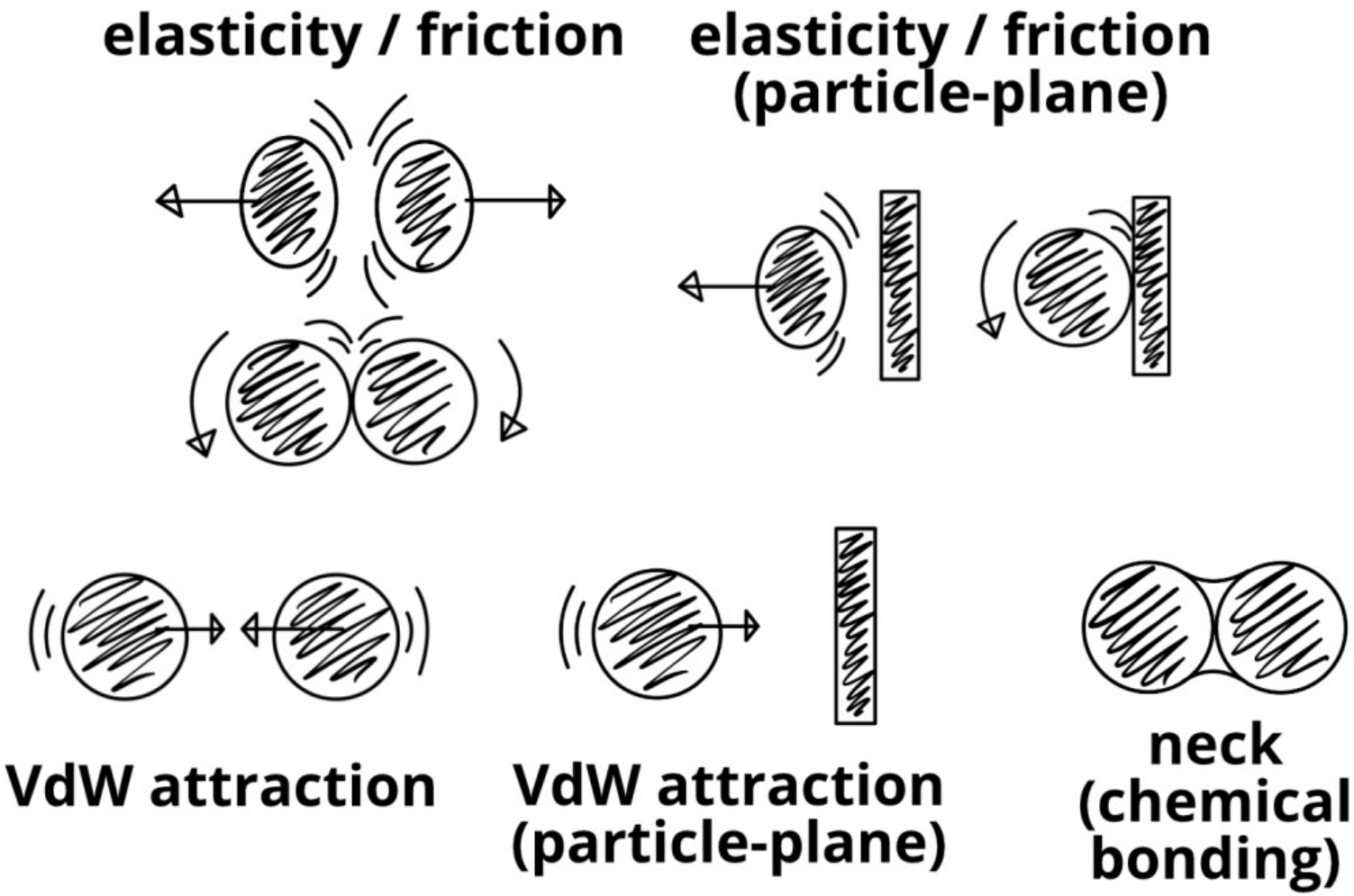
Tangential degrees of freedom

AFM spectroscopy experiments as a parametrization tool





Simulation of AFM experiments



