Quantification and Segmentation of Electron Tomography Data – Exemplified at $ErSi_2$ Nanocrystals in SiC

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Background & Motivation

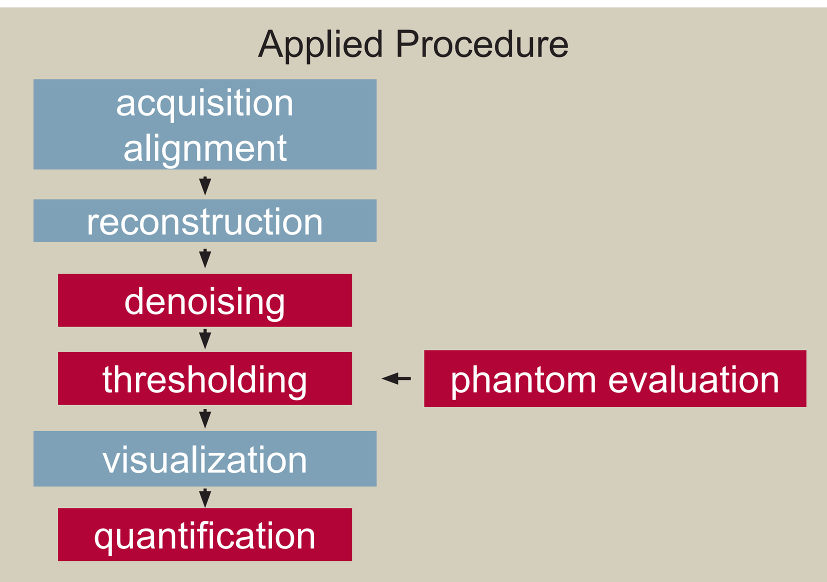
SiC is a promising material for optics, opto-electronic and spintronic applications [1, 2]. Doping with consequent controlled diffusion (e.g. metals for spintronics) should be involved for the most interesting applications. High concentration of structural defects, vacancies and interstitial atoms, generated by high energy implantation, dramatically complicate diffusion processes and an evolution of dopant species. In order to understand the diffusion and growth mechanisms of dopants in SiC matrix we studied the model system: 4H-SiC implanted with Er. Erbium was selected because of its high atomic number and thus high contrast in HAADF-STEM. Z-contrast electron tomography was applied to reveal structural features of the nanoparticles [4, 5]. For application related questions the result of the growth process is important and has to be quantified as a next step by characterization of the geometrical properties. As the segmentation is most crucial for reliable quantification of tomography data, it has to be performed in a best objective manner.

Therefore, in this work the SIRT reconstruction algorithm is first applied on a phantom from which the appropriate threshold is derived. This threshold is applied during the segmentation of the experimental data of which the quantification is carried out. The aim is to characterize the 3D shape of the $ErSi_2$ particles by their volume and aspect ratio.

