Calculation of optimum contrast for HRTEM images of SiC and graphene at medium and lower voltages

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Aberration-corrected transmission electron microscopy offers the possibility to utilize the coefficient of spherical aberration in addition to defocus as free parameter for optimizing resolution and contrast. NCSI (negative C_S imaging) conditions (negative C_S and over-focus) give optimum contrast when imaging weak phase objects at medium voltages [1, 2]. However, the values change for thick specimens, where the contribution of amplitude contrast dominates [2, 3]. Interestingly, at 80kV experiments, for one-atom-layer materials it has been reported that dark atom contrast (positive C_S and under-focus) seems to be preferable [4, 5].

In this work we evaluate optimum contrast conditions (C_S and defocus) by HRTEM image calculations for different sample thicknesses. SiC in [11-20] projection has been chosen as an example for a two component material, in which the light C atom columns are placed close to the heavier Si atom columns (dumbbell distance is 0.109nm). Optimum contrast for practical relevant thicknesses from 10-70A are evaluated at 300kV and 80kV. Graphene has been chosen as a one atom thick material; optimum contrast only depends on the microscope parameters.

Exit wave calculations were performed using the software Musli based on multislice approach [6]. Microscope parameters were then applied under optimizing for highest resolution both, defocus and C_S; C_S was varied in the range of +20 to -20µm. For the determination of optimum contrast of Si and C atom columns in SiC dumbbells, a restriction was added regarding the shape and separation of the atom columns. By variation of these parameters, optimum contrast has been calculated following the formula $C=(I_a-I_b)/I_b$, where I_a is the atom column intensity and I_b is the intensity of the background. The atom column intensity was determined from the average intensity of nine pixels around the atom column center; I_b was determined from the histogram, where the largest number of pixels was addressed to the same grey scale.

In Fig.1(a) HRTEM images of [11-20] 4H-SiC are shown for different sample thicknesses for optimized C_S and defocus conditions at 300kV. It was found that Si and C atom columns show the same behavior: negative C_S is preferred for optimum contrast in the thickness range studied, however combined with positive defocus only up to a sample thickness of about 4nm (see Fig. 1(b) and (c)). For the case of 80kV, the optimum compromise between contrast and resolution was obtained for positive C_S for thicknesses larger than 3nm.

[1] C.L.Jia, M.Lentzen, K.Urban. Microsc.Microanal.10(2004)174-184
[2] M.Lentzen. Ultramicroscopy 99 (2004) 211-220
[3] Z. Zhang and U. Kaiser Ultramicroscopy 2009, DOI.10.1016.ultramic.2009.04.004
[4] A. Chuvilin, J. Meyer, G. Algara-Siller, U. Kaiser 2009 submitted
[5] J. C. Meyer, A. Chuvilin, G. Algara-Siller, J. Biskupek, U. Kaiser, Nanoletter, 2009 DOI:10.1021/nl9011497
[6] A. Chuvilin and U. Kaiser Ultramicroscopy 104 (1) (2005) 73-82

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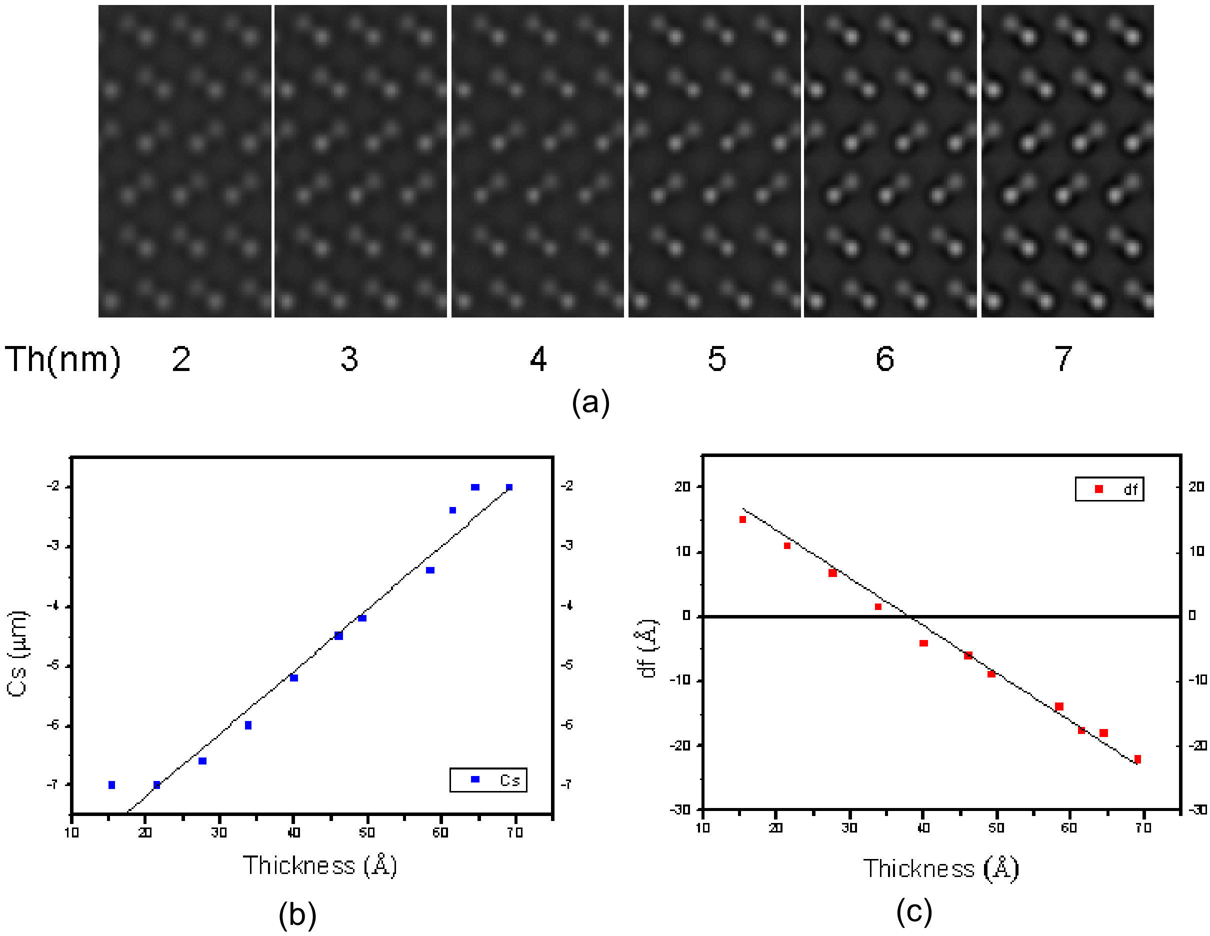

Figure. (a) Image calculations (300kV) for [11-20] 4H-SiC at different thicknesses for optimized C_S/defocus conditions, showing bright atom contrast always. (b) and (c) present the corresponding C_S and defocus conditions, respectively. It is seen that negative C_S and positive defocus (NCSI conditions) are preferred at small thickness, while negative C_S and negative defocus are preferred at larger thicknesses.

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