Discrete element method model for restructuring of soot aggregates

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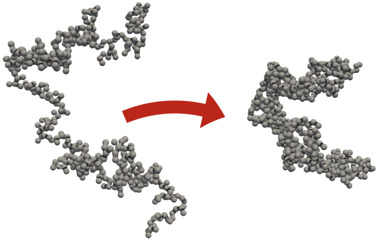
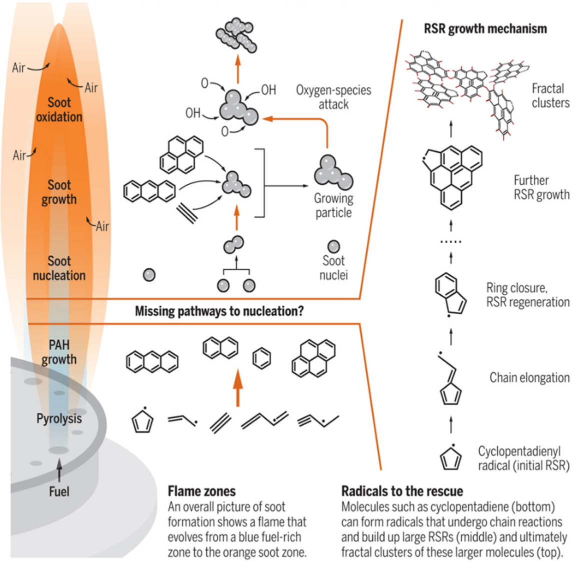
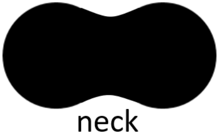
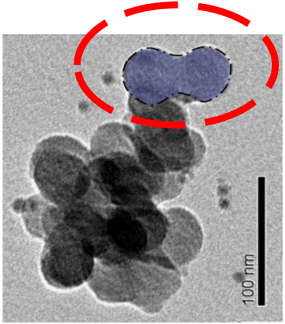
June 6, 2024



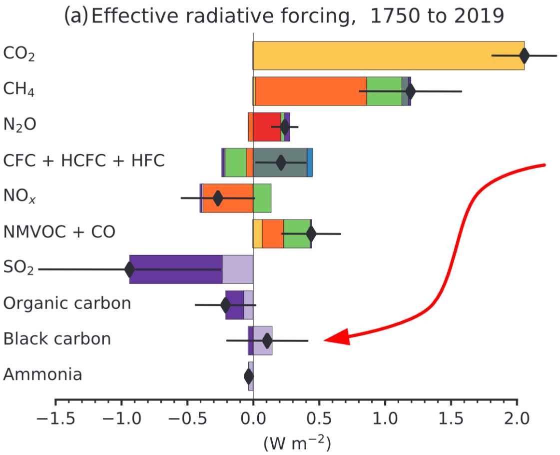
Formation of soot







Climate impact of soot

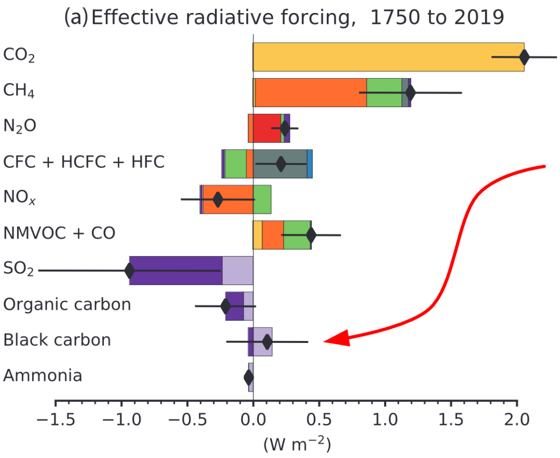


a

- Soot (black carbon) is a major contributor to climate change

[a] IPCC. *Climate Change 2021: The Physical Science Basis*. 2021. Chap. 6.4: SLCF Radiative Forcing and Climate Effects