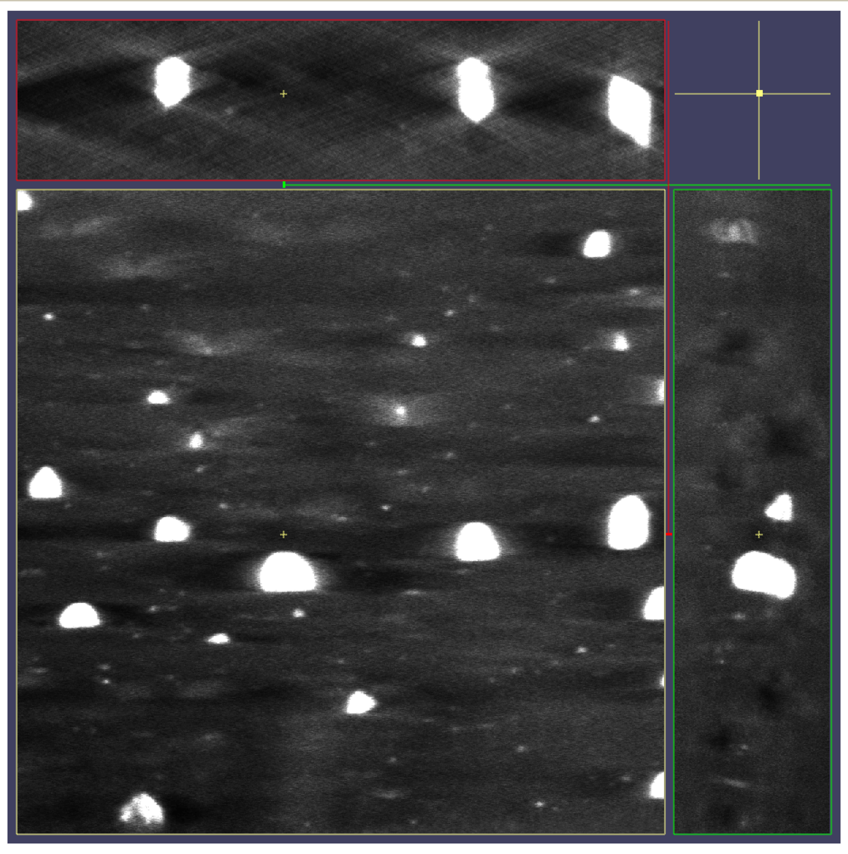
Experiment, Acquisition & Tools

Specimen creation: hexagonal 4H-SiC, implantation of Er (1016 cm^{-2}, 700°C) and annealing (3 min, 1600°C) [2, 3]
TEM investigation: FEI Titan 80-300, single-axis ±75° (Saxton scheme) HAADF-STEM tomography
Data evaluation: FEI Inspect3D®, IMOD [6], MATLAB® Wavelet Toolbox, Xmipp [7], Avizo®

(a)

