Atoms in Motion: Electron Beam Driven Dynamics in Experiment and Simulation

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With recent advances in aberration corrected electron optics, scanning transmission electron microscopy (STEM) has proven its excellent capability of characterising nanomaterials. In principle, with STEM chemical information can be extracted at the level of individual atoms. Due to the high current densities occurring in a highly focused electron beam, however, interpretation of STEM data is often impeded by continuous beam induced sample changes [1]. This is especially true for systems with a high percentage of weakly bound surface or interface atoms, which is characteristic for nanoparticles and other nanoscaled materials. Hence, beam induced processes pose a main limitation to nanomaterial characterisation in the STEM. Despite its significance, knowledge about beam induced dynamics is still very limited.

Here, we will report on STEM experiments performed on metallic clusters, grown inside superfluid helium nanodroplets. This method guarantees exceptional cluster purity and offers high flexibility in terms of morphology and composition [2].

We apply both experimental and computational methods to elucidate electron beam induced dynamics down to the single atom level. On the one hand, we perform time-resolved STEM experiments, which allow to observe the dynamics of clusters and single atoms under the controlled influence of the electron beam. Image series consisting of several hundred images are evaluated using automatic image processing techniques. On the other hand, we develop a computational framework to simulate elastic electron damage processes in solids, to obtain deeper insights into the observed dynamics. Our approach is based on a combination of molecular dynamics and Monte Carlo techniques [3].

We will show different examples where our framework can be applied:

Figure 1a shows an STEM HAADF image series for a Janus type AgAu cluster on an amorphous carbon support, while illuminated with 300 keV electrons. The two cluster phases show highly different dynamics under electron irradiation, due to differences in atomic mass and binding energies between Au and Ag. While the Au part mostly retains its size during the experiment, the Ag cluster exhibits significant mass loss due to surface sputtering. This behaviour is reproducible using above mentioned simulations (Figure 1b & c).

Deeper understanding of electron beam induced dynamics not only helps to develop strategies to prevent sample damage, which is important especially for analytical and quantitative STEM analysis. Electron induced motion of single atoms on the surface or inside crystalline materials may also be useful to estimate surface energies, analyse defect generation and investigate diffusion processes. Figure 1d shows the electron driven diffusion of Au atoms inside an AlAu alloy, for instance.

Moreover, such diffusion processes can also be used to tailor nanostructures in a highly localized manner as shown in the time-lapse series in Figure 1e, where beam induced segregation of a Ni-Au nanoalloy is demonstrated.

References:

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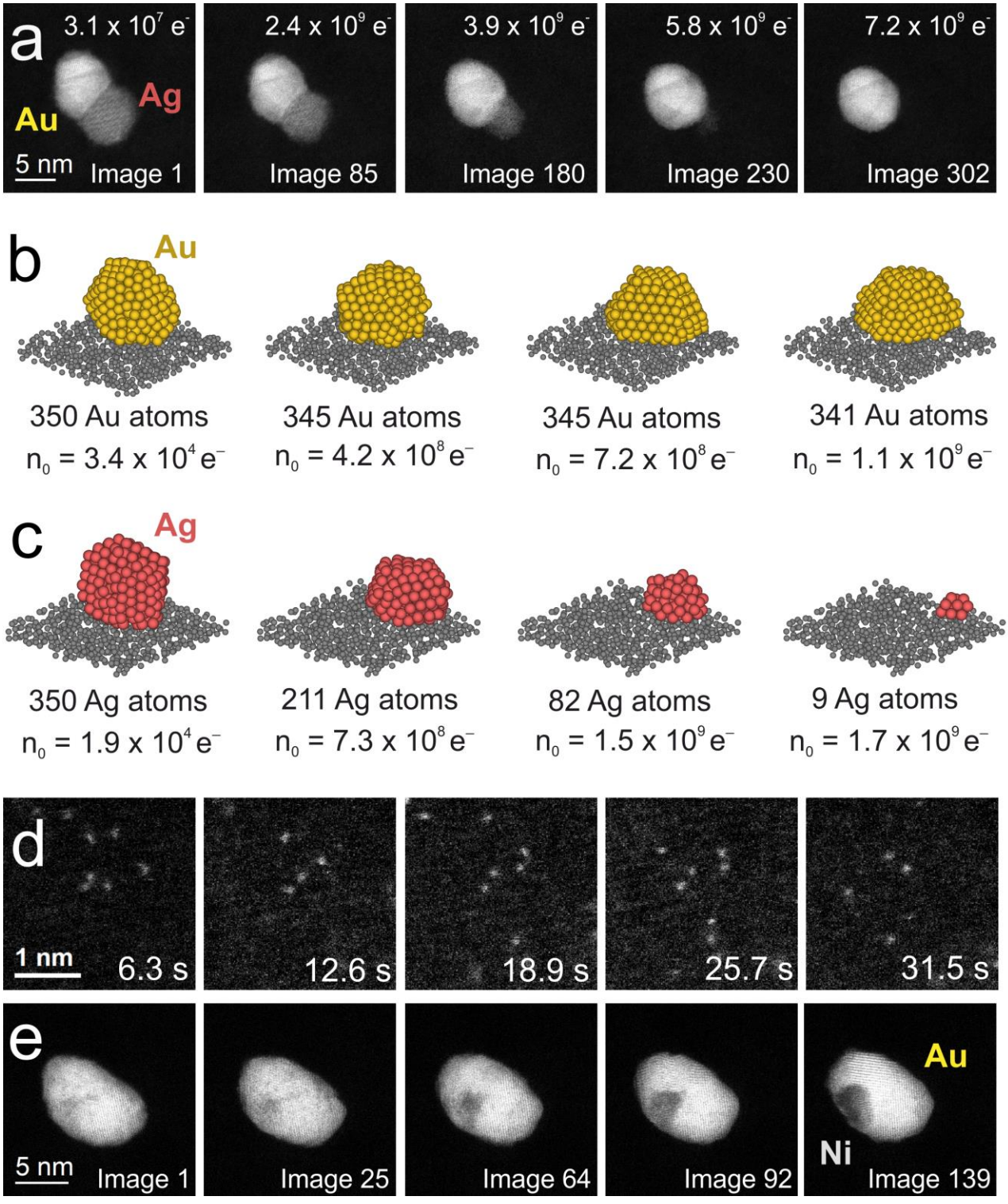

Figure 1: (a) Experimental HAADF image series of a AuAg Janus particle showing the effect of selective Ag sputtering, dependent on the applied dose in no. of electrons. (b, c) Simulation of beam induced dynamics in carbon supported clusters initially comprised of either 350 Au or Ag atoms, demonstrating significant surface sputtering of Ag atoms at 300 keV electron energy. (n_0 denotes the applied dose in no. of electrons) (d) Beam driven diffusion of Au atoms inside an Al - matrix. (e) Electron beam induced phase separation in a NiAu nanoalloy (electron energy was 300 keV in each series).