Climate impact of soot

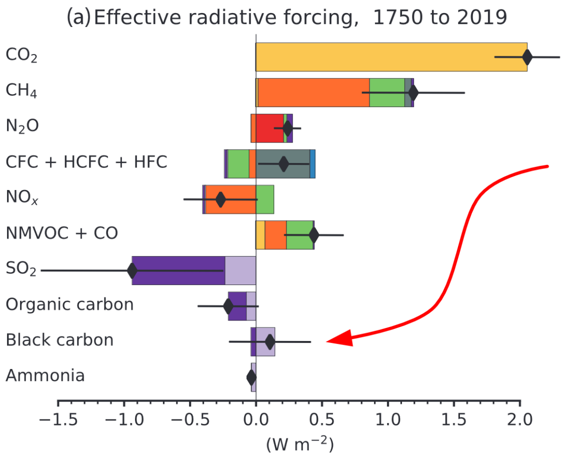


a

- Soot (black carbon) is a major contributor to climate change
- Uncertainty in climate forcing by soot remains large

[a] IPCC, *Climate Change 2021: The Physical Science Basis*

Climate impact of soot

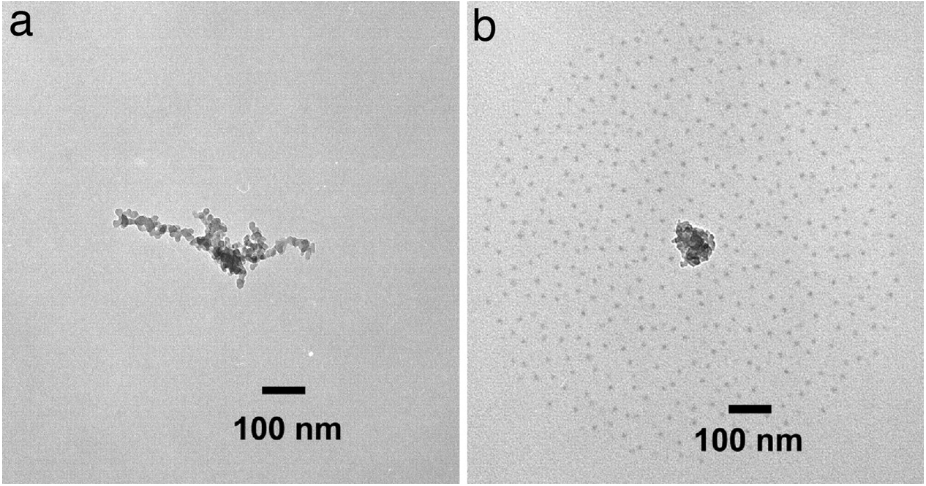


[a]

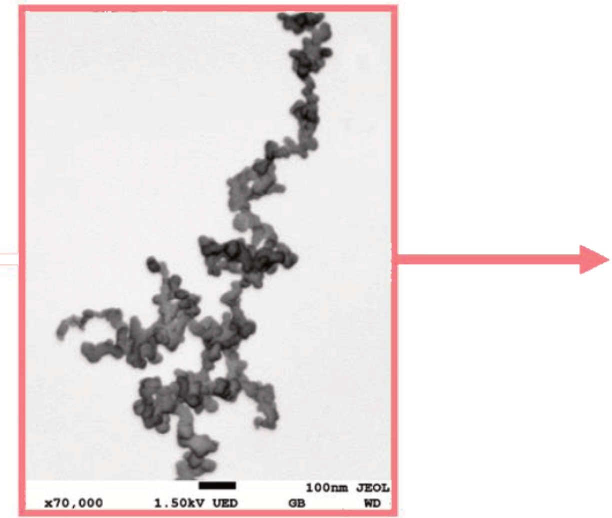
- Soot (black carbon) is a major contributor to climate change
- Uncertainty in climate forcing by soot remains large
- Determination of climate forcing by soot is complicated by:
  - Complex morphology of soot particles
  - Transformations that soot particles undergo in the atmosphere

