

# Gold Nanoparticles on MgO - A Revisit using Cs-Corrected STEM

Han, Y; Li, Z

DOI:

[10.1017/S1431927611010233](https://doi.org/10.1017/S1431927611010233)

License:

None: All rights reserved

*Document Version*

Publisher's PDF, also known as Version of record

*Citation for published version (Harvard):*

Han, Y & Li, Z 2011, 'Gold Nanoparticles on MgO - A Revisit using Cs-Corrected STEM', *Microscopy and Microanalysis*, vol. 17, no. S2, pp. 1872-1873. <https://doi.org/10.1017/S1431927611010233>

[Link to publication on Research at Birmingham portal](#)

**Publisher Rights Statement:**

© Cambridge University Press

Eligibility for repository checked July 2014

**General rights**

Unless a licence is specified above, all rights (including copyright and moral rights) in this document are retained by the authors and/or the copyright holders. The express permission of the copyright holder must be obtained for any use of this material other than for purposes permitted by law.

- Users may freely distribute the URL that is used to identify this publication.
- Users may download and/or print one copy of the publication from the University of Birmingham research portal for the purpose of private study or non-commercial research.
- User may use extracts from the document in line with the concept of 'fair dealing' under the Copyright, Designs and Patents Act 1988 (?)
- Users may not further distribute the material nor use it for the purposes of commercial gain.

Where a licence is displayed above, please note the terms and conditions of the licence govern your use of this document.

When citing, please reference the published version.

**Take down policy**

While the University of Birmingham exercises care and attention in making items available there are rare occasions when an item has been uploaded in error or has been deemed to be commercially or otherwise sensitive.

If you believe that this is the case for this document, please contact [UBIRA@lists.bham.ac.uk](mailto:UBIRA@lists.bham.ac.uk) providing details and we will remove access to the work immediately and investigate.

## Gold Nanoparticles on MgO – A Revisit using Cs-Corrected STEM

Y. Han and Z.Y. Li

Nanoscale Physics Research Laboratory, School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, UK

Previously, high-resolution transmission electron microscopy (HREM) has been commonly used for the purpose of understanding the 3D structures of Au nanoparticles [1,2]. However, the phase contrast images may only be interpretable with the help of simulations, with accurate structural models required for the first instance. This can be a real challenge in detecting low-coordination Au atoms in the nanoparticles, which has been reported to be the most important factor determining the catalytic activities [3]. In comparison, high-resolution aberration-corrected scanning transmission electron microscopy (AC-STEM) imaging has been applied successfully in the characterisation of metallic nanoparticles on various substrates [4,5]. The high-angle annular dark-field (HAADF) images taken under STEM mode exhibit an advantage of allowing us to see single atoms directly and analyzing the contrast quantitatively [4-6].

In this context, Au nanoparticles deposited on MgO smoke crystals at room temperature via thermal evaporation were characterised using a 200kV spherical aberration corrected JEM 2100f STEM equipped with a JEOL HAADF detector. Fig.1a is a low-magnification micrograph of the sample and Fig. 1b is an atomic-resolution image showing one of the Au nanoclusters supported on one side surface of a MgO. This cluster roughly adopted a half truncated octahedron shape with the electron beam aligned with the [001] zone axis of the MgO. To obtain quantitative information about atomic arrangement of the cluster, high-frequency noises were first filtered using fast Fourier transform (FFT). The maximum intensities were then used to locate the positions of the atomic columns. The MgO substrate recorded in the same image was used to achieve an absolute scale. Both the in-layer (parallel to the interface) spacings and layer-to-layer spacings (vertical to the interface) were measured, with the average values plotted in Fig. 2. Here the atomic layers parallel to the Au/MgO interface were numbered from the Au/MgO interface. It can be seen that, away from the interface, the average lateral spacing firstly adopted  $d_{002}$  of MgO (layers 1,2). It then went down (layers 3-8) towards the  $d_{002}$  value of bulk Au, and finally showed a strong relaxation (layers 9-11). Interestingly, the vertical spacing displayed an overall contraction as the layer moving away from the interface. This is the first direct evidence that the relaxation for the atoms in the top two layers (lateral) was strongly coupled with a vertical contraction for Au nanoparticles on MgO(100) surface. It is noted that out-of-plane contractions for surface atoms in Au nanoparticles of 3-5 nm in diameter on carbon support had been suggested by coherent diffraction [7]. The contraction estimated here is 0.17 Å, being comparable with that reported in reference [7] for the {001} surface atoms, at 0.13 Å. The present study demonstrated that the latest advancement in AC-STEM could provide vast unprecedented opportunities to access direct atomic information at surfaces and interfaces. Combined with time evolving measurements, one should be able to study the dynamic behaviors of nanoparticles on a variety of supports in atomic details.

