# The Influence of Contrast Delocalization on TEM Image Interpretation

Anna Altberg, Yaron Kauffman and Wayne D. Kaplan
Department of Materials Engineering, Technion, Haifa, Israel

## The Problem

Determining the real size of a nano-particle can be a tricky business. How much can we base our determination solely on a TEM image? What is the influence of contrast delocalization on TEM image interpretation?

To answer these questions, two simulations of MgO [001] nano-particles were done. Figure 1 displays a simulated image for Scherzer defocus, for a standard TEM. Figure 2 displays a simulated image for negative CS conditions for an aberration-corrected TEM. Figure 3 displays the simulated phase of the exit wave function for the same particle. Obviously contrast delocalization can't be ignored, even for the simple measurement of particle size at the nanometer length-scale. So, the following questions are raised:

How much delocalization, and where is the delocalization?

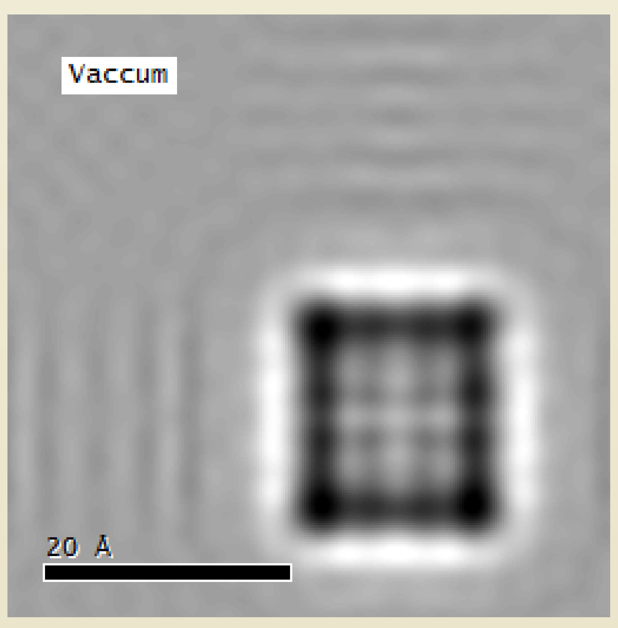


**Figure 1:** MgO [001] for Schertzer conditions:

Δf=-54nm, Cs=1.2mm

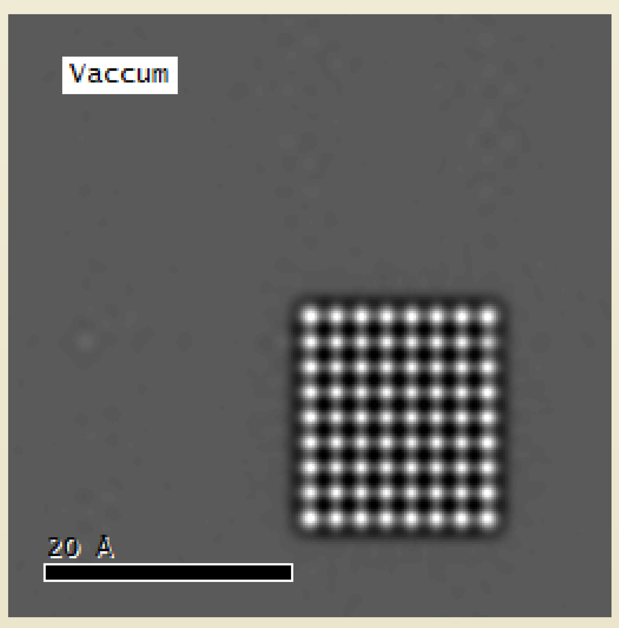


**Figure 2:** MgO [001] for negative Cs conditions:

Δf=4nm, Cs=-0.007mm

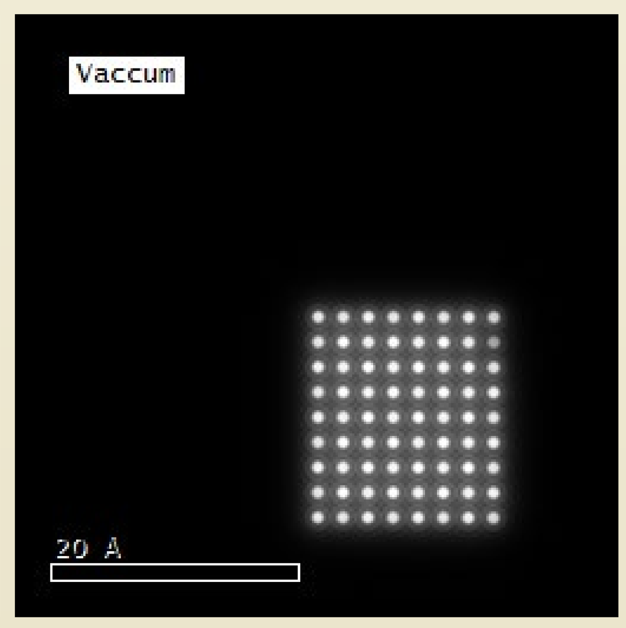


**Figure 3:** Phase of the exit wave function for MgO [001]

## Introduction

Imperfections in TEM electromagnetic lenses limit the resolution of the microscope. One of the main defects that limits performance is the spherical aberration of the objective lens. Spherical aberration occurs when the lens field behaves differently for off-axis beams. As a result, a point object is imaged as a disk of finite size, which limits our ability to magnify detail because the detail is degraded by the image process.

The objective lens aberration function is : $\chi(g)=\frac{1}{2}\Delta f\lambda g^2+\frac{1}{4}C_S\lambda^3 g^3$, where $\Delta f$ is defocus, $C_S$ is the spherical aberration coefficient, $\lambda$ is the wave length and g is the spatial frequency.