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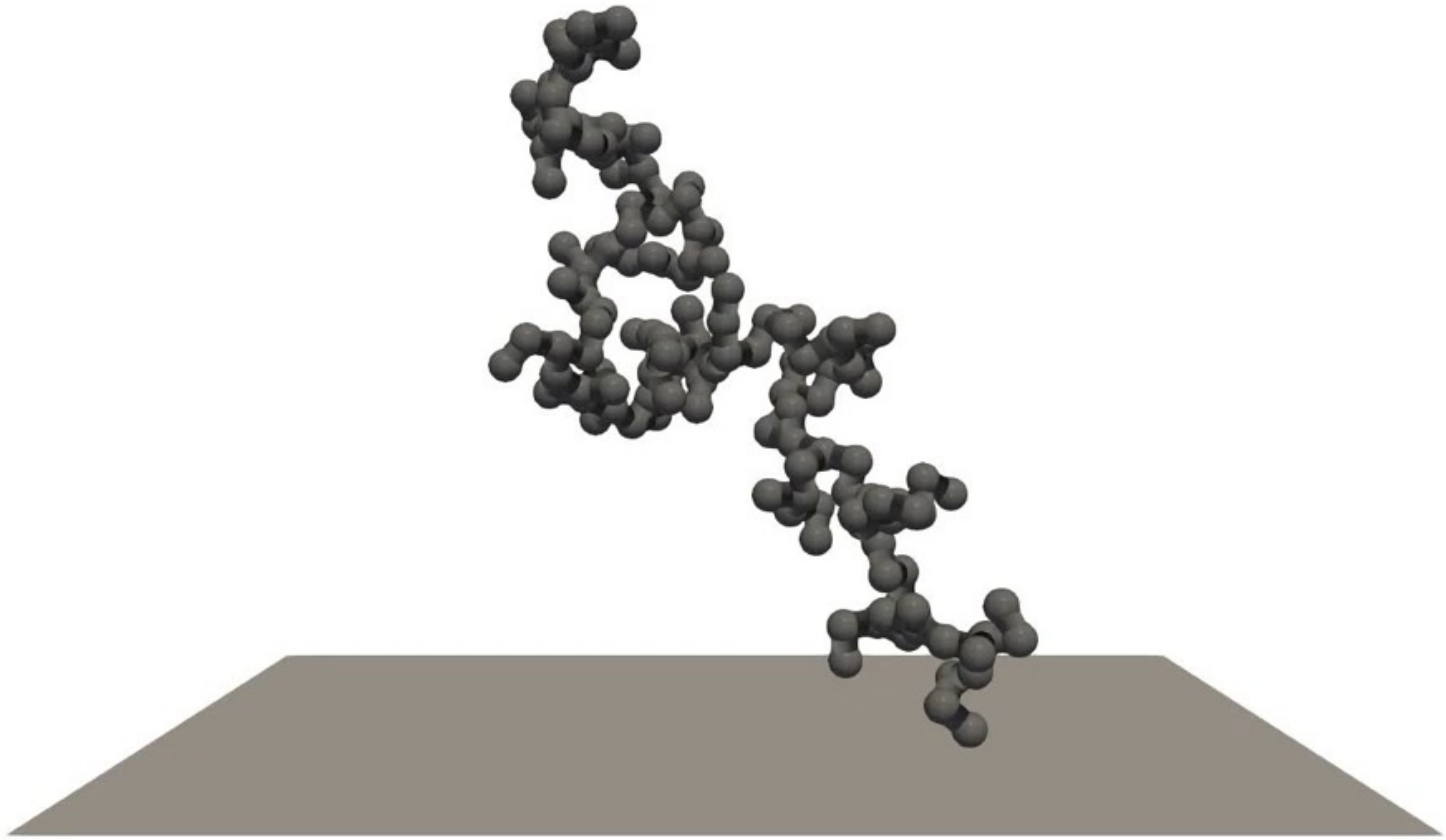
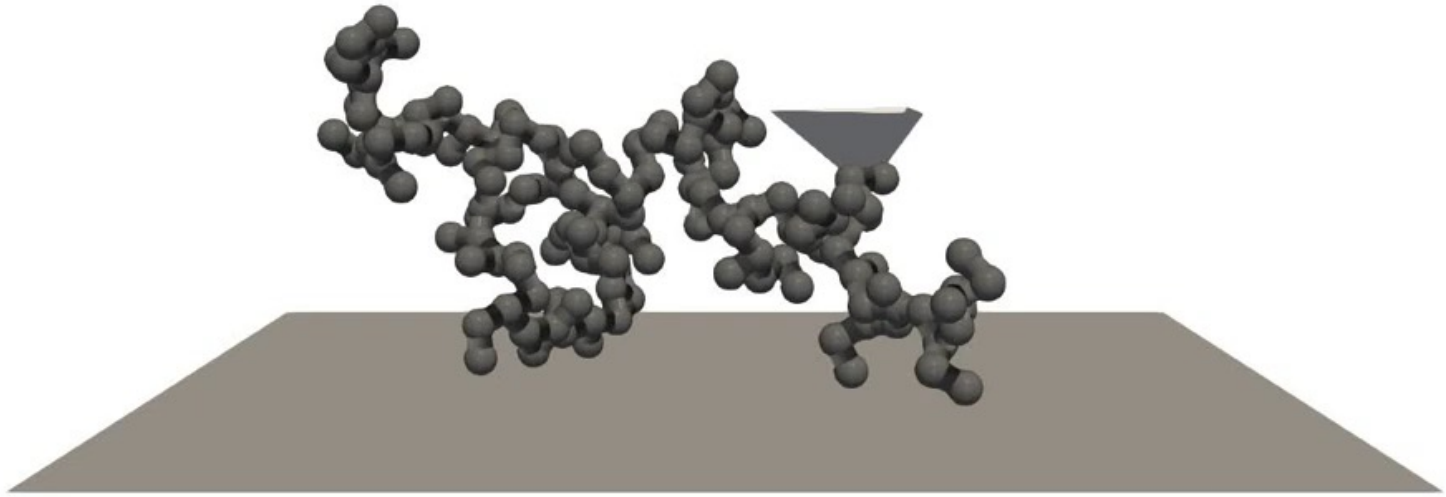
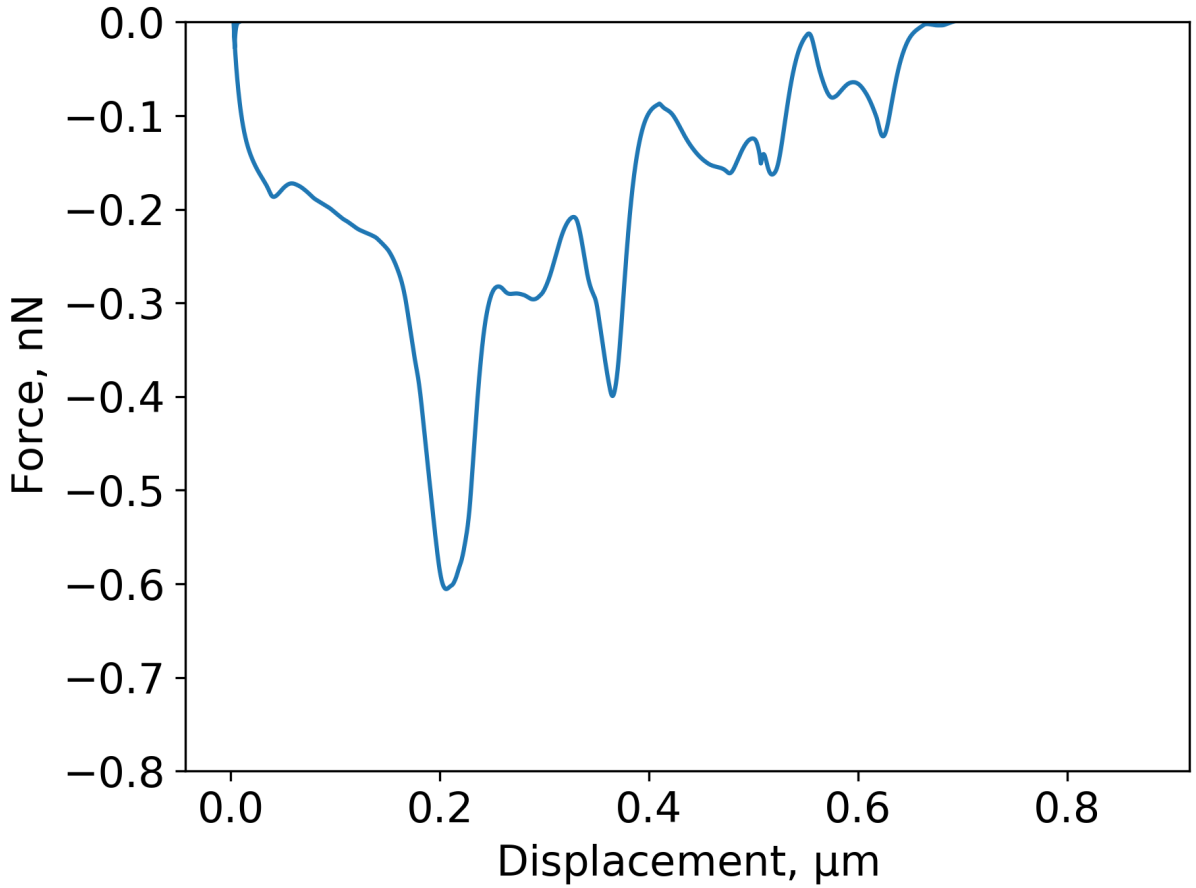
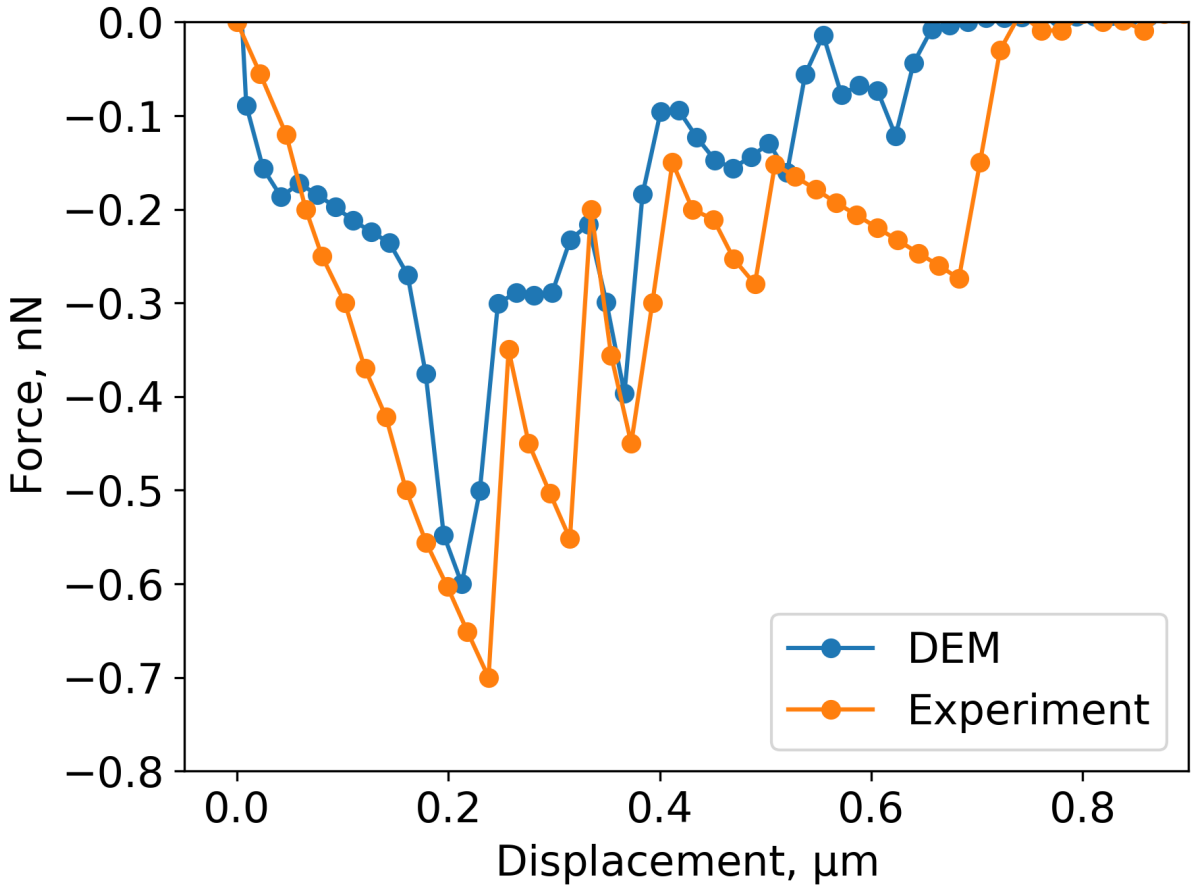


