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Atomic-resolution imaging of lattice imperfections in semiconductors by conjoined aberration-corrected HRTEM and exit-plane wavefunction retrieval

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Keywords (user supplied):	spherical aberration correction, exit-plane wavefunction reconstruction, dislocation core structure



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**ATOMIC-RESOLUTION IMAGING OF LATTICE IM-
PERFECTIONS IN SEMICONDUCTORS BY CON-
JOINED ABERRATION-CORRECTED HRTEM AND
EXIT-PLANE WAVEFUNCTION RETRIEVAL**

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ABSTRACT

With the amelioration of the instrumental information limit and the simultaneous minimization of image delocalization, high-resolution transmission electron microscopy is presently enjoying exceeding popularity with respect to the atomic-scale imaging of lattice imperfections in solid state materials. In the present study the benefits derived from the deliberated combination of spherical aberration corrected imaging together with the numerical retrieval of the exit-plane wavefunction from a focal series of micrographs are illustrated by highlighting their combined use for the atomic-scale characterization of lattice defects frequently observed in common semiconductor materials. For these purposes, experimental analyses will review the core structure of Lomer dislocations at $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ -heterointerfaces and focus on atomic lattice displacements associated with extrinsic stacking faults in GaAs, as well as on the core structure of chromium implantation induced Frank partial dislocations in GaN at directly interpretable contrast features. Supplementary, practical advantages of the retrieval of the exit-plane wavefunction for the subsequent numerical elimination of residual lens aberrations are demonstrated.

Key words: High-resolution transmission electron microscopy, spherical aberration correction, exit-plane wavefunction reconstruction, lattice defects, disloca-

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tion core structure, stacking faults, semiconductors,
GaAs, GaN

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1. INTRODUCTION

Over the past fifty years, transmission electron microscopy has become the technique of choice whenever structural properties associated with lattice imperfections in solid state materials have been investigated experimentally. Even though enormous progress has been made in the characterization of dislocations, stacking faults and internal boundaries in these common semiconductor materials, there is still much to learn about the precise atomic configuration in the vicinity of these structural imperfections. Above and beyond purely scientific curiosity this task is also of technological interest as further improvements in applied semiconductor research stand in need of an amended understanding of the interaction between structural and electronic properties with advancing miniaturization [i, ii]. To put it another way, the detailed evaluation of electronic features induced by lattice imperfections and the elucidation of the atomic structure of these imperfections are interdependent [iii, iv].

Recently of particular interest with high-resolution transmission electron microscopy is (i) the pursuit of sub-Ångström resolution at medium acceleration voltages [v, vi, vii] in close communion with (ii) the straightforward interpretability of micrographs [viii, ix, x] characterized by (iii) a rather low image delocalization in the vicinity of lattice imperfections [xi, xii]. Two sophisticated techniques to accomplish all three of these objectives simultaneously, not within reach during operation of "traditional" medium voltage instruments equipped with field emission gun emitters, have attracted much interest in recent years.

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5 On the one hand, double hexapole corrector elements
6 enabling a compensation of detrimental lens aberrations
7 are practically usable these days [xiii, xiv]. As a re-
8 sult, the aberration coefficient C_s emerges as an addi-
9 tional parameter for extending the point resolution at
10 phase contrast imaging conditions to the information
11 limit together with the simultaneous maximization of
12 phase contrast and the minimization of contrast delo-
13 calization [xv]. Moreover, when employing a negative C_s
14 value combined with a certain overfocus setting $Z_{\text{opt}} > 0$,
15 not only a substantial contrast improvement is achieved
16 but low-nuclear charge elements can also be imaged at
17 bright atom contrast features in the vicinity of high-
18 nuclear charge atoms [viii, ix].

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30 On the other hand, numerical techniques enable the res-
31 toration of the phase $\Phi(\mathbf{r})$ and the amplitude $A(\mathbf{r})$ of
32 the exit-plane wavefunction from a focal series [xvi,
33 xvii, xviii] or an illumination tilt direction series
34 [xix, xx] of experimental micrographs. By this means,
35 all spatial information up to (focal series) or even
36 beyond (tilt direction series) the axial information
37 limit of the instrument can be retrieved, also allowing
38 for a subsequent elimination of residual lens aberra-
39 tions still present in aberration corrected microscopy
40 [xxi, xxii, xxiii, xxiv].