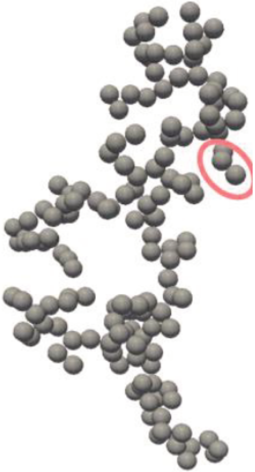
[a] IPCC, *Climate Change 2021: The Physical Science Basis*

Morphology and composition of soot particles

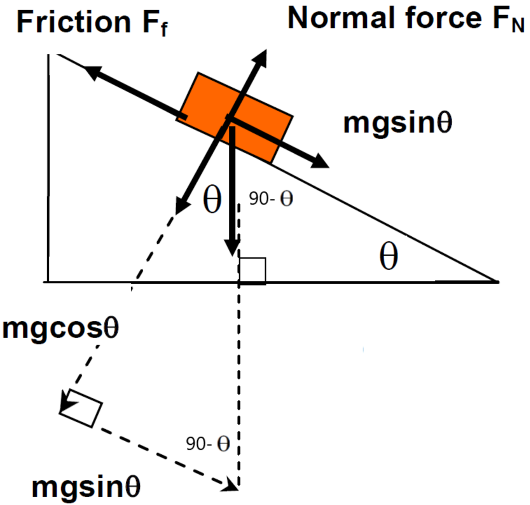


Representation of soot in a simulation





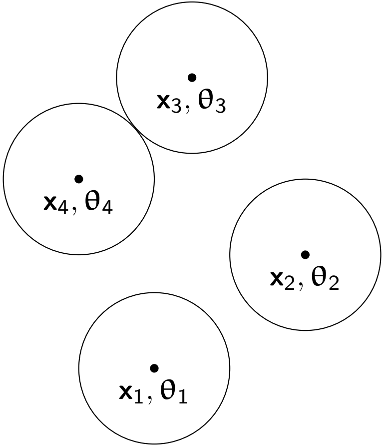
Newton's equations of motion



$$\mathbf{f} = m\mathbf{a} = m\frac{d^2\mathbf{x}}{dt^2}$$

$$\boldsymbol{\tau} = I\boldsymbol{\alpha} = I\frac{d^2\boldsymbol{\theta}}{dt^2}$$

Problem statement



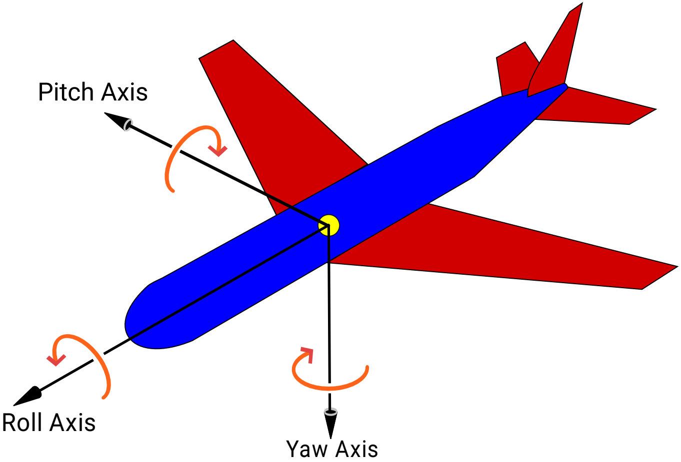
System of interacting particles

$$\underbrace{\mathbf{x} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix}}_{\text{positions}}$$

$$\underbrace{\boldsymbol{\theta} = \begin{bmatrix} \theta_{11} & \theta_{12} & \theta_{13} \\ \theta_{21} & \theta_{22} & \theta_{23} \\ \vdots & \vdots & \vdots \\ \theta_{N1} & \theta_{N2} & \theta_{N3} \end{bmatrix}}_{\text{orientations}}$$