## References

- [1] B. Pauwels, G. Van Tendeloo, W. Bouwen, L.T. Kuhn, P. Lievens, H. Lei, M. Hou, *Phys. Rev. B* 62 (2000) 10383.
- [2] S. Giorgio, M. Cabie, C.R. Henry, *Gold Bull.* 41 (2008) 167.
- [3] M. Haruta, *Gold Bull.* 37 (2004) 27.
- [4] Z.Y. Li, N.P. Young, M. Di Vece, S. Palomba, R.E. Palmer, A.L. Bleloch, B.C. Curley, R.L. Johnston, J. Jiang, J. Yuan, *Nature* 451 (2008) 46.
- [5] S. Van Aert, K.J. Batenburg, M.D. Rossell, R. Erni, G. Van Tendeloo, *Nature* 470 (2011) 374.
- [6] Y. Liu, C.J. Jia, J. Yamasaki, O. Terasaki, F. Schüth, *Angew. Chem. Int. Ed.* 49 (2010) 5771.
- [7] W.J. Huang, R. Sun, J. Tao, L.D. Menard, R.G. Nuzzo, J.M. Zuo, *Nature Mater.* 7 (2008) 308.
- [8] The authors acknowledge the Engineering and Physical Sciences Research Council (UK) and the Birmingham Science City project (AWM) for support.

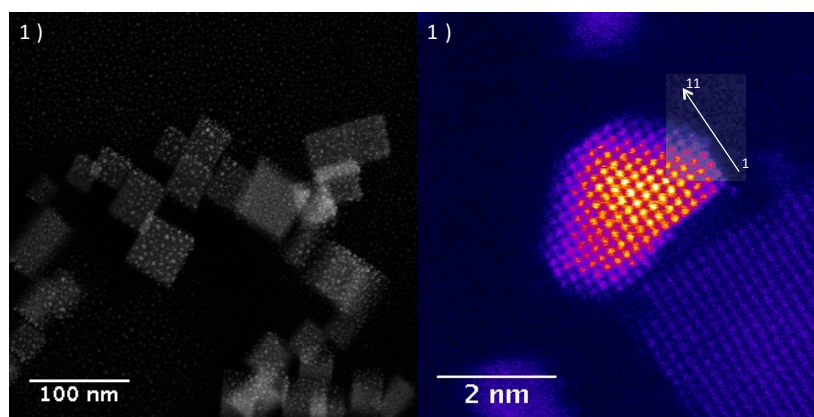


FIG. 2. (a) Overview of the Au nanoparticles on MgO crystals. (b) HAADF-STEM image of a Au nanoparticle supported on MgO. The atomic layers parallel to the Au/MgO interface were numbered from the Au/MgO interface.

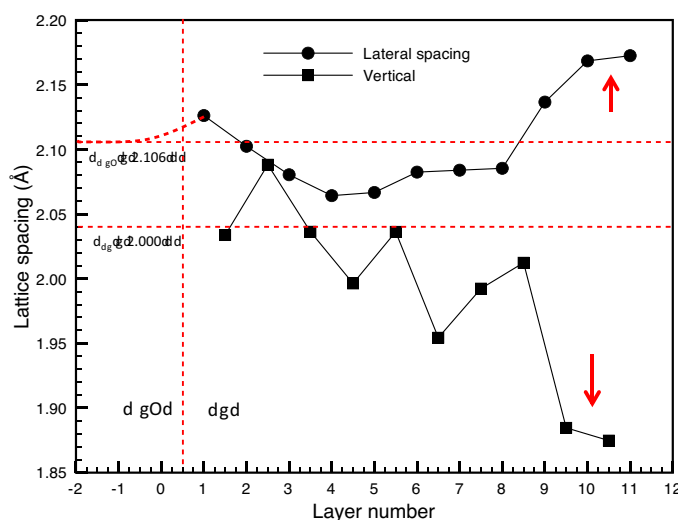


FIG. 3. The average lateral and vertical lattice spacings vs. layer number. The occurrence of lateral relaxation for the atoms in the top two layers coupled with a strong vertical contraction is indicated by the arrows. The half units in the x-axis for the vertical values are used to demonstrate their relative positions with the lateral values.

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.