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Coherent Scattering in the STEM

J. S. Wall

Biology Dept., Brookhaven National Laboratory, Upton, NY 11973

The central tenet of mass measurement in the STEM (Scanning Transmission Electron Microscope) is the proportionality between the mass of all atoms in the path of the beam and the large angle annular detector signal. Since this is a dark field signal, from a wave optic point of view one might expect a quadratic dependence on thickness (scattered amplitude squared). However, Fertig and Rose[1] showed that the quadratic term is only important if the atoms are close together or the angular collection range of the annular detector is small. They showed how to calculate the "coherence volume" for any detector geometry. This is an ellipsoid of revolution with the long axis along the beam direction. Atoms within that volume would have enhanced scattering. Simulation software allows us to examine this question under a number of conditions closer to experiment.

We have adapted the multi-slice software of Kirkland[2] to simulate STEM imaging of biological specimens. Currently we can simulate a $25nm^3$ volume containing up to 10^7 atoms specified by atomic number and floating point atomic coordinates. Structures can be from Biology (Protein Data Bank) or Materials Science and placed on an amorphous carbon film of any desired thickness or embed in amorphous ice or negative stain. The probe wavefront entering the top surface of the specimen is simulated wave optically (aperture angle, wavelength, defocus and spherical aberration), propagated through the specimen using the multi-slice method, and propagated to the detector plane wave optically. There the amplitude is squared and integrated over the angles subtended by the various detectors. The entire process must be repeated for each point in the scan raster, requiring roughly 1 sec per pixel for a moderately complicated specimen.

During the propagation through specimen, the beam intensity distribution (at the top of the specimen) is convoluted with the scattering cross sections of all atoms in each slice and this incoherent intensity is summed. This gives a point-by-point comparison to the simple approximation normally used for STEM calculations.

In the first simulation we have used two gold atoms on various thicknesses of amorphous carbon substrate. One gold atom is at the surface of the substrate and the second is above the first (unsupported) at distances of 0.2 to 9.8 nm and displaced laterally in increments 0f 0.025nm. Fig. 1 shows the total simulated integrated intensity for all pixels within a radius of 0.4nm for the small angle (SA=15-40mR) and large angle (LA=40-250mR) for BNL STEM1 (V_0=40 keV, C_s=0.6mm, aper=14mR, dF=60nm) as the second atom moves away from the first. Note that the value of 4 expected for the coherent case is not reached on either detector and the LA detector is much less affected than the SA detector.

A simulation of tobacco mosaic virus (TMV) on 4nm thick amorphous carbon provided another example of departure from ideal behavior. Fig. 2 shows the correlation of LA and SA signals compared to the convolution of atoms in the path of the beam with the beam intensity profile. Note the much better behavior of the Large Angle signal.

1. J.Fertig, H.Rose, (1977) Ultramicroscopy, **2**, 269-279.
2. E.J.Kirkland, "Advanced Computing in Electron Microscopy", Plenum (1998).
3. Supported by USDOE and NIH P41-EB-002181.