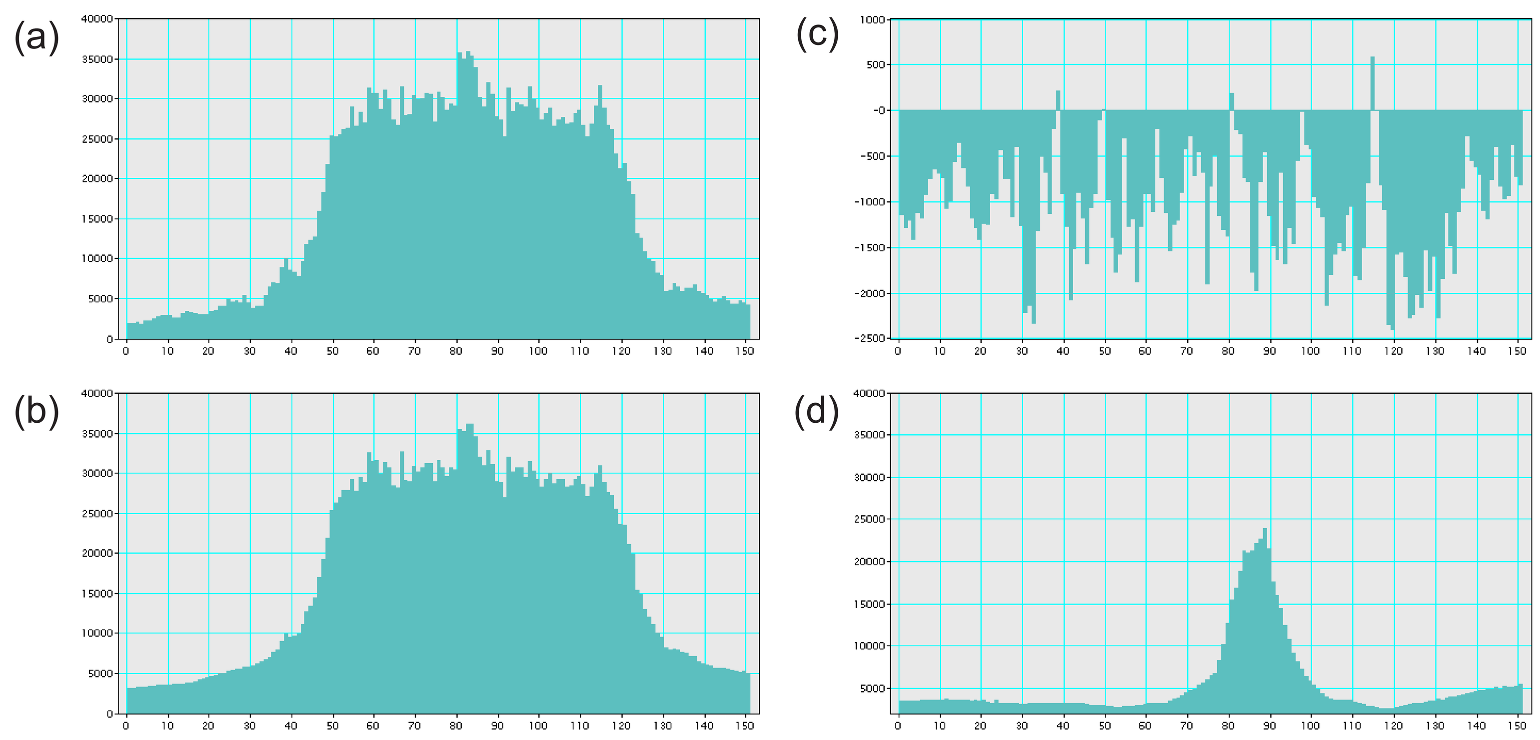


(b)



Overview: (a) sketch of applied procedure (blue: tomography procedure, red: issues of this work), (b) directional views in IMOD [6] of 3D tomogram of $ErSi_2$ nanocrystals