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49 The objective of the present contribution is to demon-
50 strate the benefits accruing from the deliberated com-
51 bination of both of these state-of-the-art techniques
52 for the atomic scale imaging of structural imperfec-
53 tions in semiconductor materials. Special emphasize
54 will be put on conceptual vantages for the characteri-
55 zation of lattice defects at atomic resolution and for
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the quantification of atomic column positions in the vicinity of lattice imperfections in semiconductor materials.

2. METHODOLOGICAL BACKGROUND: NEGATIVE SPHERICAL-ABERRATION CORRECTED IMAGING IN TANDEM WITH THE NUMERICAL RETRIEVAL OF THE EXIT-PLANE WAVEFUNCTION

In aberration-corrected microscopy a high amount of negative phase contrast may be obtained simultaneously with a widely minimized image delocalization, when setting the constant of spherical aberration to an optimized value [ix, xv]

$$C_s = -64/27 \lambda^{-3} g_{\max}^{-4} \quad (1)$$

and choosing an overfocus setting of the objective lens

$$Z_{\text{opt}} = 16/9 \lambda^{-1} g_{\max}^{-2} \quad (2)$$

with λ and $1/g_{\max}$ denoting the electron wavelength and information limit of the instrument, respectively. A corresponding set-up of the instrument yields direct interpretable high-resolution micrographs accompanied by a residual image delocalization of

$$R = 16/27 g_{\max}^{-1} \quad (3)$$

Using an aberration corrected CM-200 FEG ST instrument, the aforementioned parameters amount to $Z_{\text{opt}} = 11.6$ nm, $C_s = -40.6$ μm and $R = 80$ pm when putting to use an electron wavelength of $\lambda = 2.51$ pm and an information limit of $1/g_{\max} = 125$ pm with the latter value measured from a Young's fringe analysis of images taken with the microscope utilized in this study [xv].

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5 The associated partially coherent phase contrast trans-
6 fer function, displayed in Figure 1, extends up to $1/g_{\max}$
7 and is characterized by a broad pass-band with a phase
8 deviation close to $\pi/2$. Simplifying the imaging process
9 to linear theory, a weak phase object is then imaged
10 under bright atom contrast conditions [xxv] and a sub-
11 stantial contrast improvement is achieved since the
12 linear phase contrast and the nonlinear dark field sig-
13 nal add rather than subtract as is usual when applying
14 "traditional" high-resolution imaging modes [xxvi]. In
15 the strict sense Eqns. (1) to (3) base upon a first or-
16 der expansion of the aberration function, thus neglect-
17 ing any detrimental impact of higher order lens aberrations.
18 As the hexapole corrector of the CM-200 FEG ST
19 allows for a sufficient correction of aberrations up to
20 the third order [xxvii] and higher order aberrations
21 will become relevant not until $1/g_{\max}$ becomes smaller
22 than 100 pm [xxviii, xxix], these aberrations do not
23 need to be considered for the instrument under consid-
24 eration.
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40 The numerical retrieval of the exit-plane wavefunction
41 $\Psi(\mathbf{r})$ from a focal series of micrographs provides auxil-
42 iary improvements as it is basically free from nonlin-
43 ear imaging artifacts and the impact of the low fre-
44 quency gap in information transfer is considerably re-
45 duced by the combination of many images taken at dif-
46 ferent foci. As improvements of the instrumental reso-
47 lution limit still gather pace, this aspect is of spe-
48 cial importance when imaging common semiconductors at
49 atomic resolution since the structural information is
50 predominantly carried by the low-frequency {111} re-
51 flections. Furthermore, by extracting information from
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5 about $N = 20 \dots 30$ images, the signal-to-noise ratio
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7 at high spatial frequencies can be substantially in-
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9 creased. Even the application of small C_s values, which
10 is a prerequisite to obtain phase contrast, induces a
11 parasitic delocalization whereas $\Psi(\mathbf{r})$ is ideally free
12 from any delocalization induced artifacts.
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16 Moreover, the availability of $\Psi(\mathbf{r})$ allows for the nu-
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18 merical *a posteriori* measurement of residual lens aber-
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20 rations. This aspect is of special practical importance
21 as experience shows that not all aberrations of the mi-
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23 croscope are sufficiently constant over the period of
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25 operation or cannot be determined before the experiment
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27 with sufficient accuracy. In detail, the measurement of
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29 even aberrations, i. e. the defocus Z and the twofold
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31 astigmatism A_1 , may be carried out by processing the
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33 weak signal originating from amorphous overlayers [xxi]
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35 while odd aberrations, i. e. the axial coma B_2 and the
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37 threefold astigmatism A_2 , may be determined by sampling
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39 a variety of discrete aberration azimuths and magni-
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41 tudes up to twice their arguable limits according to
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43 [xxvii] followed by handpicking those aberrations at
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45 which the symmetry properties of the corresponding $\Phi(\mathbf{r})$
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47 and $A(\mathbf{r})$ images correlate best with the supposed lat-
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49 tice structure [xxii]. Irrespective of this procedure
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51 even more sophisticated approaches are available to
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53 tackle the problem of measurement of odd aberra-
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55 tions [xxx].
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59 Finally, since $\Psi(\mathbf{r})$ is complex-valued, we may evaluate
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"local" diffraction patterns from specimen areas as
small as desired. When evaluated during operation of
the microscope, the judgement of the symmetry proper-
ties of these "local" diffraction patterns is a most