Delocalization is the term for phenomenon in which image details are displaced from their true locations in the image plane [1]. The maximum delocalization distance in the image plane R($\vec{g}$) can be calculated from: $R(\vec{g}) = max\left|\frac{\partial\chi}{\partial\vec{g}}\right| = \max|\Delta f\lambda\vec{g}+\mathrm{Cs}\lambda^3\vec{g}^3|$.

If the defocus ($\Delta f$) and Cs were zero, than there would be no contrast delocalization and no spherical aberration, but at the same time, the information we would get from the image would be limited (poor contrast). Therefore, all HRTEM images will contain delocalization to some degree.

The delocalization effect is especially severe for a microscope equipped with a field emission gun (FEG) due to their high coherence which transfers delocalized spatial frequencies [1].

## Where and how much delocalization?

One of the methods to measure the size of a particle, **free of delocalization**, is to retrieve the complex electron wave function (amplitude and phase) at the exit surface of the specimen using holographic techniques [2]. In this method, the exit wave function is retrieved using a defocus series of experimental micrographs, the measured contrast transfer function of the microscope, and a numerical procedure (see figure 4) [3].

Figures 5-7 experimentally demonstrate the delocalization phenomena. Figure 5 is a TEM micrograph of an MgO particle acquired using a FEG source at 300kV, at Δf=-4nm and with $C_S$=1.2mm. Figure 6 is an image of the same particle acquired at the same conditions except $C_S$=-0.005mm, and figure 7 is the amplitude of the reconstructed exit wave function (acquired at $C_S$=-0.005nm). An intensity line-profile was determined for the same region all 3 micrographs. Since the amplitude of the exit wave displays the particle without residual delocalization, the real particle size can be measured based on this micrograph. As expected, the micrograph of the particle acquired with Cs-corrected TEM, displays a small degree of delocalization, while the micrograph acquired with a regular TEM displays considerable delocalization, which can lead to significant errors (>7%) in the measurement of particle size at the nanometer length-scale.