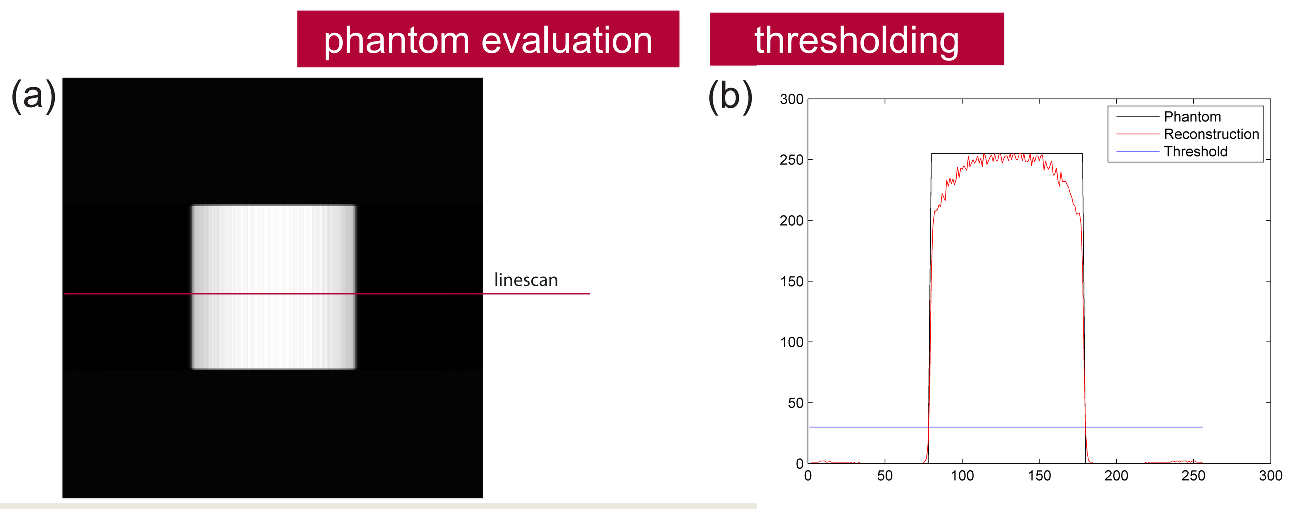
denoising



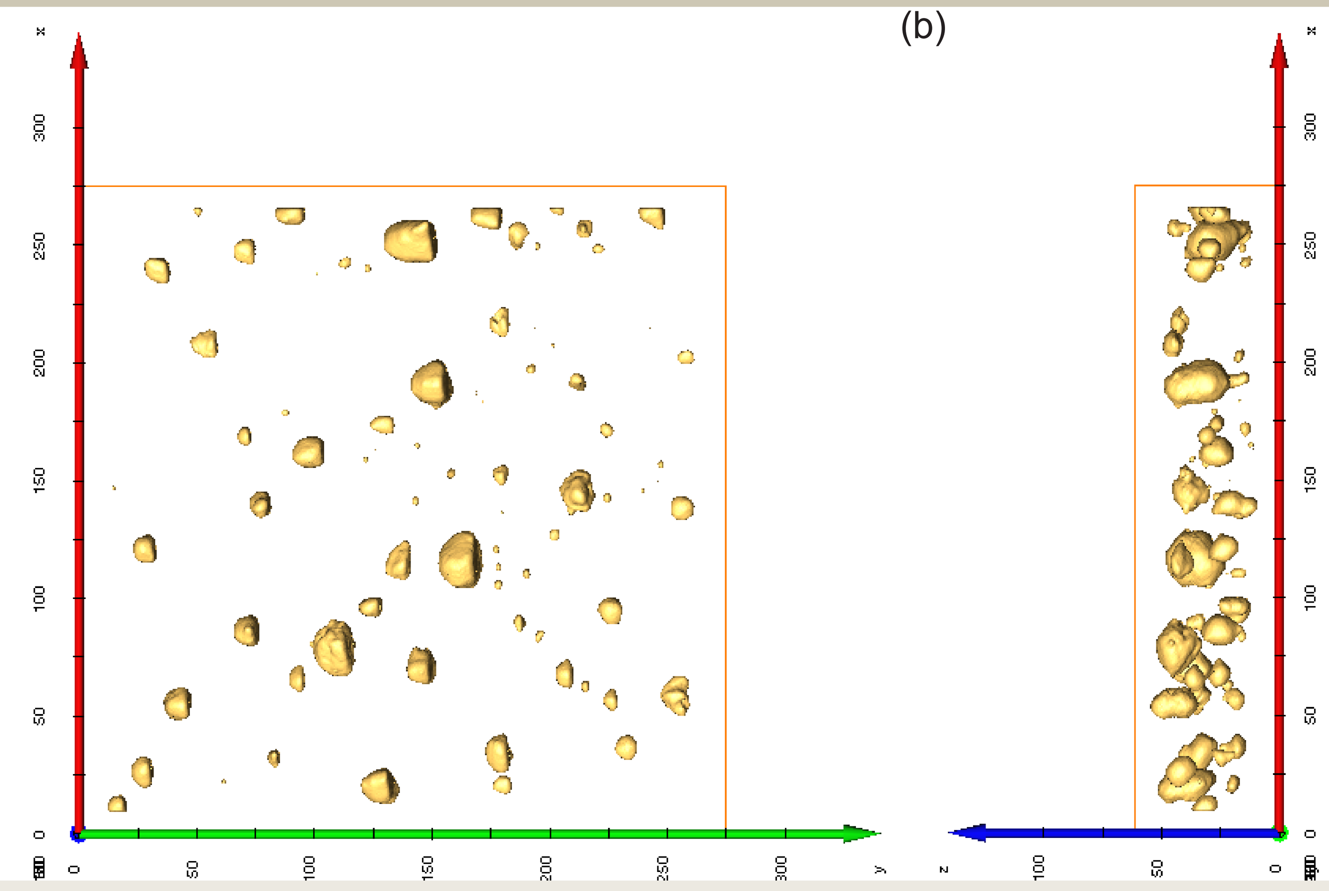
Effect of wavelet denoising on 3D tomogram in cross-sectional views: (a) original, (b) denoised, (c) difference of original and denoised intensity, and (d) a different, smaller particle, which was denoised