Find $\mathbf{x}(t)$ and $\boldsymbol{\theta}(t)$

Rotational degrees of freedom



Discrete element method

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

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

Discrete element method

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

$$\mathbf{a}_i = \frac{1}{m}\left[\underbrace{\mathbf{F}_{i,\mathrm{u}}}_{\text{field force}} + \underbrace{\sum_{j=1}^{N}\mathbf{F}_{ij,\mathrm{b}}}_{\text{binary force}}\right]$$

Field force: gravity, electric field, viscous drag, *etc.*
Binary force: friction, elasticity, van der Waals attraction, *etc.*

Discrete element method

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

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

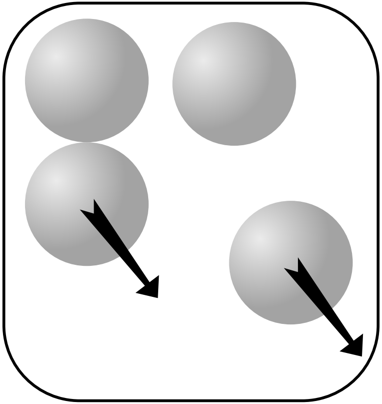
Also, inter-particle friction can result in rotation:

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

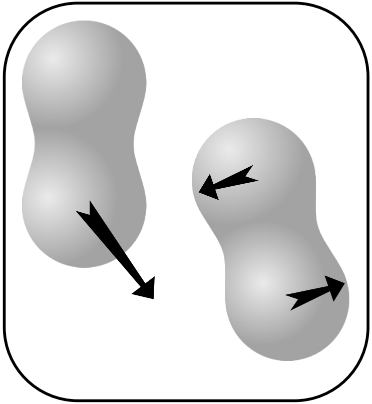
Remark

A multi-body problem is approximated as a system of two-body problems

Types of contacts in a soot aggregate

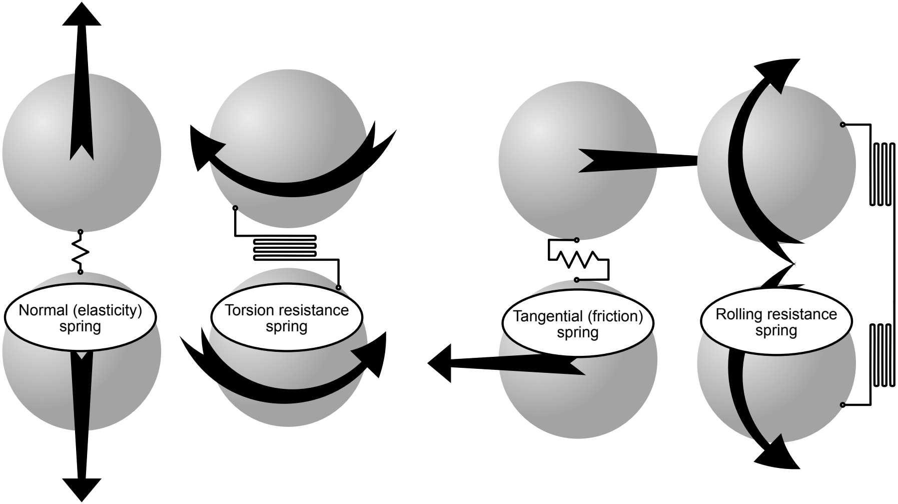


Non-bonded contact under tension



Bonded contact under tension

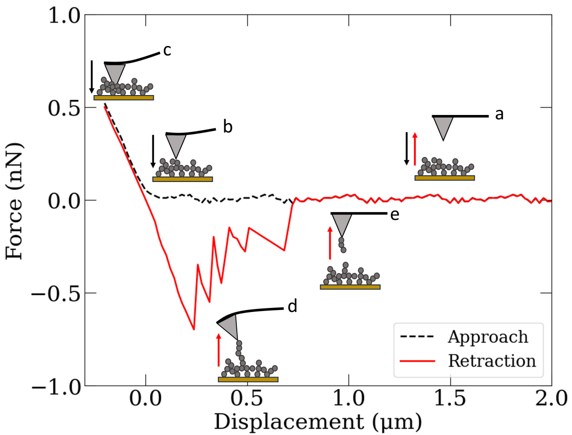
Degrees of freedom in a pair

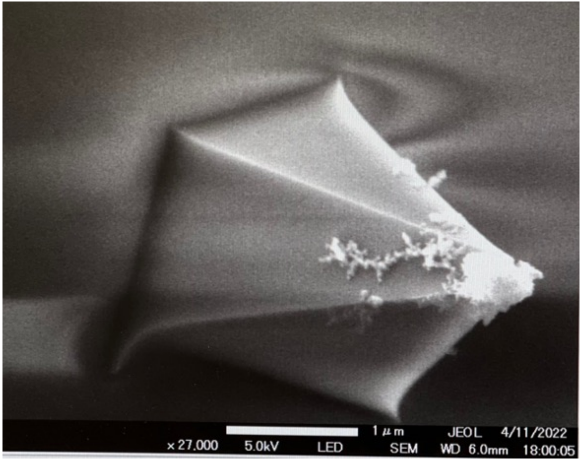


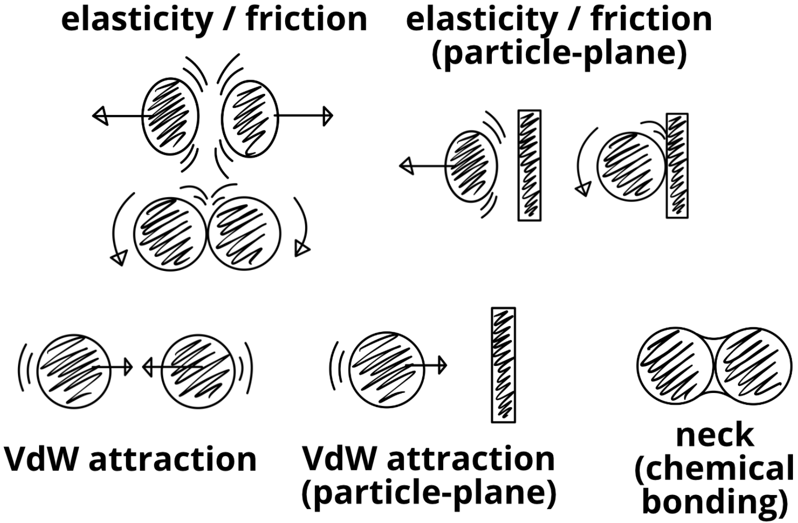
Normal degrees of freedom

Tangential degrees of freedom

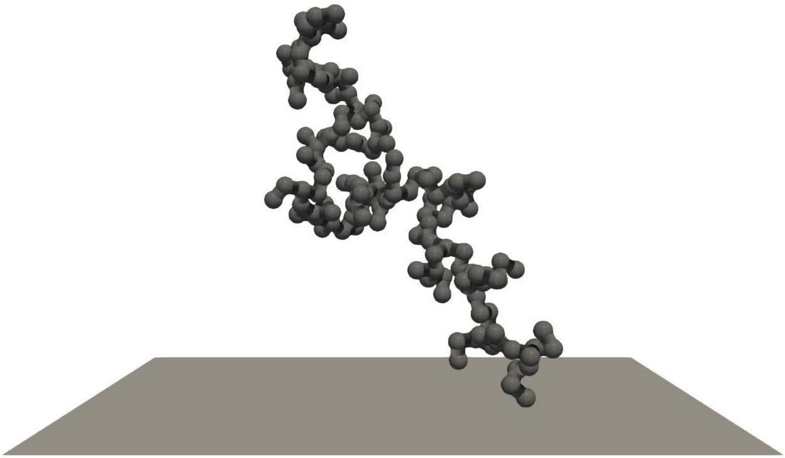
AFM spectroscopy experiments as a parametrization tool