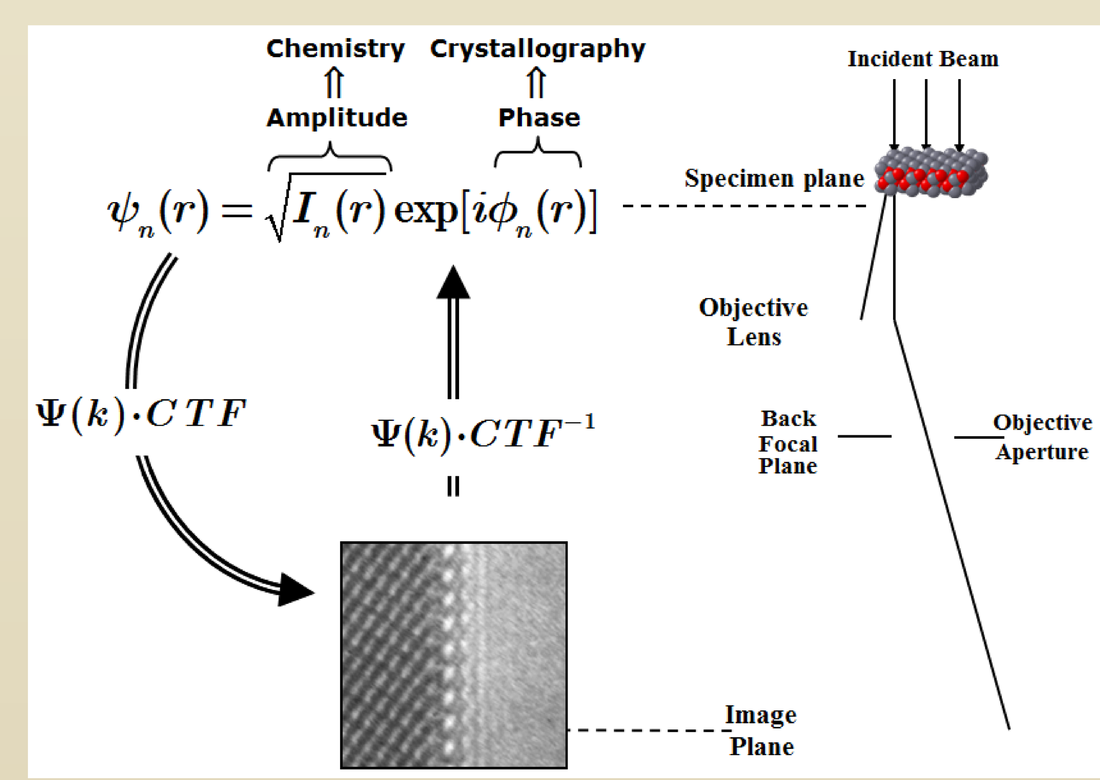


**Figure 4:** A schematic representation of the concept of exit wave reconstruction [4]

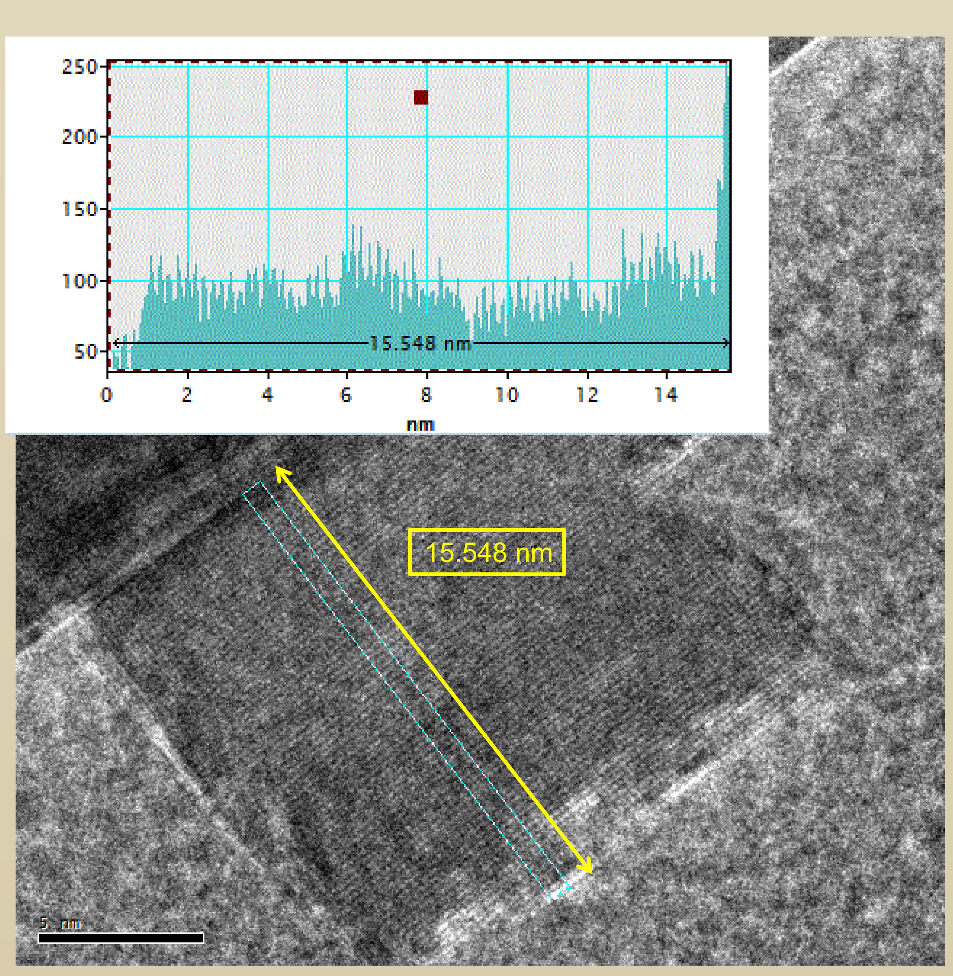


**Figure 5:** MgO [001], 300kV, Δf=-4nm, Cs=1.2mm

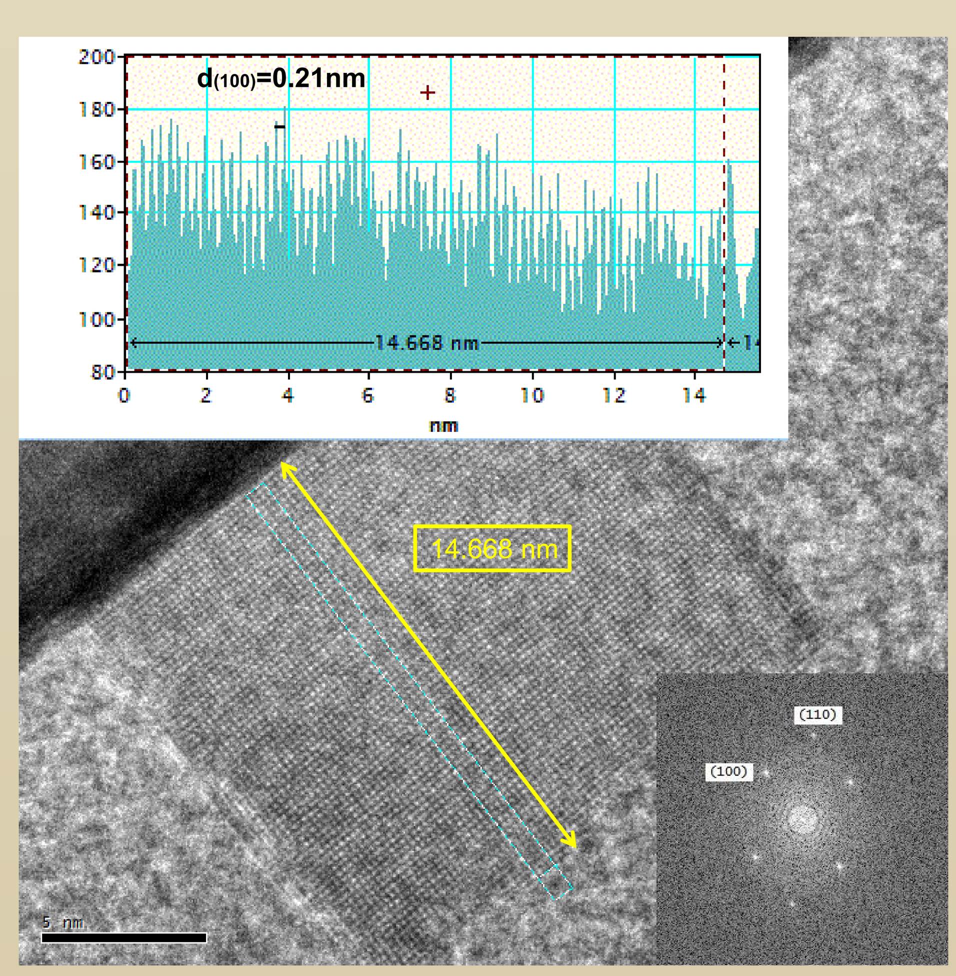


**Figure 6:** MgO [001], 300kV, Δf=-4nm, Cs=-0.005mm

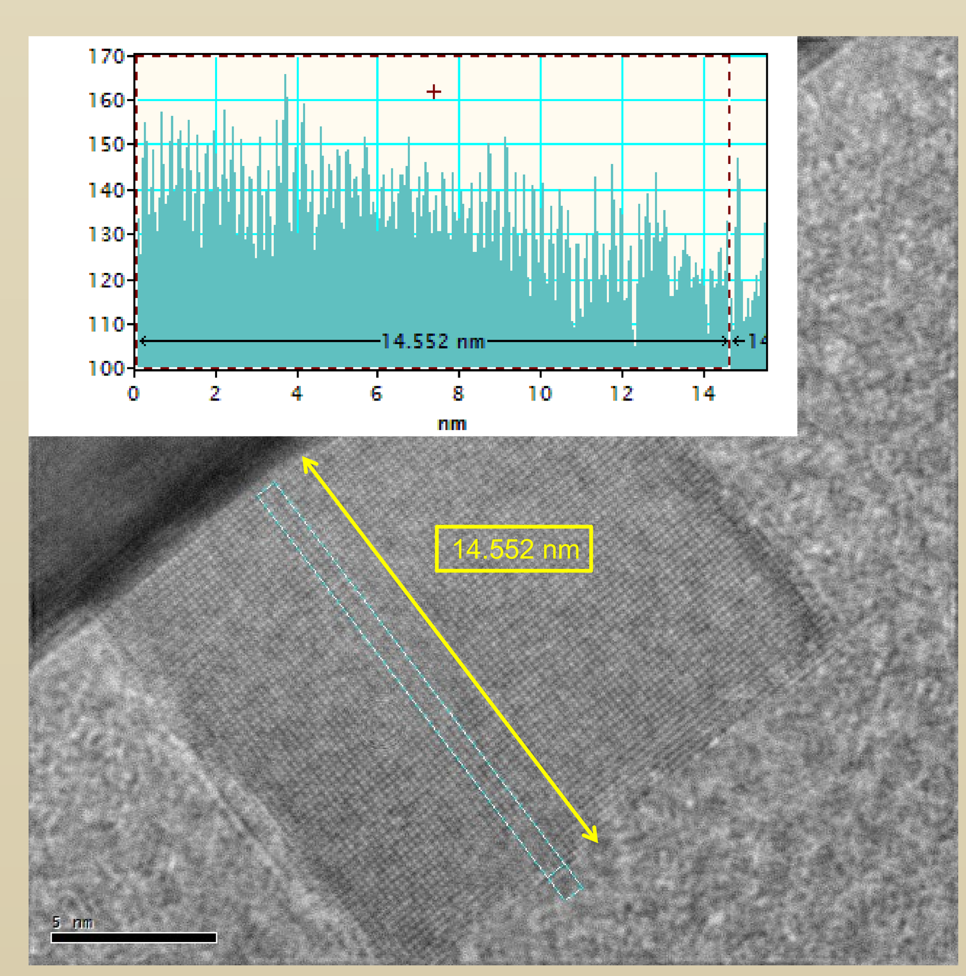


**Figure 7:** Amplitude of the exit wave function from MgO [001].

Another option to asses the delocalization in the image is to calculate the maximum delocalization distance in the image plane $R(\vec{g})$ at a specific (experimentally determined) value of focus. For example, for an image acquired at 300kV with an information limit of 0.08nm, $\Delta f$ =- 4nm and Cs = -0.005nm: $R(\vec{g})=0.18\mathrm{nm}$ , while for an image acquired at the same conditions but with Cs = 1.2mm, $R(\vec{g})=17.82\mathrm{nm}$. For a particle 10nm in diameter, this would correspond to a 4% error in measurement of the particle diameter, versus and error of more than 150% *!!!*

**To conclude**, this work demonstrates the importance of contrast delocalization on the determination of particle size at the nanometer length-scale.

## References

*[1] M.T. Otten and W.M.J. Coene, High-Resolution Imaging on a Field Emissin TEM, Ultramicrosopy, 48[1-2]: 77-91,1993*
*[2] H. Lichte, Optimum Focus for Taking Electron Holograms, Ultramicroscopy, 38[1]: 13-22, 1991*
*[3] A. Thust, W.M.J. Coene, M. Op de Beek and D. Van Dyck, Focal-Series Reconstruction in Hrtem: Simulaton Studies on Non-Periodic Objects, Ultramicroscopy, 64[1-4]: 211-230, 1996*
*[4] Y. Kauffmann, Ph.D. Thesis, Department of Materials Engineering, Technion, 2006*