phantom evaluation

thresholding

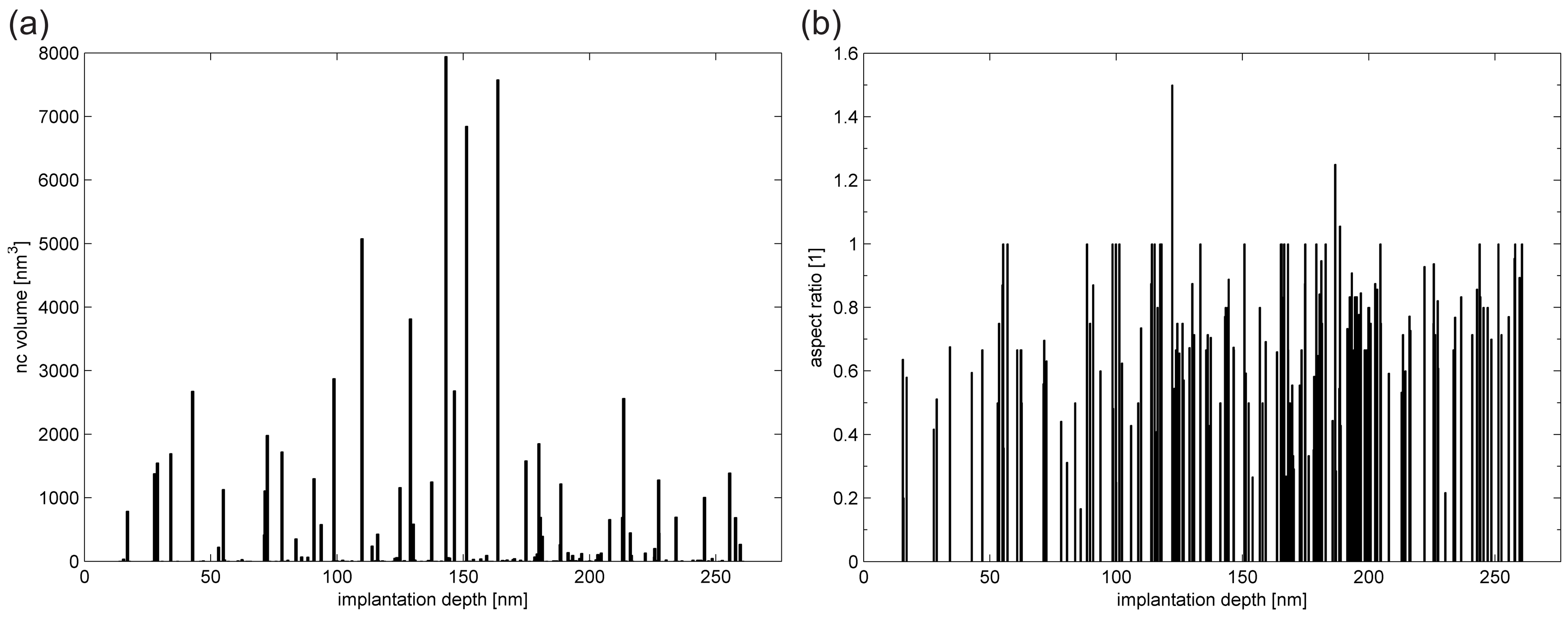


Evaluation of the influence of the reconstruction algorithm on the particle shape: (a) cubic box-phantom created by XMIPP [7] and reconstructed by SIRT (Inspect3D®), (b) linescan across the box and for comparison the linescan of the phantom is overlapped and the estimation of the threshold is pointed out



Nanoparticles visualized by surface rendering with the obtained threshold from the phantom: (a) xy-plane, (b) xz-plane (scale is nanometer)

quantification



Quantification of the nanocrystals by Avizo® (XQuant) along (relative) implantation depth: (a) volume distribution, and (b) aspect ratio = ylength/Max(xlength,zlength), revealing most particles are not enclosed in a cube, but a flat cuboid

(a) Volume

Min [nm^3]	0.2
Max [nm^3]	7943.3
Mean [nm^3]	326.1
StdDev [nm^3]	1032.3
Sum [nm^3]	76635.7
TotVol [nm^3]	4.7e+06
Fraction [%]	1.6%

(b) Aspect Ratio

	unweighted	weighted (V>500nm^3)
Mean [1]	0.49	0.70
Median [1]	0.59	0.68
StdDev [1]	0.38	0.16

Results of the quantification: (a) volume distribution, and (b) aspect ratio; the unweighted aspect ratio, as depicted in the right plot above, and the weighted to enhance the most significant volumes, as depicted in the left plot above, revealing an aspect ratio of about 0.7

Summary

With the application of wavelet denoising the noisy tomogram is enhanced as a primary step for further visualization processing. With artificially generated phantoms an estimate for the exact segmentation threshold is selected. After binarization the particles are visualized and automatically quantified. The size-distribution shows that at a certain implantation depth the nanoparticles have grown biggest, but over almost the entire range to a smaller size. The aspect ratio reveals that most particles are flat-grown or hill-shaped. In order to judge the obtained quantification results the influence of the form and the size of the used phantom has to be evaluated as a next step.

References

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