Simulation of adhesion-moments depending on the van der Waals interactions between rough particles and smooth walls in gaseous environment

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Objects of the project

- Examination of the adhesion moment
- Particle on a wall
- Gaseous Environment
- Atomic scale
- Two different models:
  - Smooth particle
  - Rough particle
- Simulation to calculate the moment distribution
- Estimation of contact resistance versus external stresses
Scanning principle

- Scanning of a 3-dimensional space
- Three different principles
- Starting point is set → one atomic radius distance away from the point of origin of the coordinate system
- From starting point one line of points is scanned
- At the end of one row (marked by the diameter of the particle), scanning starts again in the next column
- A plane is built and then the planes are stacked to a space
- At every scanned point the simulation decides, whether there is an atom of the particle or not
- If this check is positive, the van der Waals force is calculated and added to a total adhesion force
Examples and adhesion force

Fig.1: 40 nm particle cut open

Fig.2: 103 nm particle surface

Equation for the van der Waals force between an atom and the wall:

\[ F_{\text{atom-wall}} = \frac{A}{\pi \rho 2D^4} \]
Flaws in the particle lattice

- Simulated lattice is perfect
- Real lattices are not
- Lattice flaws must be built and were realised by a porosity:
  - Each atom gets a random number \(1 \leq x \leq 100\)
  - Porosity is set in percent
  - Atoms with a random number below the porosity value are ignored in the calculations
- Result: Lattices with high porosity (many flaws) build up less adhesion force
Flattening and effective force range

Fig. 4: Adhesion force against flattening factor for different particle diameters

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Adhesion moment

- Not depending on the force direction for a smooth particle
- Depending on the force direction for a rough particle
- Anisotropic behaviour of the contact
Fig. 5: Adhesion moment against force angle, flattening factor 0.0, rough particle
Fig. 6: Adhesion moment against force angle, flattening factor 0.5, rough particle
Thank you for your attention.

Questions?

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