exponential of the Hamiltonian was made with the Lanczos method [5].

The optical response of smaller clusters is found to be critically dependent on the atomic structure, even for clusters of the same or very similar size. Very few consistent trends or patterns with size or structure can be identified. The addition of a ligand coating [$(PH_3)_{12}Cl_6$] to a 55 atom cluster was found to smooth the optical absorption profile, giving better agreement with experimental data. It also reduced the differences between the optical response of structures with a cuboctahedral or icosahedral core.

For the largest structures studied here a convergence in the optical absorption spectra is seen and there is less variation as a consequence of small changes in the atomic arrangements, as we might expect.

[1] A. Castro, M. Marques, H. Appel, M. Oliveira, C. Rozzi, X. Andrade, F. Lorenzen, E. Gross, A. Rubio, *Physica Status Solidi. B. Basic Research* **2006** *243*, 2465. [2] N. Troullier, J. Martins, *Solid State Communications* **1990,** *74*, 613. [3] D.M. Ceperley, B.J. Alder, *Physical Review Letters* **1980,** *45*, 566. [4] F. Nogueira, A. Castro, M. Marques, in *A Primer in Density Functional Theory*, edited by C. Fiolhais, F. Nogueira, and M.A.E. Marques Springer: Berlin, **2003,** 218. [5] A. Castro, M. Marques, A. Rubio, *The Journal of Chemical Physics* **2004,** *121*, 3425.

Keywords: nanocrystal, optical, density_functional_theory

MS.65.2

Acta Cryst. (2011) A**67,** C148

Chemical mapping at atomic-column resolution by STEM-EDX

C. H. Chen and M. W. Chu, *Center for Condensed Matter Sciences, National Taiwan University, Taipei, (Taiwan).* E-mail: chchen35@ntu.edu.tw

Chemical mapping at atomic-column resolution by energy-dispersive X-ray spectroscopy (EDX) in spherical aberration-corrected scanning transmission electron microscope (STEM) was demonstrated in InGaAs, achieving an element-specific resolving power for the dumbbell atomic columns, InGa and As, separated by 1.47 Å. The structural imaging and the chemical information in the two-dimensional map are directly correlated. Comparisons with the other existing mapping technique of STEM in conjunction with electron energy-loss spectroscopy were discussed from aspects of ionization interactions.

Keywords: scanning transmission electron microscopy, energy dispersive X-ray spectroscopy, chemical mapping

MS.65.3

Acta Cryst. (2011) A**67,** C148

Three-dimensional atomic imaging of crystalline nanoparticles

Sandra Van Aert,[a] Sara Bals,[a] Joost Batenburg,[b] Gustaaf Van Tendeloo,[a] [a]*Electron Microscopy for Materials Research, University of Antwerp, Antwerp (Belgium).* [b]*Centrum Wiskunde & Informatica, Amsterdam (The Netherlands).* E-mail: sandra.vanaert@ua.ac.be

Nanomaterials in general and nanoparticles in particular play a key role in modern technology and devices because of their unique physical and chemical properties. These properties are controlled by the exact three-dimensional morphology, structure and composition. Therefore, development of new techniques to determine the structure atom by atom in 3D would allow the properties of the resulting materials to be better understood, increasing the number of applications. The strong interaction of electrons with matter makes electron microscopy a promising technique to achieve atomic resolution in 3D. Electron tomography enables the recovery of the shape of nanoparticles in 3D from a series of projection images. The resolution that can be obtained in 3D using conventional tomography ranges on the nanometer scale although in 2D atomic resolution has been feasible for nearly four decades. In order to help close the gap between the sub-ångstrom resolution that can be reached in 2D and the coarser resolution in 3D, a new method has been devised combining high-angle annular dark field (HAADF) scanning transmission electron microscopy (STEM), model-based statistical parameter estimation theory and discrete tomography [1].

Discrete tomography [2] has been proposed as a promising technique for atomic resolution tomography in which prior knowledge about the discrete nature of atoms and their lattice structure is exploited. However, an important requirement is that one should be able to determine the number of atoms in each atomic column with great precision from a set of images taken under zone-axis orientations. We therefore employed a quantitative method to analyze HAADF STEM images [3]. It is generally known that such images show Z-contrast allowing one to visually distinguish between chemically different atomic column types. However, if the difference in atomic number of distinct atomic column types is small or if the signal-to-noise ratio is poor, direct interpretation of HAADF STEM images is inadequate. A performance measure which is sensitive to the chemical composition is the total intensity of scattered electrons. These intensities can now be quantified atomic column - by - atomic column using a parametric model describing the contrast of HAADF STEM images. Next, the unknown parameters of the model including the scattered intensities can be estimated by optimizing a criterion of goodness of fit. As such differences in (averaged) atomic number of only 3 can be identified [3]. The high chemical sensitivity is an advantage that could be further exploited to count the number of atoms in a column with an error of only 1 atom. In [1] this method has been proven to work on a metal nanocluster embedded into a stabilizing matrix with the same crystal structure. By counting the number of atoms from two different viewing directions, it has been shown that the three-dimensional structure can be reconstructed at atomic resolution. Recent results show that the method also works for more challenging structures including free-standing nanoclusters.

[1] S. Van Aert, K.J. Batenburg, M.D. Rossell, R. Erni, G. Van Tendeloo *Nature* **2011,** *470*, 374-377. [2] J.R. Jinschek et al. *Ultramicroscopy* **2008,** *108*, 589-604. [3] S. Van Aert, J. Verbeeck, R. Erni, S. Bals, M. Luysberg, D. Van Dyck, G. Van Tendeloo *Ultramicroscopy* **2009,** *109*, 1236-1244.

Keywords: 3D, electron microscopy, nanocrystal

MS.65.4

Acta Cryst. (2011) A**67,** C148-C149

Bonding and electronic structure of nanomaterials and interfaces with electron energy loss spectroscopy

G.A. Botton, M.C.Y. Chan, S. Hosseini Vajargah, F. Nan, D. Rossouw, S. Woo, G. Zhu, *Department of Materials Science and Engineering, Canadian Centre for Electron Microscopy, McMaster University, Hamilton, (Canada).* E-mail: gbotton@mcmaster.ca.

Electron microscopy is an invaluable tool to study the detailed structure of materials. Many of the analytical methods available in the transmission electron microscope, electron energy loss spectroscopy (EELS) in particular, provide detailed compositional and spectroscopic information with unprecedented spatial resolution. In today's modern instruments, energy resolution down to 0.1eV with an electron beams approaching 0.1nm size is possible.

Various examples of applications of electron microscopy will be