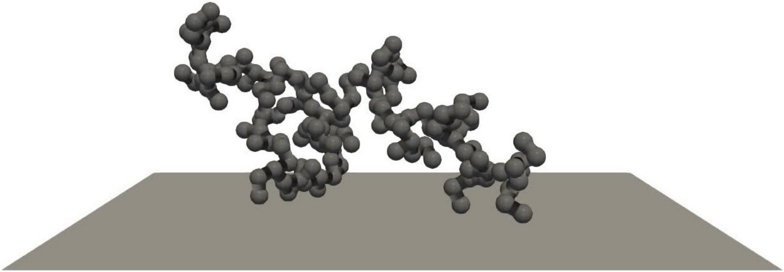



elasticity / friction
elasticity / friction (particle-plane)
VdW attraction
VdW attraction (particle-plane)
neck (chemical bonding)

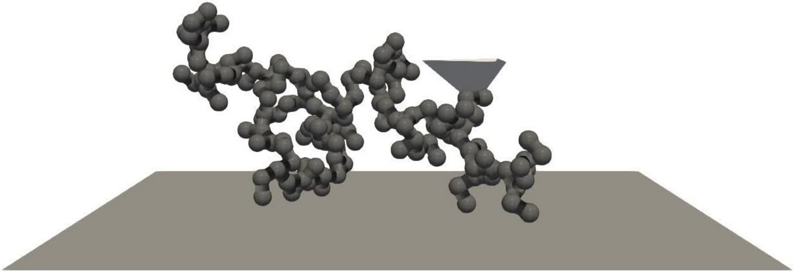
Simulation of AFM experiments



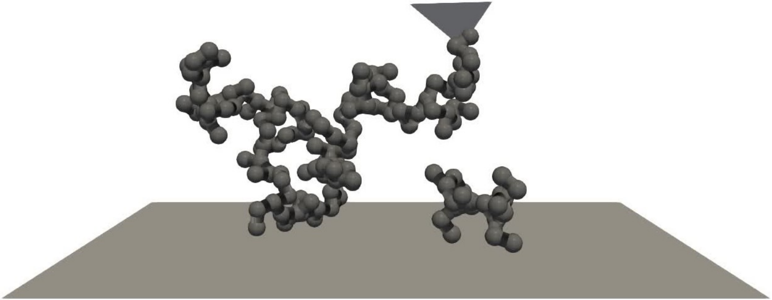
Simulation of AFM experiments



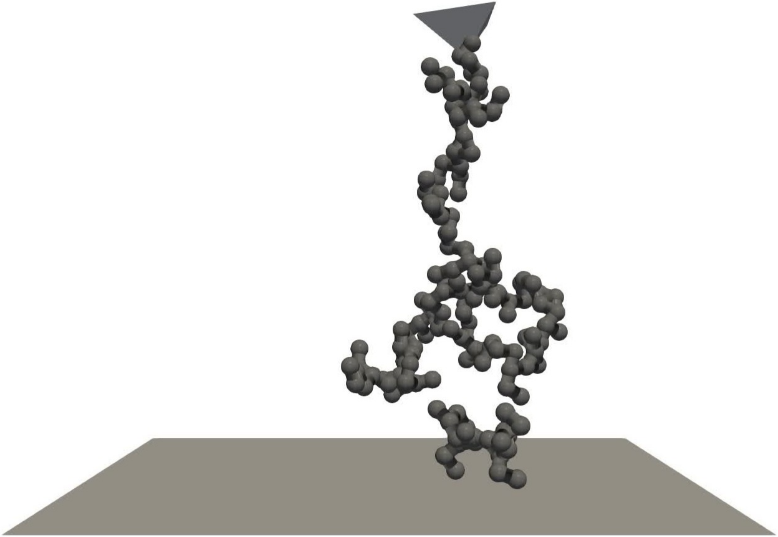
Simulation of AFM experiments



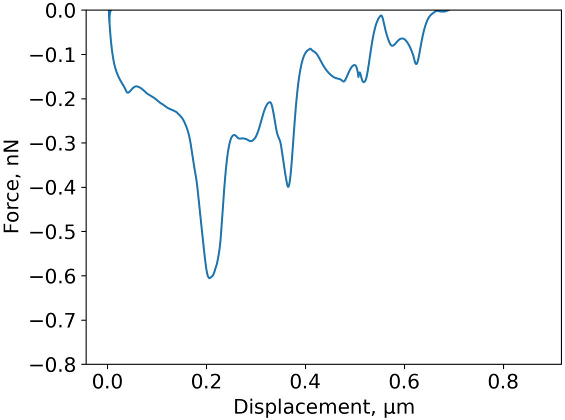