Simulation of AFM experiments

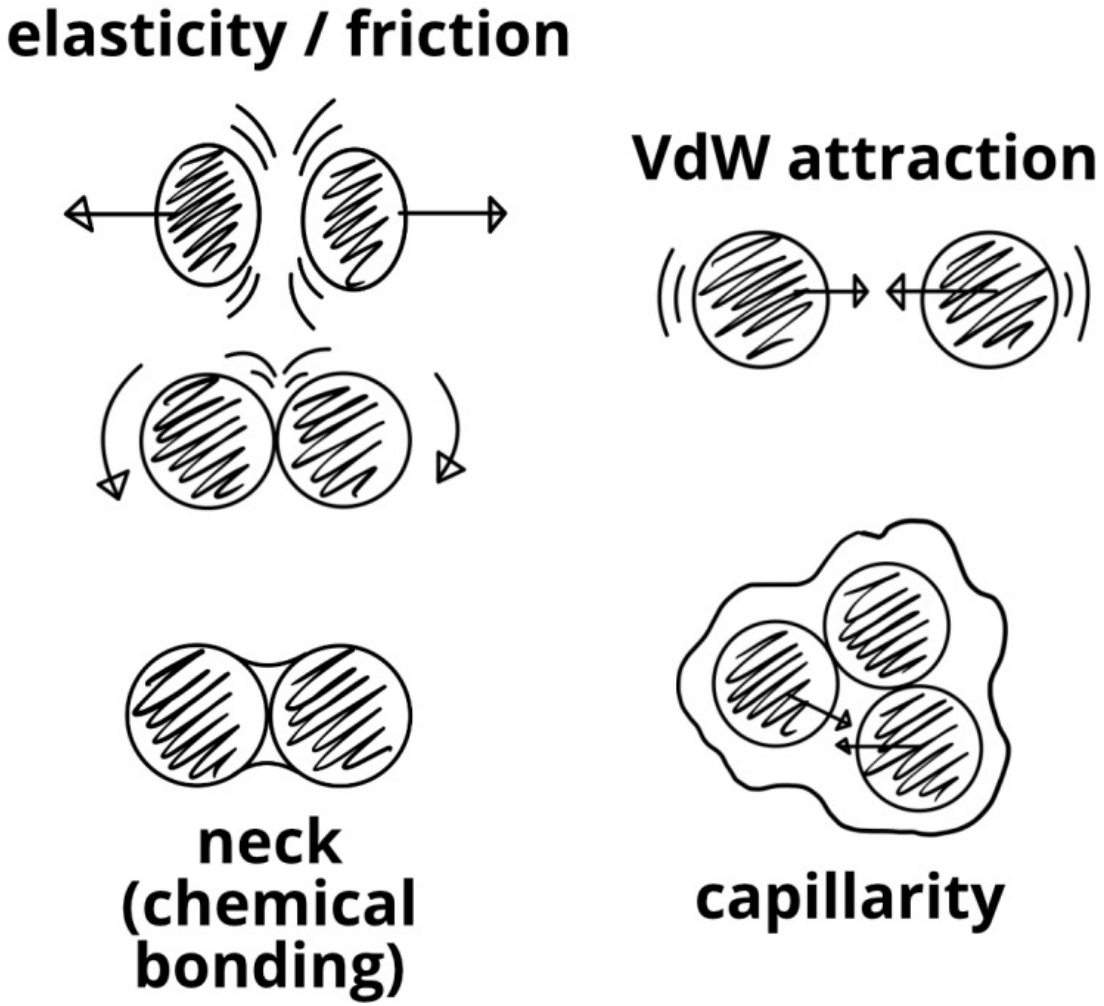


AFM force-displacement curves





Simulation of aggregate restructuring



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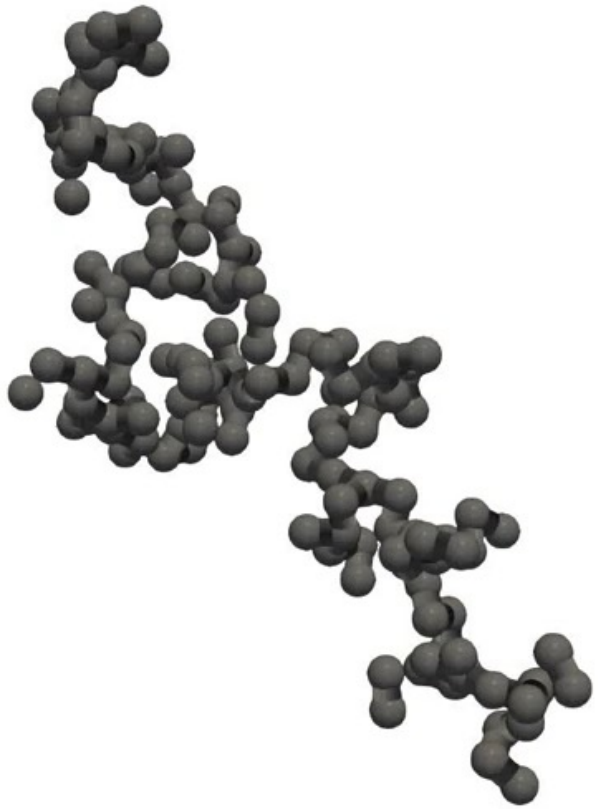
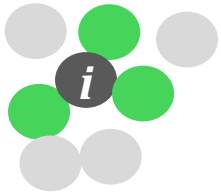


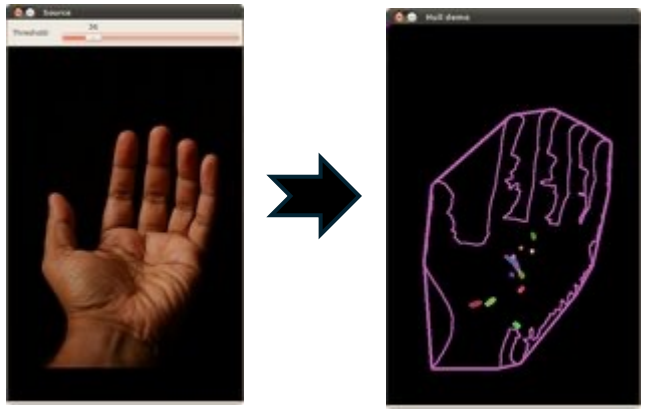
Restructuring effects on aggregate geometry

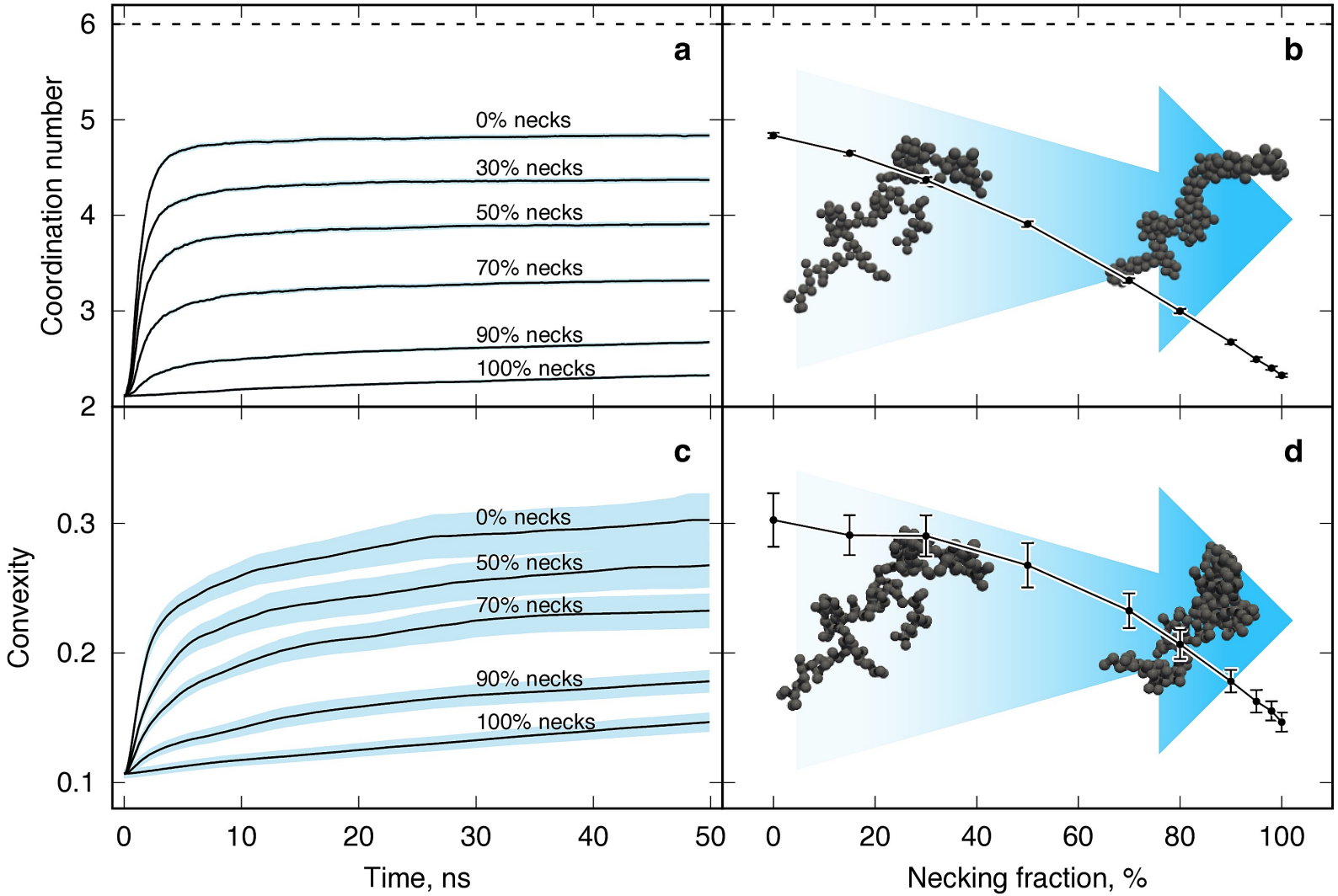
$$\text{Coordination} = \frac{1}{N}\sum_{i=1}^{N} N_{\text{nb},i}$$