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5 convenient tool for the proper orientation of specimen
6 areas under investigation. By this means, a proper zone
7 axis alignment of the samples with an accuracy below
8 3 mrad is ensured while the vast majority of samples
9 aligned by "traditional" procedures demonstrates off-
10 zone-axis orientations above 10 mrad [xxxi].

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16 To set aright the common fallacy that the aforemen-
17 tioned benefits coming along with the restoration of
18 the exit-plane wavefunction do not necessitate the use
19 of spherical aberration corrected instrumentation but
20 rather suggest an increase of the instrumental resolu-
21 tion solely, e. g. by monochromatisation of the elec-
22 tron source, it is emphasized that the *a posteriori*
23 measurement of residual lens aberrations requires a
24 sufficient pre-reduction of the very same aberrations.
25 Moreover, image delocalization in a non-corrected in-
26 strument will generally not be less than [xi]

$$R_L = C_s / 4 \lambda^3 g_{\max}^3 \quad (4)$$

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38 and only to be within reach at Lichte's defocus of
39 least confusion

$$Z_L = -3/4 C_s \lambda^2 g_{\max}^2 \quad (5)$$

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45 which, alas, comes along with the great disadvantage
46 that the phase contrast transfer function exhibits a
47 large number of rapid contrast oscillations at medium
48 spatial frequencies, and the corresponding contrast re-
49 versals make the resulting image quite difficult to in-
50 terpret. Moreover, image delocalization according to
51 Eqn. (4) does not only have a detrimental effect on the
52 spread out of structural information in the vicinity of
53 lattice imperfections but also to data acquisition at
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5 marginal areas of the recording medium. In other words,
6 the rather large image delocalization of uncorrected
7 instruments represents a serious limitation for the us-
8 able field of view of the charge-coupled device (CCD)
9 camera detector.
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13 14 15 16 17 **3. EXPERIMENTAL SETUP**