Simulation of AFM experiments



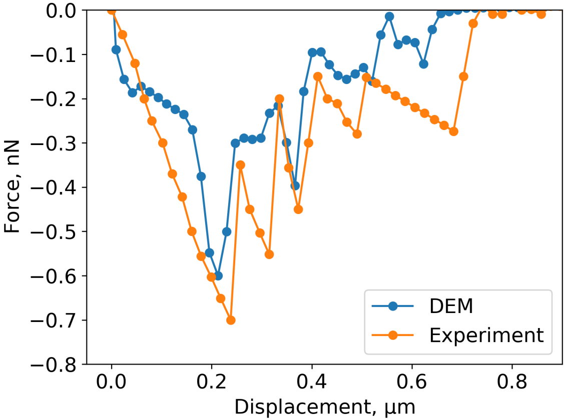
Simulation of AFM experiments



AFM retraction (force-displacement) curves

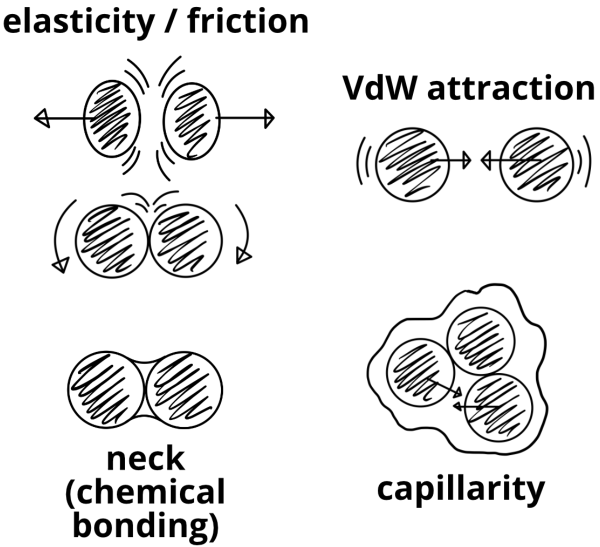


Simulated force-displacement curve

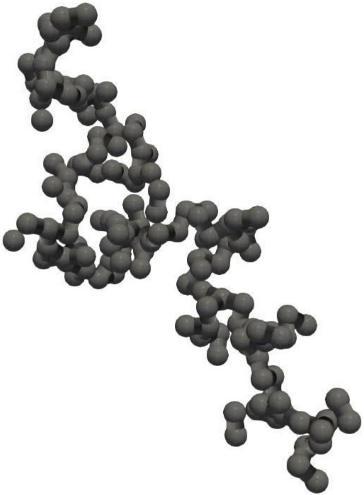


Simulation and experiment overlaid

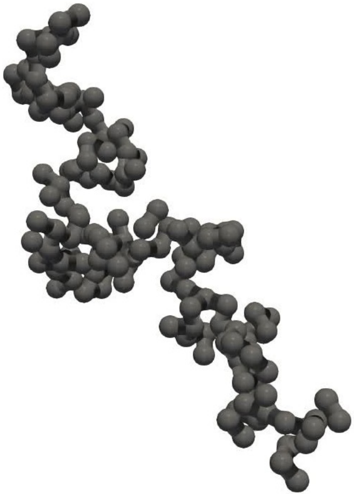
Simulation of aggregate restructuring experiment