$$N_{\text{nb},i} = 3$$

$$\text{Convexity} = \frac{V_{\text{aggregate}}}{V_{\text{convex hull}}}$$





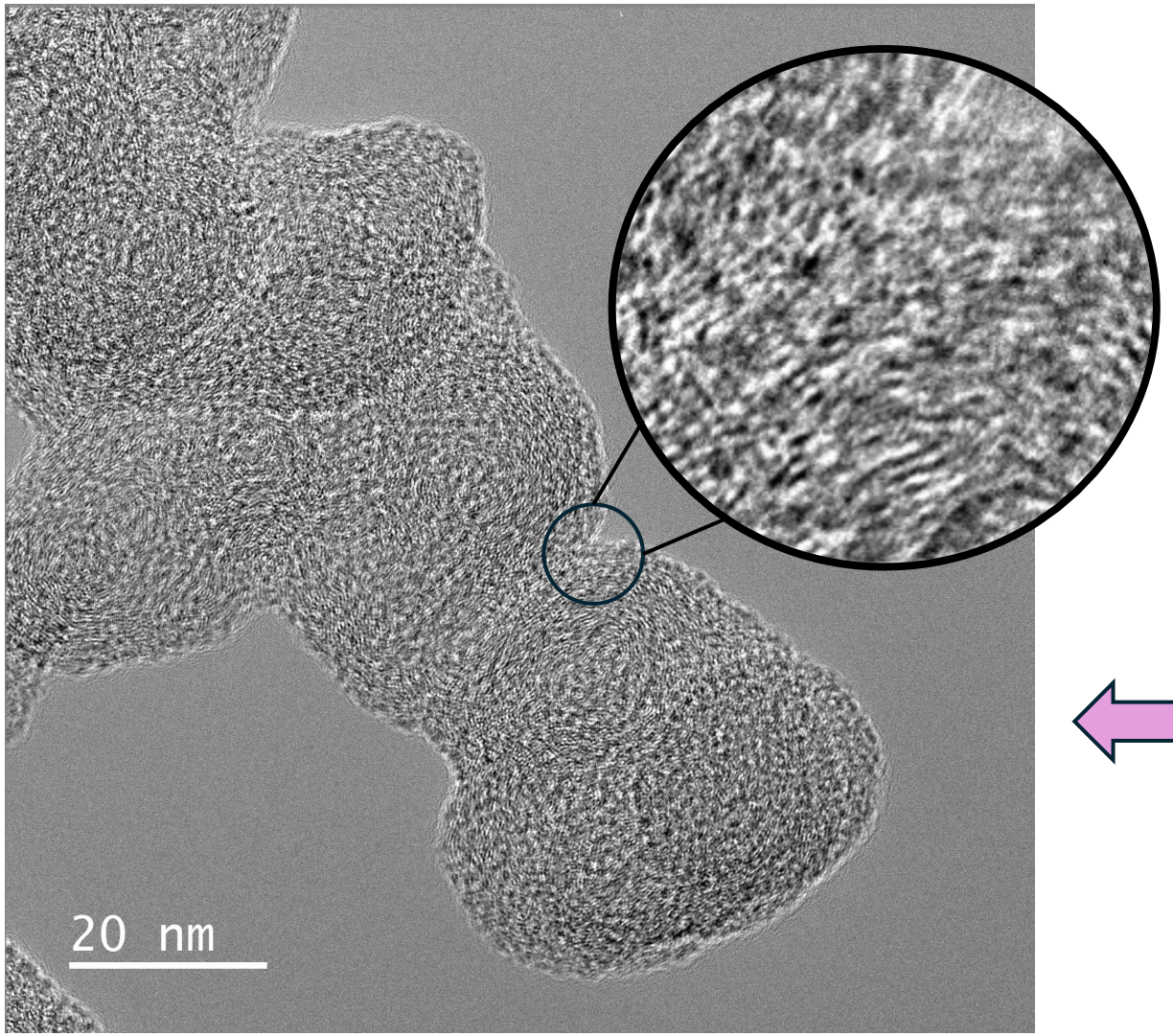
Summary of the developed framework

- Developed a DEM contact model
- The model can reproduce AFM spectroscopy experiments
- Restructuring simulations qualitatively behave as expected from experiments

Future work:

- Parametrize the restructuring simulations based on experimental data
- Develop a parametrization for soot restructuring in large-scale aerosol models based on simulations

