# *In situ* studies of high-purity mono- and bimetallic nanostructures in experiment and simulation

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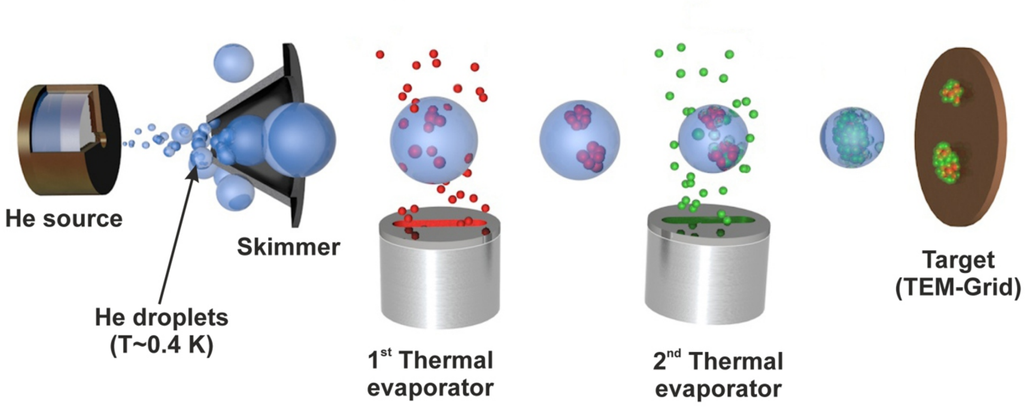
## Introduction

- We performed in situ STEM heating experiments of metallic nano structures and interfaces
- Study of diffusion processes between different metals on an atomic scale
- High-purity clusters and nanoalloys synthesised with superfluid helium droplets
- Computational modelling of temperature- and beam induced diffusion processes

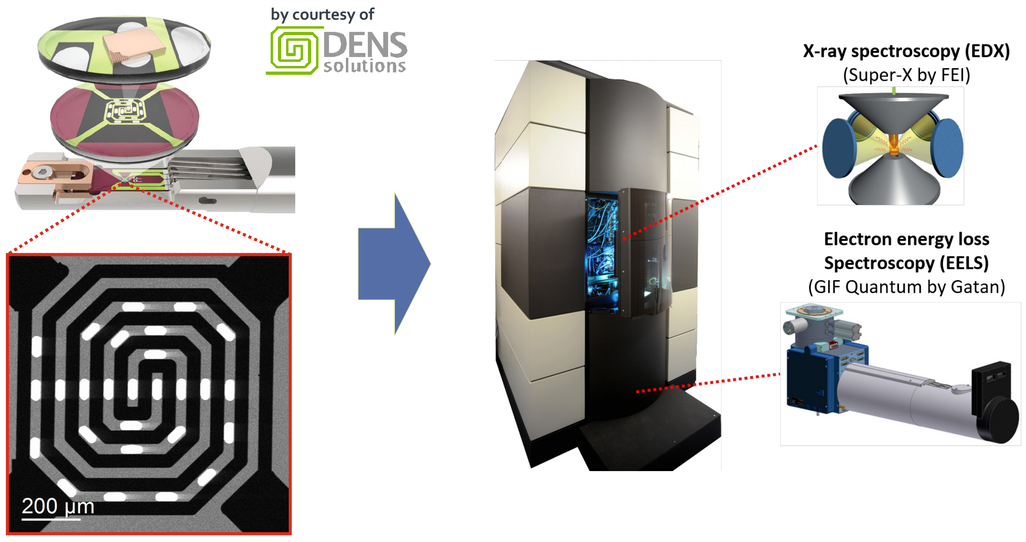
## Methods

**Synthesis of metallic clusters and nanoalloys:**




+ High purity structures (UHV, no surfactants) [1, 2]
+ With variable morphologies
+ Clusters can be deposited on any surface

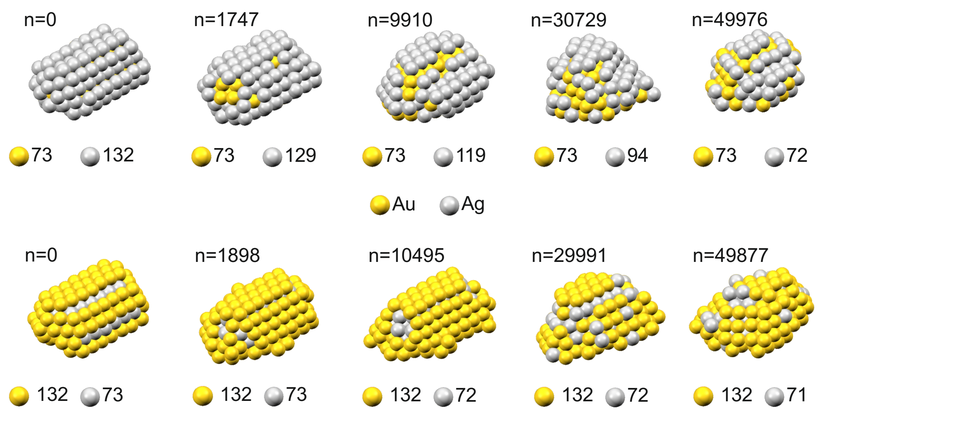
**HR-STEM *in situ* analysis:**




- DENS Wildfire D6 holder with FEI Titan$^3$ G2 60-300
- Precise and fast temperature control up to 1300 °C
- Allows to utilize resolution and high analytical capability of the microscope

