Microsymposia

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 [(PH3),2Cl] 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.

F. Nogueira, A. Castro, M. Marques, in A Primer in Density Functional Theory,
2004, 121, 3425.

Keywords: nanocrystal, optical, density functional theory

MS.65.2


Chemical mapping at atomic-column resolution by STEM-EDX
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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


Three-dimensional atomic imaging of crystalline nanoparticles
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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.

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Keywords: 3D, electron microscopy, nanocrystal

MS.65.4


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