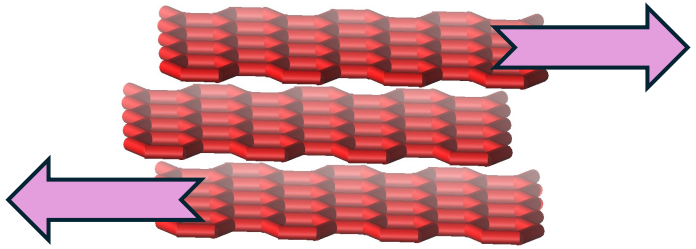
Parametrization – microstructure



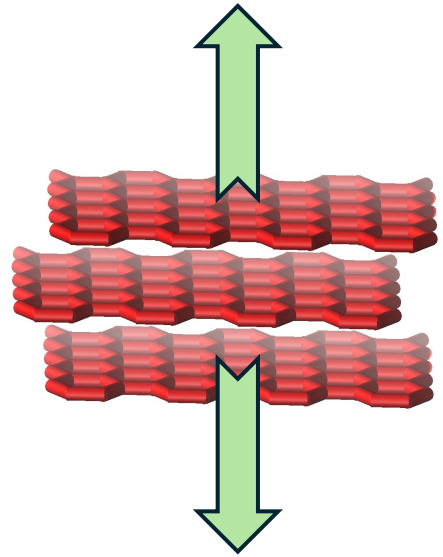
HRTEM image by Xena Mansoura, EMSL

Microstructure affects:

