Physical Resolution Limits of Single Particle 3D Imaging with X-rays and Electrons

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Recent years have witnessed a boost of methods aiming at 3D imaging of single particles with nm resolution in life-science applications or sub Angstrom resolution in inorganic materials. New X-ray imaging methods such as lensless diffractive imaging combined with powerful phase reconstruction methods such as hybrid I-O or oversampling have proven their potentiality. Simultaneously we also witness a steady improvement in the brightness of the synchrotron sources or the development of Free Electron X-ray laser sources which allow to use extremely fast pulses and methods to combine the data of many identical particles or to orient them physically prior to the diffraction experiment. Combining these methods will continue to push the resolution even further.

Ultimately this evolution will be hampered by physical limits that cannot be surpassed such as radiation damage of the specimen and limits on the brightness and pulse duration etc.

For electron imaging the development of aberration correctors pushes high resolution electron microscopy into the domain where individual atoms can be resolved. Furthermore the brightness of the advanced electron sources exceeds that of the synchrotron. One reaches the situation where the information in real space i.e. in the image approaches the information in Fourier space i.e. the diffraction pattern. Then HREM or lensless diffractive methods will yield the same information.

Since the interaction between electrons and atoms is orders of magnitude larger as compared to X-rays but with less radiation damage, electron imaging methods have the potentiality for higher resolution. In HREM of inorganic materials the limit is posed by the total dose -Rose Criterium - which is limited by displacive radiation damage or by the combination of brightness and recording time. The figure of merit is the ratio between the elastic and inelastic cross section for the electron interaction.

The ultimate goal of all imaging methods is to visualise the ultimate building blocks. In case of electron imaging this are the constituting atoms. In case of X-ray imaging of life particles this may be larger but well known subunits. Once the building blocks can be resolved it is in principle possible to refine their positions quantitatively in the sense as done by classical electron diffraction techniques. Precise positions of the building blocks can then be used as input data for ab-initio calculations in order to understand the properties and eventually design new structures.

For HREM the ultimate challenge is to quantitatively determine atom positions in an amorphous structure with high precision. However, the information density, the number of data per unit area exceeds the physical capacity of the electron microscopic information channel. The only way out is to explore also the third dimension, i.e. electron tomography with atomic resolution. For amorphous materials which are subject to radiation damage it may require a lower voltage and the use of a Cs and Cc corrector. Since HREM is a parallel imaging technique it is suited for tomographic reconstruction. However we have doubts about the practical usability of optical sectioning by HAADF STEM.