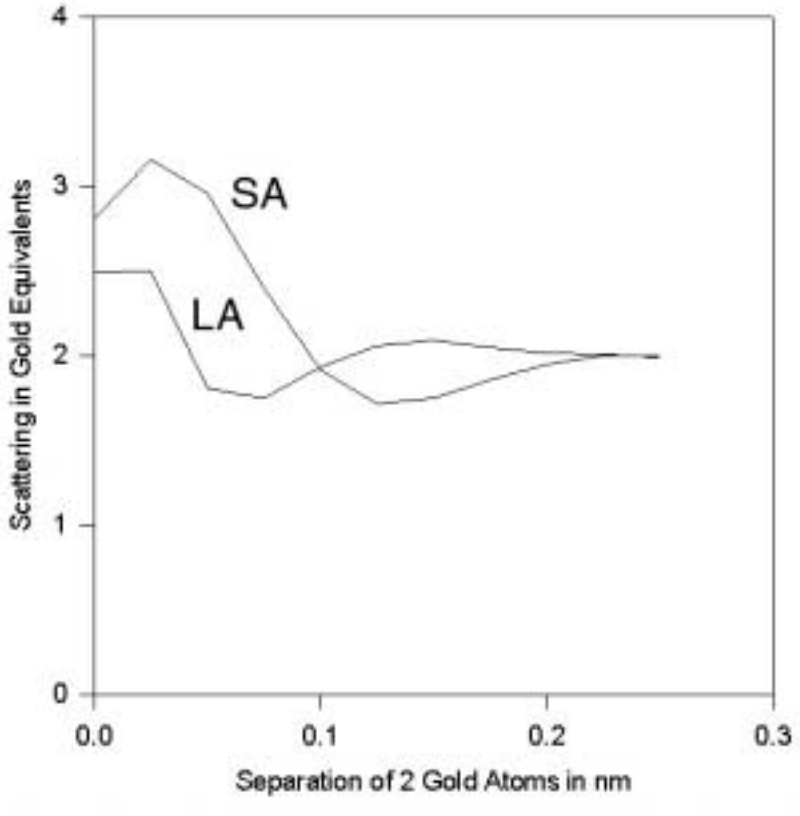
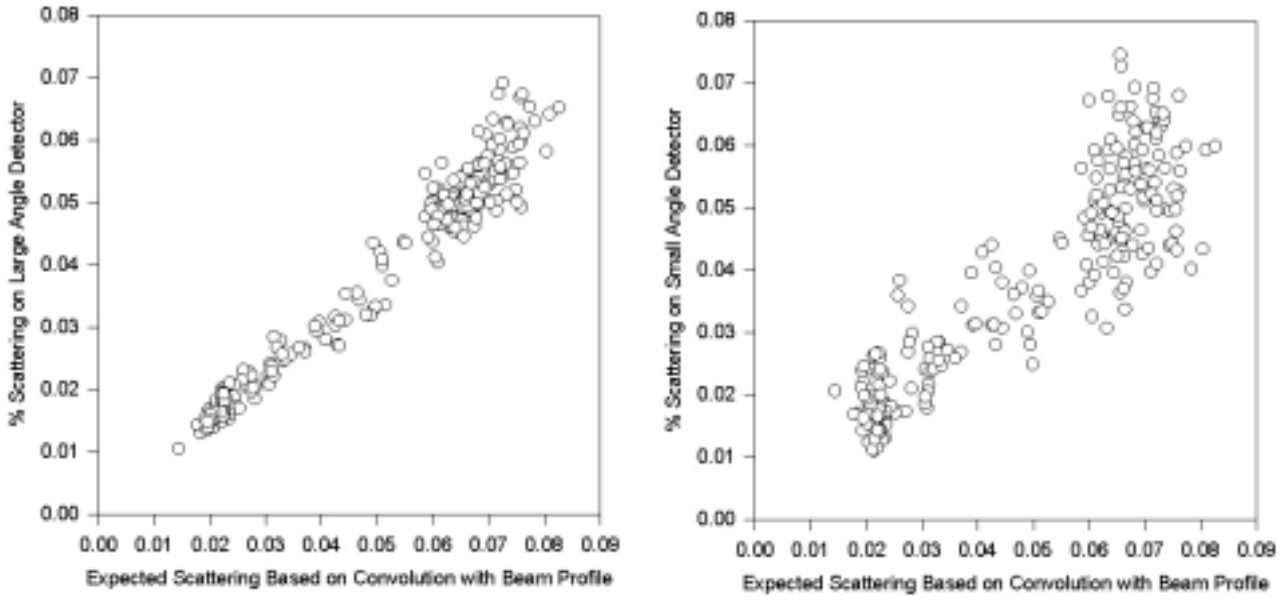


Figure 1. Effect of coherent scattering on the total signal from a pair of gold atoms as a function of their separation.

Figure 2. Correlation of Large Angle (LA) and Small Angle (SA) signals with the value expected form the convolution of the incident beam intensity distribution with all atoms in the path of the beam. Specimen was TMV on 4nm amorphous carbon.



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