- Ultimate mechanical properties
- Anisotropy

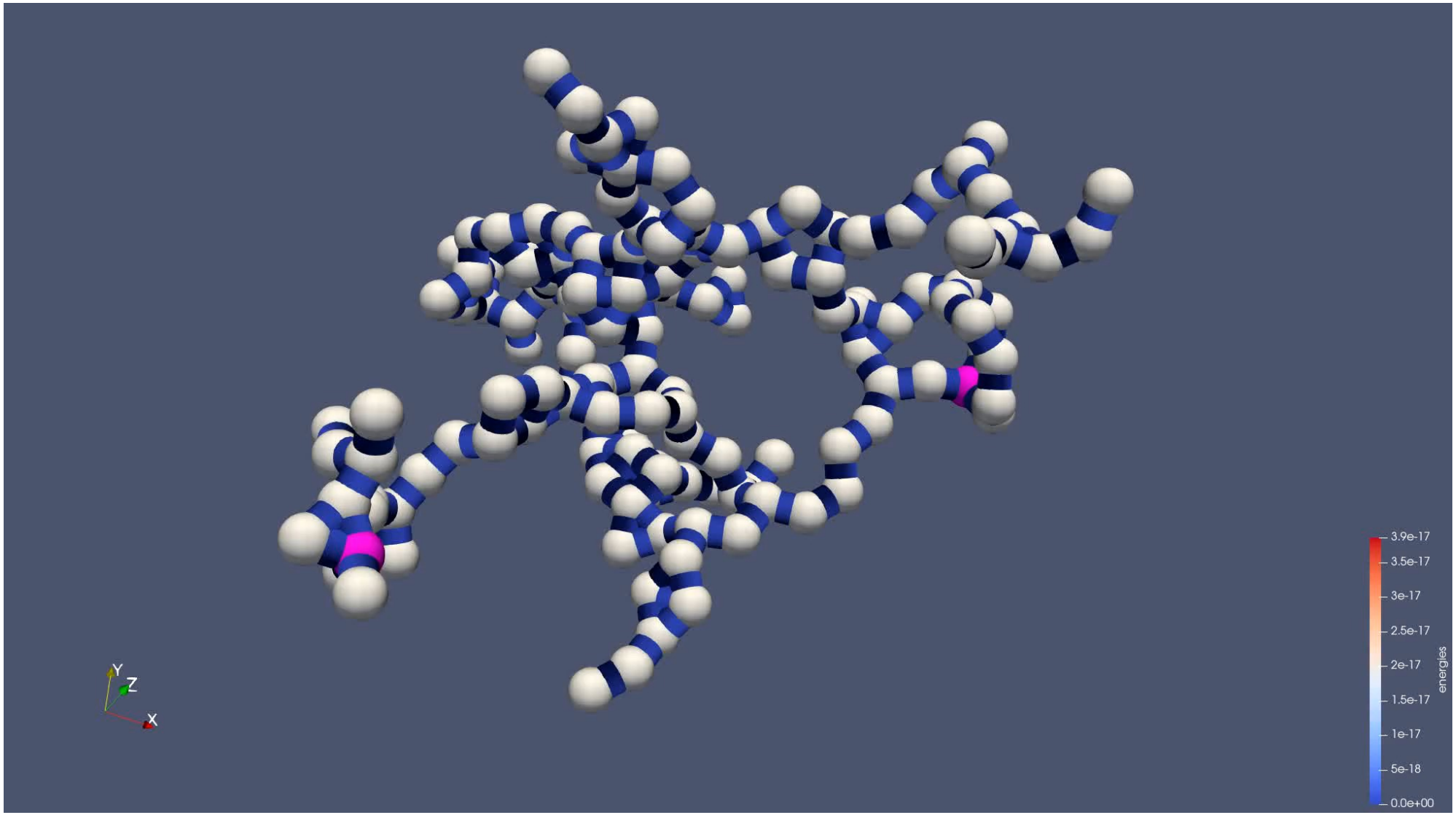


Shear strain on a graphite layer

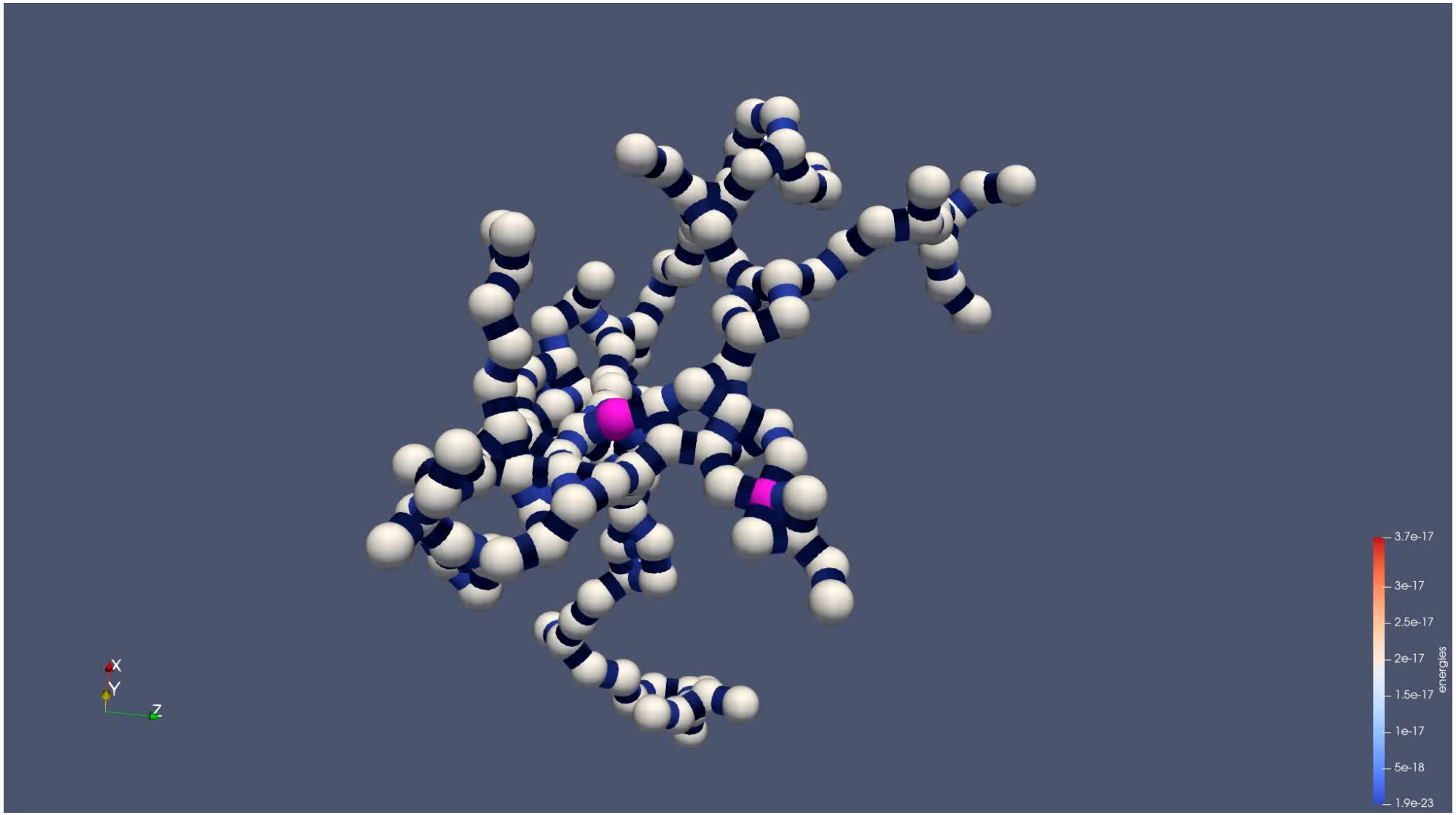


Normal strain on a graphite layer