**Simulation of beam induced atom dynamics:**

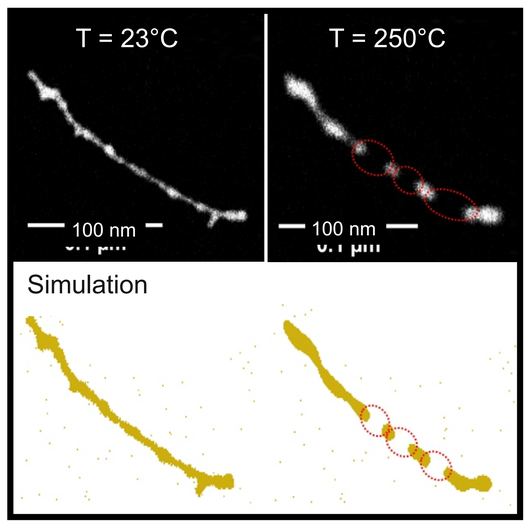
- Beam induced displacements and sputtering on metallic nanostructures dominated by “elastic” interactions of the nuclei with the electrons [3]
- Simulation with Molecular Dynamics on AuAg clusters




n... no. of simulated displacement events

## Results

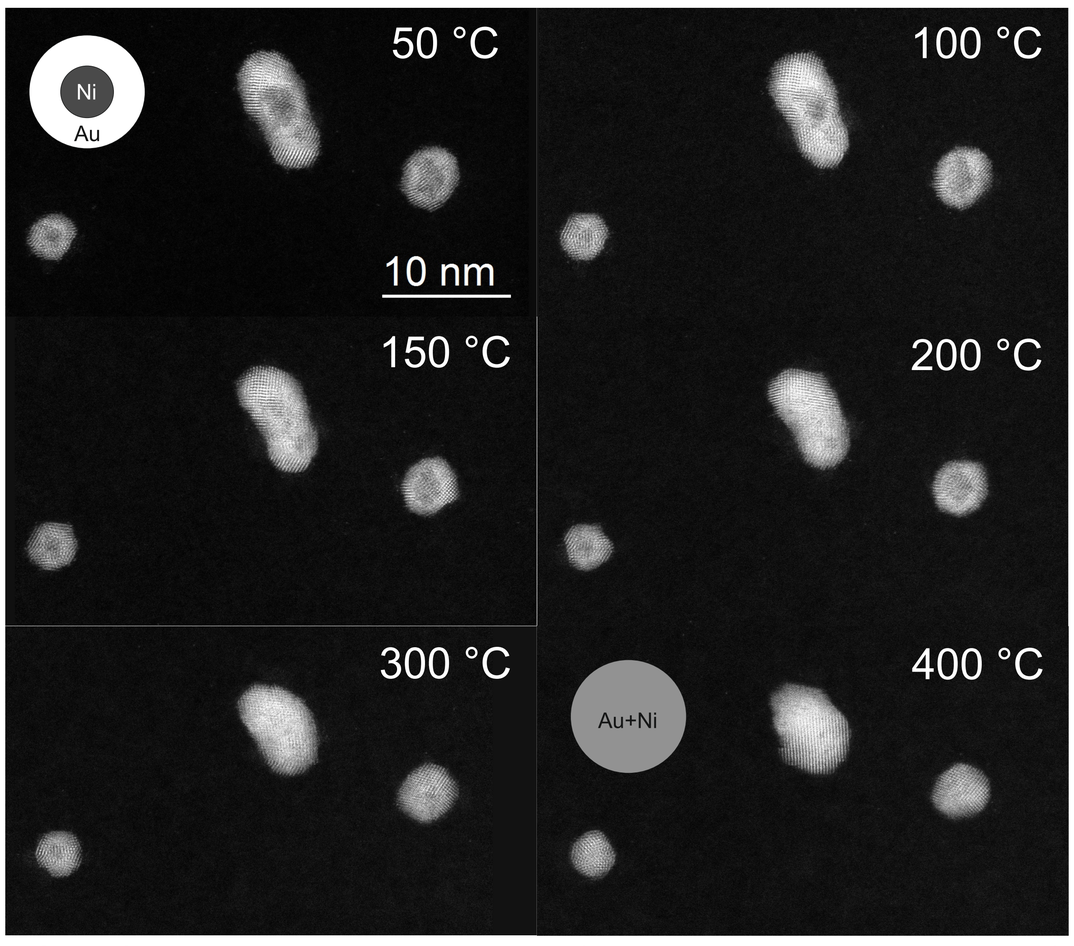
**Rayleigh breakup of Au nanowires: Experiment & Simulation**




- Rayleigh breakup (RB) is well known in fluids
- RB also occurs in solids on the nanoscale
- RB of metallic nanostructures starts far below melting temperatures
- Mediated by surface diffusion
- Simulation with a cellular automaton (no. of nearest neighbours maximised) [4]

**Alloying of Ni-Au core-shell clusters:**

- Au-Ni phase diagram exhibits large miscibility gap; provokes spinodal decomposition in the bulk system
- Question: Thermodynamics of Ni-Au in a nanoalloy?
- Bimetallic clusters (70 at.% Au) are supported by 5 nm amorphous carbon
- Direct comparison of different sizes and morphologies




- Significant morphology change (thermodynamic equilibirum)
- Irreversible alloying at temperatures above ~150°C
- Larger particles alloy easier than smaller ones

## References/ Literature

[1] Volk, A. et al. The impact of doping rates on the morphologies of silver and gold nanowires grown in helium nanodroplets. Phys Chem Chem Phys 18, 1451–459 (2016).
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