Simulation of aggregate restructuring experiment



Simulation of aggregate restructuring experiment



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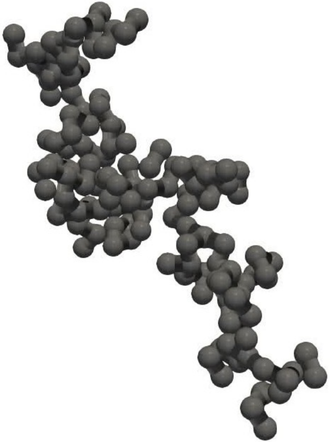

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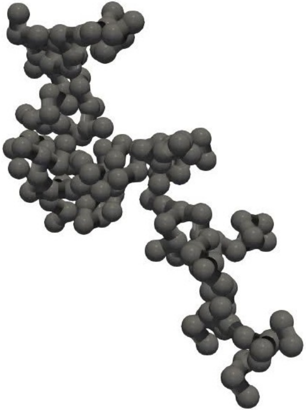
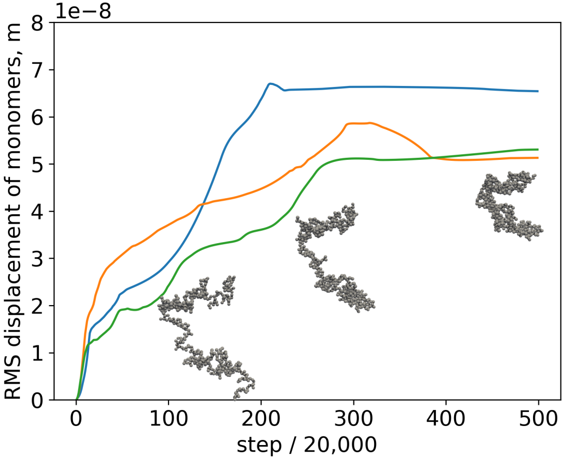
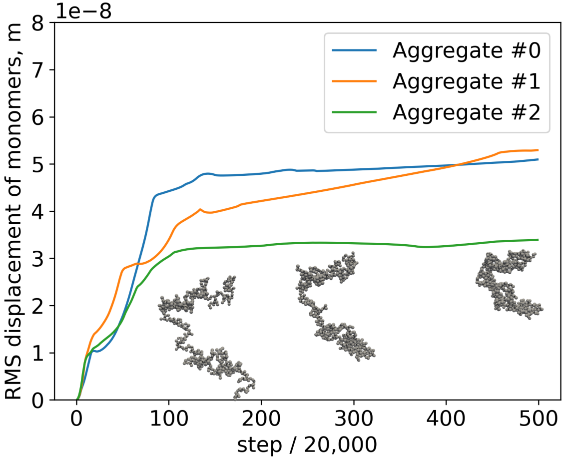


Restructuring primary particle displacement curves



70% necking



90% necking

Conclusions & future work

Conclusions:

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

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Future work:

- Parametrize the restructuring simulations based on experiments
- Develop a parametrization for soot restructuring in large-scale aerosol models based on simulations
- Apply the DEM model to simulation of industrial carbon blacks

Acknowledgement

- Ali Hasani for experimental AFM data
- Ashoka Tholangamuwe Gedara for annotated force-displacement curve
- U.S. NSF award #AGS-2222104