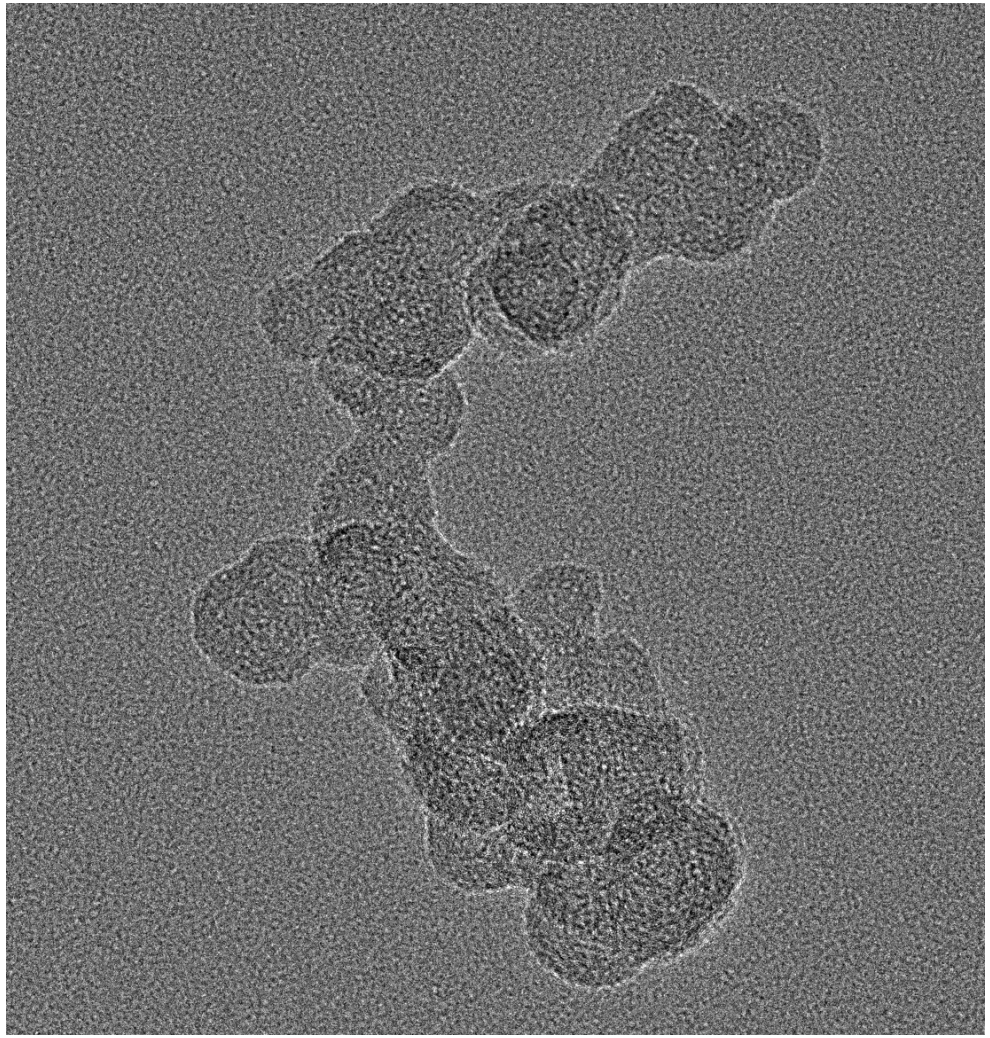
Shear strain in an aggregate



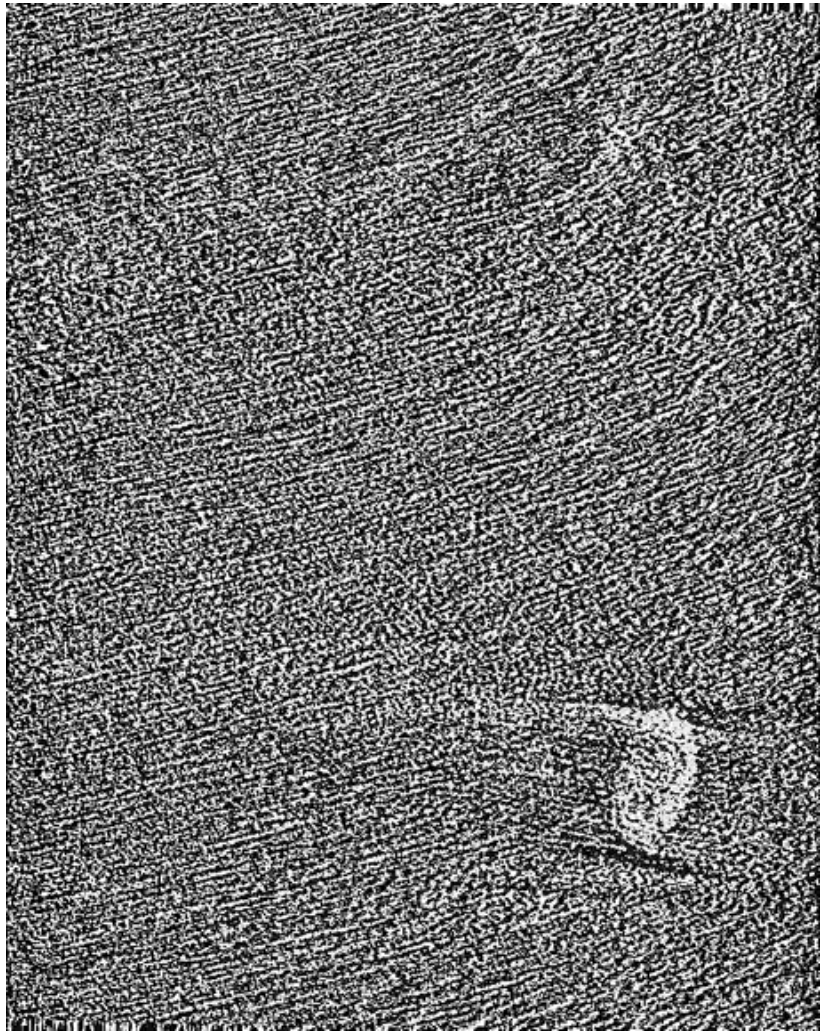
Shear strain in an aggregate



Parametrization – neck geometry

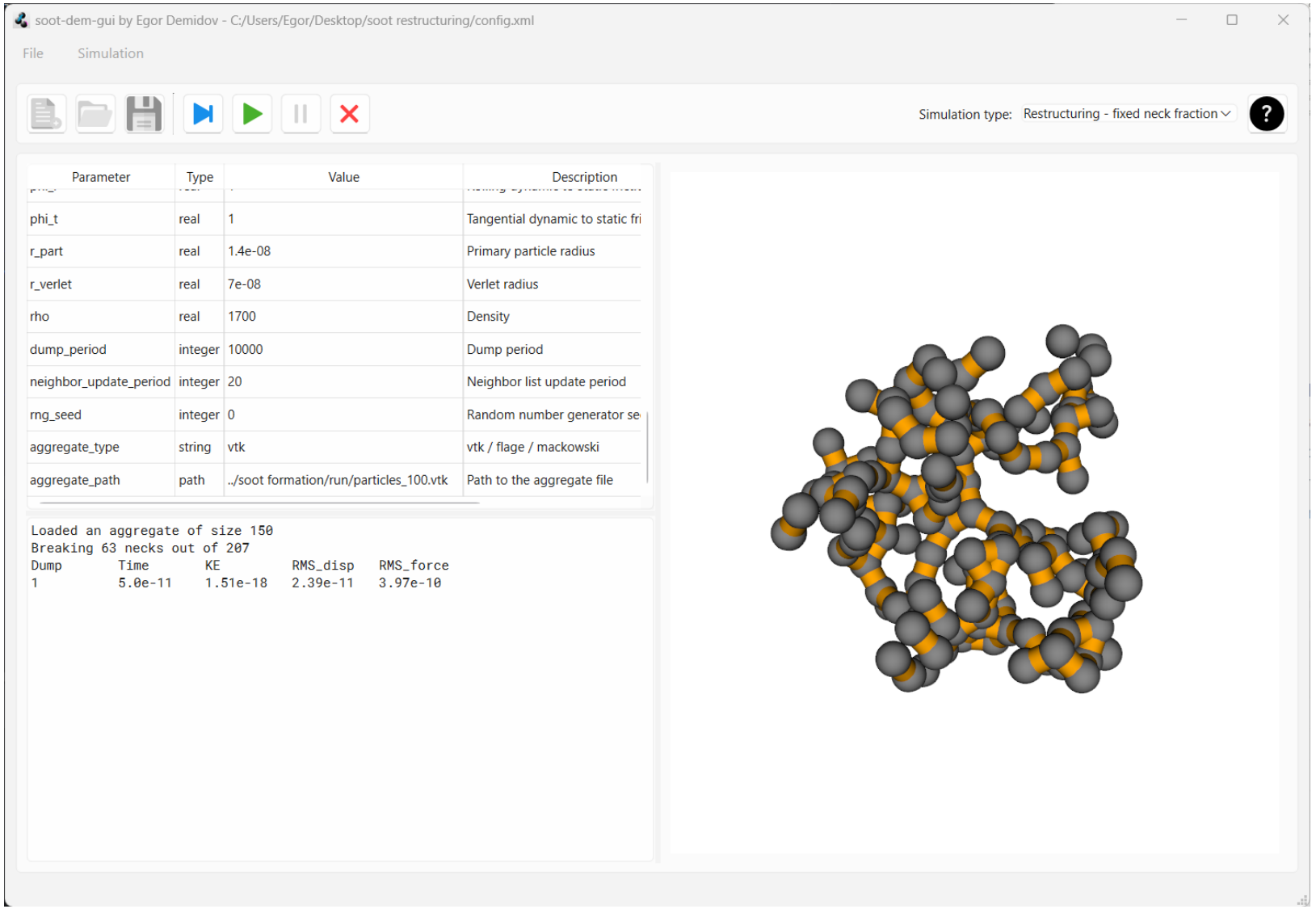


TEM tilt series, EMSL



TEM tomography reconstruction, EMSL

Try our soot mechanics engine



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EMSL

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