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19 This study utilizes a Philips CM-200 FEG instrument
20 equipped with a computer-controlled electromagnetic
21 hexapole system for the correction of the spherical ab-
22 erration of the objective lens [xxvii]. An optical
23 coarse adjustment of the hexapole corrector elements
24 was performed by analysing Zemlin tableaus taken from
25 amorphous specimen areas with an incident electron beam
26 tilted up to 20 mrad from the optical axis [xxxii] thus
27 yielding an initial estimate on the quality of higher-
28 order aberration corrections. Setting down an optimized
29 negative $C_s = -40 \mu\text{m}$ the magnitudes of residual aberra-
30 tion coefficients were limited to $A_1 \leq 2.0 \text{ nm}$ for the
31 two-fold astigmatism, to $A_2 \leq 170 \text{ nm}$ for the three-fold
32 astigmatism and to $B_2 \leq 55 \text{ nm}$ for the axial coma
33 [xxvii].
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46 Focal series of about $N = 20 \dots 30$ images were re-
47 corded using a 1k x 1k CCD camera system at a sampling
48 rate of about 20 pm per picture element. This corre-
49 sponds to an image discretization well below the Ny-
50 quist frequency with respect to half of the instrumen-
51 tal information limit $1/(2 g_{\text{max}}) = 65 \text{ pm}$ and represents
52 an adequate sampling to tap the full potential of the
53 instrument facing that the modulation transfer function
54 of many CCD cameras is known to exhibit a rather poor
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5 transfer at higher spatial frequencies. The focal range
6 of each series included the focus setting with $Z_{\text{opt}} =$
7 11.6 nm for optimized phase contrast. From these series
8 the exit-plane wavefunction was retrieved for the fre-
9 quency band between 1 nm^{-1} and 8 nm^{-1} applying a dough-
10 nut-shaped restoration filter.
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19 **4. ATOMIC RESOLUTION IMAGING AT A DECENT SIGNAL-TO-NOISE**
20 **RATIO: CORE STRUCTURE OF MISFIT DISLOCATIONS AT $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$**
21 **/GaAs HETEROINTERFACES**
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24 As a first materials science example of use, we report
25 on the core structure of Lomer type pure edge disloca-
26 tions [xxxiii] at the heterointerfaces between lattice-
27 mismatched sphalerite semiconductors. In view of the
28 multiplicity of conceivable lattice positions of the
29 pulled out half-plane's terminal point, numerous core
30 models have been proposed for this type dislocations
31 [xxxiv, xxxv] but owing to the hitherto insufficient
32 instrumental resolution previous high-resolution analy-
33 ses required elaborate support by numerical image simu-
34 lations merely to draw indirect conclusions on the cor-
35 responding dislocation core structures [xxxvi, xxxvii,
36 xxxviii].
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47 In the present analysis we focus on an $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epi-
48 layer with a thickness of 35 nm that was grown by mo-
49 lecular beam epitaxy on a GaAs(001) substrate and sub-
50 sequently overgrown with a GaAs capping layer of 55 nm
51 in thickness whereby growth conditions were chosen as
52 specified in a previous analysis [xxxix].
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5 Figure 2(a) displays an optimum focus micrograph $I(\mathbf{r})$ of
6 a Lomer dislocation with a Burgers circuit yielding a
7 projected closing vector $\mathbf{b} = a/2 [\bar{1}\bar{1}0]$ in the proximity
8 of the interface between the $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayer and the
9 GaAs(001) substrate viewed with a $[\bar{1}\bar{1}0]$ zone axis orien-
10 tation of the sample. Far-off the dislocation core, the
11 image contrast is dominated by clearly separated pairs
12 of contrast dots constituting atomic dumbbells at dis-
13 tances of $a/4 \cdot 141 \text{ pm}$ with $a = 565 \text{ pm}$ denoting the
14 lattice parameter of the substrate material.
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23 However, two conspicuous contrast artifacts become evi-
24 dent from close inspection of the Z_{opt} micrograph of the
25 GaAs matrix displayed in Figure 2(e). Firstly, non-
26 structure related spurious intensity peaks are observed
27 in between the atomic column positions which are due to
28 an expended transfer of low spatial frequencies at se-
29 vere phase offsets, especially of the strongly excited
30 $\{111\}$ beam amplitudes [xxvi]. Secondly, a kidney-shaped
31 distortion of the dumbbells is observed. As can be
32 shown from quantitative measurements on the associated
33 "local" diffraction pattern displayed in Figure 2(b),
34 these distortions are not due to any potential misori-
35 entation of the sample but instead result from para-
36 sitic lens aberrations amounting to $A_1 = 2.2 \text{ nm}$ (83°),
37 $B_2 = 110 \text{ nm}$ (83°), and $A_2 = 150 \text{ nm}$ (43°) with the values
38 in parentheses indicating the respective azimuth angles
39 inclined with the $[001]$ direction [xxx]. For that rea-
40 son, the phase $\Phi_{\text{unc}}(\mathbf{r})$ of exit-plane wavefunction re-
41 trieved from a focal series of $N = 30$ micrographs and
42 displayed in Figure 2(e) still shows distortions of the
43 contrast dumbbells as long as these residual aberrations
44 are not considered during the initial step of the
