Structural properties of Au clusters on MgO


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Summary: Au-clusters deposited on MgO are studied by means of high resolution electron microscopy (HREM). The preferred morphology of the deposited clusters is truncated octahedral or truncated half-octahedral, depending on the size of the clusters. Precise measurements on HREM images show that the Au lattice expands at the interface to accommodate to the MgO lattice.

1. Introduction.

Recently a lot of attention is paid to the study of nanoparticles and clusters. The investigation of clusters is not only interesting from a fundamental point of view e.g. magnetic properties depend on the cluster structure [1], but also from a more applied point of view e.g. catalysis [2]. The crystal structure of the cluster is closely related to the physical and chemical properties; HREM is the only way to visualise the crystal lattice and to achieve information on the structure of individual clusters.

In this contribution, Au clusters deposited on MgO are studied. The Au clusters are deposited on MgO cubes. With the use of HREM, not only the morphology of the clusters is determined but also an epitaxial relation between the Au clusters and the MgO substrate is derived. The lattice parameter of MgO is 4.20 Å and the lattice parameter of Au is 4.08 Å. This means that there is a small lattice mismatch of 3%. By precise measurements on the HREM images, it is shown that at the Au/MgO interface the Au lattice is adapting itself to the MgO.


Microscope grids on which MgO single crystalline cubes are deposited by burning MgO powder in air are used as substrates for the Au clusters. The Au clusters are fabricated in a laser vaporisation cluster source [3] and deposited by low energy cluster beam deposition (LECBD) [4] on the MgO cubes. The low cluster kinetic energy (E_{kin} < 1 eV/atom) prevents fragmentation of the clusters and minimises the interaction with the substrate upon impact.

Images are taken with a JEOL 4000 EX microscope. Precise measurements of the lattices of Au and MgO are done using the DALI program (Digital Analysis of Lattice Images) of Andreas Rosenauer [5]. Before measuring the lattice distances, a Wiener filter is applied to the images to reduce the noise.

3. Results.

The morphology is determined by projections of the particles parallel to the interface Au/MgO (cross section) in two different orientations: <011> and <001>. In the <011> zone axis, also projections perpendicular to the interface (top view) helped to determine the morphology. Fig. 1a shows a cluster (2.5 nm) in cross section in the [011] orientation. The profile of the particle is limited by 4 <112> directions and 2 <011> directions. This indicates that the cluster has an octahedral shape and is asymmetrically truncated at the top and the interface. HREM images taken in the <001> orientation also show truncations at the corners of the Au octahedrons. Smaller clusters (around 1 nm) are half octahedron shaped. The same morphologies are also observed for other metal clusters deposited on MgO [6].

The epitaxial relation between Au clusters and MgO could be derived from the HREM-images: (001)_{Au} // (001)_{MgO} and [100]_{Au} // [100]_{MgO}. This epitaxial relation was also seen in studies of larger Au particles on MgO [7,8].
Fig. 1b shows the (220) lattice distances of a Au cluster and the MgO substrate in the [011] orientation. From this graph, it is clearly seen that the interface between Au and MgO is between the layers 11 and 12. The (220) distances in the Au layers close to the interface decrease from 1.472 ± 0.013 Å (in layer 11) to 1.451 ± 0.010 Å (in layer 9). For the layers above (n<9) it reaches the bulk value of Au. The dilatations of the (220) lattice in layers 1 and 2, layers close to the top of the particle, are delocalisation effects of the microscope and are also observed in other studies of metal clusters [9]. The same behaviour as shown in fig. 1b is also seen for clusters in the <001> orientation. Here the d_{300} distance is accommodated to the MgO substrate.

**Figure 1:** a) Au cluster deposited on MgO. b) Graph of the (220) distances through the cluster shown in a. The accommodation in the cluster is clearly seen. Layer 1 and the interface are both indicated on the photo and on the graph.

4. Conclusion.

We can state that all Au clusters deposited on MgO are single crystals with the fcc structure. From cross section and plan view images, it is determined that clusters with a size of 2 nm have a truncated octahedral shape. For smaller particles (1 nm) a truncated half-octahedral shape is observed. These morphologies are only limited by {111} and {001} faces, which are energetically the most stable ones.

From the HREM images of clusters in <001> and <011> orientations the epitaxial relation is determined: (001)_{MgO} // (001)_{Au} and [100]_{MgO} // [100]_{Au}. By precise measurement of the (220) lattice distances in the deposited particle, it is concluded that near the interface between Au and MgO, the Au lattice dilates in the first two or three contact layers to adapt to the lattice of MgO.

5. Acknowledgements.

B.P. and P.L. are grateful to FWO-Flanders (Belgium) for financial support. L.T.K. has received financial support from SNF (Danish Research Council).

6. References.