Characterizing amorphous specimen by using the three particle structure factor

Vrana, S.[1], Peterlechner, M.[2] and Kohl, H.[1]

[1] Physikalisches Institut, WWU Münster, Germany, [2] Institut für Materialphysik, WWU Münster, Germany

The structure of amorphous specimens is traditionally determined using their pair distribution function or its Fourier transform, the two particle structure factor. However, this describes only the distribution of atomic distances. Information about bond angles is lost. This would be accessible if the triple correlation function $g_3(\vec{r_1},\vec{r_2},\vec{r_3})$ or its Fourier transform could be measured [1].

Structure factors can be directly obtained from experimental images [2]. For linear contrast transfer the structure factor $S^{(1)}(\vec{q}) = \sum_j exp\left(i\vec{q}\cdot\vec{r_j}\right)$ is closely related to the Fourier transform of the measured intensity. For thin phase objects the Fourier transform of the intensity can be written as $I(\vec{q}) = S^1(\vec{q})L(\vec{q})$ where L is the contrast transfer function. As a first approximation, we assumed ideal contrast transfer, hence $L(\vec{q}) = 1$. The two particle structure factor $S^{(2)}$ is then calculated as the square of its absolute value and finally the three particle structure factor is obtained as $S^{(3)}(\vec{q_1},\vec{q_2}) = S^{(1)}(\vec{q_1})S^{(1)}(\vec{q_2})S^{(1)}(-\vec{q_1}-\vec{q_2})$ where $\vec{q_1}$, $\vec{q_2}$ are spatial frequencies in two dimensions [2].

Since $S^{(3)}$ has 4 degrees of freedom, we had to find a representation that condenses the information into less dimensions. Assuming that amorphous matter is isotropic on a macroscopic scale we averaged over one spatial angle and considered $S^{(3)}$ as a function of now only three variables $q_1 = |\vec{q_1}|$, $q_2 = |\vec{q_2}|$ and $\phi = \angle(\vec{q_1},\vec{q_2})$. Then we reduced the number of degrees of freedom even more by taking $q_1 = q_2 =: q$ and varying only q and ϕ. This approach was inspired by [3].

We have calculated $S^{(3)}$ for reconstructed phase of amorphous carbon (figure 1. The reconstructed focus series was taken with an aberration corrected FEI Titan Themis G3 30 at 300keV). The obtained three particle structure factor (figure 2) looks very noisy and shows no structure except the sharp peak at $q \approx 0.4\ \text{Å}^{-1}$ and $\phi = 120°$ that was shown to stem from the gold nanocluster by performing the analysis only for that part of the image. The line profile for q between $0.1\ \text{Å}^{-1}$ and $0.25\ \text{Å}^{-1}$ (figure 3) shows a peak for 120°. This suggests the presence of some structures with bond angles of 120°.

We are now systematically searching for ways to reduce the noise.

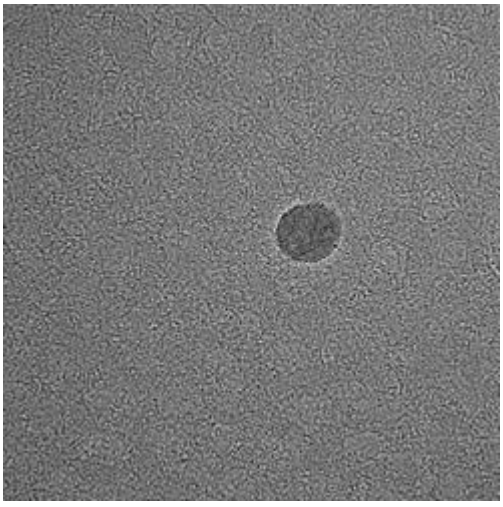

Figure 1:TEM image of amorphous carbon with a gold nanocluster on top of it.

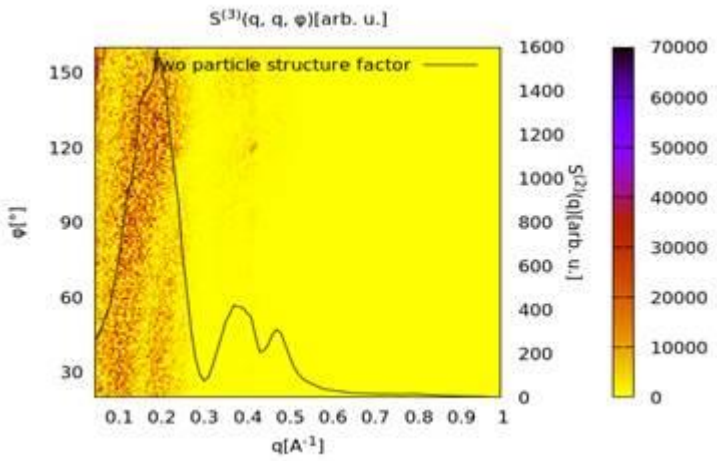

Figure 2: The two and three particle structure factor of amorphous carbon. The line shows the two particle structure factor mapped against the right axis. The color map shows the three particle structure factor.

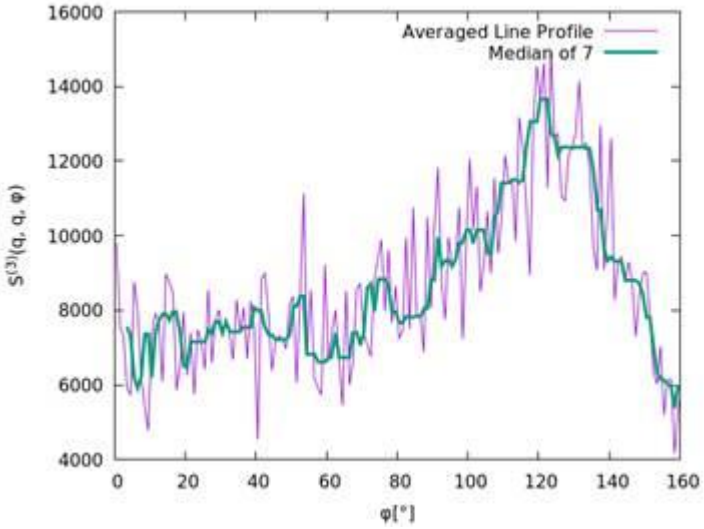

Figure 3: Averaged profile of the three particle structure factor of amorphous carbon for q between $0.1\,Å^{-1}$ and $0.25\,Å^{-1}$. The data was also filtered using a median filter to reduce the noise.

References

[1] J. Ziman, Models of disorder (Cambridge University Press, 1979).

[2] M. Hammel and H. Kohl, in Inst. phys. conf. ser. 93 (1988), pp. 209"210.

[3] J. M. Gibson et al., Phys. Rev. Lett. 105, 125504 (2010).