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5 reconstruction process. By contrast, the phase image
6 $\Phi(\mathbf{r})$ is free of any distortions after the above speci-
7 fied aberrations A_i and B_i have been eliminated [xxxi].
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11 Above and beyond this, the phase image is also richer
12 in contrast compared to the Z_{opt} micrograph since there
13 are practically no limitations with respect to the tem-
14 poral and spatial coherence, thus providing a superior
15 signal-to-noise ratio at high frequencies up to the in-
16 formation limit. Additionally, the retrieved phase
17 benefits from the averaging of information from a com-
18 plete series of micrographs. When quantifying the sig-
19 nal-to-noise-ratios σ_Φ and σ_I of the $\Phi(\mathbf{r})$ and $I(\mathbf{r})$ im-
20 ages, respectively, by applying analysis procedures
21 outlined in [xl] an improvement through the restoration
22 of the exit-plane wavefunction by a factor of $(\sigma_\Phi/\sigma_I)_{exp} =$
23 4.1 is obtained. This value is in excellent agreement
24 with the ideal factor of $(\sigma_\Phi/\sigma_I)_{th} = \cdot N/2 = \cdot 30/2 = 3.9$
25 to be expected for information retrieval from a focal
26 series of $N = 30$ micrographs.
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39 When also determining the polarity of the sample by the
40 evaluation of a set of relevant reciprocal-space ampli-
41 tudes from the "local" diffraction pattern and the
42 subsequent trimming of simulated data, individual
43 bright contrast dots in the $\Phi(\mathbf{r})$ image may be directly
44 associated with gallium and arsenic columns [xxxi].
45 Corresponding atomic species are indicated in
46 Figure 2(e).
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54 The essential benefit of the combined use of the nu-
55 merical retrieval of the exit-plane wavefunction with
56 aberration-corrected imaging, however, becomes evident
57 when having a closer look at the atomic structure of
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5 the dislocation core, which is basically not resolved
6 in the single optimum focus image $I(\mathbf{r})$ but only in the
7 amplitude and phase images, respectively. Both, $A(\mathbf{r})$
8 and $\Phi(\mathbf{r})$, show the atomic arrangement down to the dis-
9 location core and reveal a detached atomic column at
10 the point of intersection of extrapolated line posi-
11 tions indicated by the horizontal and vertical arrows.
12 Relevant contrast features show mirror symmetry with
13 respect to the medial $(\bar{1}\bar{1}0)$ lattice plane indicated by
14 the upright arrows. This global symmetry behaviour
15 ranges down to the dislocation core.
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24 From the exit-plane wavefunction a core structure model
25 according to Figure 3(a) can be deduced as contrast
26 features are intuitively interpretable. The disloca-
27 tion core shows some similarity to the glide set type
28 model of a Lomer dislocation originally proposed by
29 Hornstra [xxxiv] which is displayed in Figure 3(b) and
30 characterized by an eight-atomic inner ring. The pre-
31 sent analysis, however, reveals a less compact core,
32 which is build up of a ten-sided polygon also travers-
33 ing the detached atomic column with a coordination dif-
34 ferent from the surrounding matrix. This structure also
35 deviates from rather complex mirror symmetric configu-
36 rations observed at GaAs/Si interfaces [xxxvi, xli] and
37 in Ge/Si heterosystems [xxxviii]. As surface effects in
38 the vicinity of the highly strained dislocation core
39 are likely to occur in thin electron microscopy speci-
40 mens, the retrieved core structure may certainly devi-
41 ate from that of a dislocation core embedded in bulk
42 material. This problem, however, exists in any high-
43 resolution analysis concerned with lattice defects
44 raising rather strong lattice distortions.
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5 Referring to a detailed discussion of the matter [xxxi]
6 we briefly summarize the causal connections impeding
7 the resolvability of the dislocation core in the Z_{opt} im-
8 age but evidently not in the retrieved exit-plane wave-
9 function. Numerical image calculations give clear evi-
10 dence that this non-resolvability in the single $I(\mathbf{r})$ im-
11 age will neither be due to (i) the residual image delo-
12 calization or (ii) a decreased sample thickness in the
13 vicinity of the dislocation core. Moreover, a potential
14 impact of (iii) a locally inhomogeneous strain relaxa-
15 tion of the thin specimen may be ruled out since, oth-
16 erwise, the $A(\mathbf{r})$ and $\Phi(\mathbf{r})$ images would similarly be af-
17 fected. Instead, the practically improved resolution of
18 the amplitude and phase images will be rather due to
19 (iv) an increased resistibility against time-dependant
20 electron beam induced degeneration of the sample. While
21 numerical retrieval techniques purge information from
22 intrinsically unstable amorphous overlayers by averag-
23 ing, a single Z_{opt} micrograph simply represents merely a
24 snap-shot of a sample under illumination with a certain
25 probability of an adverse atomic overlayer assembly
26 during the time of exposure [xxxi].
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46 **5. GEOMETRIC LINEARITY AT HIGH-LEVEL PRECESSION: LATTICE** 47 **DISTORTIONS ASSOCIATED WITH DISSOCIATED 60° DISLOCATIONS** 48 **IN GaAs (110)** 49 50

