

## Molecular Foundry – NCEM User’s Meeting 2008

### **Abstract Title:**

Resolution in electron microscopy - Physical limitations and a signal-to-noise ratio based alternative

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### **Short Description:** (*approximately 100 words*)

Thanks to new developments in the field of aberration corrected electron optics, materials science studies can nowadays be performed at atomic resolution. However, despite of these advantages, one should realize that the resolution is no longer limited by the electron microscope itself. Instead, in terms of classical resolution criteria, the electrostatic potential of the atoms poses fundamental limitations. Moreover, since experimental observations are never noise-free, the quality of an electron microscopy image is also limited by the signal-to-noise ratio. In order to quantify the combination of different limiting factors, the obvious performance criterion is the precision with which atom positions can be estimated.

### **Talk Summary:**

In this talk it will be shown that for the new generation of electron microscopes, the resolution is no longer limited by the instrument itself. Indeed, in the image formation process, several band-limiting factors cause a loss in resolution. Therefore, the resolution is not only determined by the width of the point-spread function of the electron microscope. The “width” of the electrostatic potential of the atoms, the effect of thermal vibrations of the atoms, the environment, and the detection have to be taken into account as well. As a result of these extensions, it should be concluded that the intrinsic “width” of the atoms themselves ultimately limits the classical resolution. Therefore, it is unrealistic to expect, for instance, that one could resolve amorphous structures.

Moreover, since electron microscopy images are never noise-free, the resolution depends fundamentally on the signal-to-noise ratio. In that sense, resolution should obviously be reconsidered in the framework of statistical parameter estimation theory. In order to extract quantitative structure information use is made of model to describe the electron-object interaction, the transfer in the microscope, as well as the image detection. This model contains unknown parameters characterizing the structure of the object, the positions of the atoms in particular. These parameters are estimated by fitting the model to the experimentally obtained images by optimising a criterion of goodness of fit. It can then be shown that the precision with which atom positions can be estimated depends both on the classical Raleigh-like resolution  $\rho$  and the available dose of imaging electrons  $N$ , according to the formula  $s \sim \rho / \sqrt{N}$ , with  $s$  the so-called Cramér-Rao Lower Bound on the standard deviation. Notice that if  $N$  is large, the precision can be orders of magnitude better than the resolution  $\rho$ .

Application of statistical parameter estimation theory to experiments shows that atomic column positions and interatomic distances can be determined with a precision in the picometer range. These results not only apply to well-resolved structures but also to projected distances beyond the information limit of the microscope which can be determined with picometer range precision.