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52 In sphalerite materials 60° dislocations with a Burgers
53 vectors of type $\mathbf{b} = a/2 \langle 0\bar{1}1 \rangle$ may dissociate into two
54 partials bounding either an intrinsic or an extrinsic
55 stacking fault [xlii, xliii, xliv, xlv]. The dissocia-
56 tion reaction is:
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$$a/2 [0\bar{1}1] \rightarrow a/6 [\bar{1}\bar{2}1] + a/6 [\bar{1}\bar{1}2] \quad (6)$$

with the Burgers vectors of both partials inclining angles of 30° and 90° with the dislocation line along the $[\bar{1}\bar{1}0]$ direction, respectively. While most analyses at the outset of quantitative high-resolution microscopy were primarily concerned with distinguishing glide and shuffle set dislocations, i. e. discriminating whether dislocations cores lie on the narrowly or widely spaced $\{111\}$ planes, by interpreting characteristic contrast features in the vicinity of the dislocations cores [xlvi, xlvii, xlviii], it is only recently that efforts have been put forth to investigate the core structure of 30° and 90° partials, both theoretically applying *ab initio* calculations [xlix, l, li] and experimentally employing advanced electron microscopy techniques [lii, liii].

In the following we shall focus on a dissociated 60° dislocation bounding a double stacking fault ribbon. Figure 4(a) displays an optimum micrograph $I(\mathbf{r})$ of the terminating zone of such an extended dislocation in GaAs viewed along the crystallographic $[\bar{1}\bar{1}0]$ direction. The image has been taken from the same specimen investigated in the previous section focusing on the GaAs capping layer in this case. The associated phase $\Phi(\mathbf{r})$ and amplitude $A(\mathbf{r})$ images displayed in Figure 4(b) and (c) allow for an accurate identification of the atomic arrangement of the stacking fault ribbons and, especially, the core structure of the dislocation terminating the defect.

As the overall lattice defect is composed of two adjacent (111) lattice planes showing similar misorienta-

tions of the atomic dumbbells, it appears inceptively reasonable to describe the entire defect as a sequence of two adjoining likewise congenerous faulted fault ribbons. Both ribbons need then to be characterized by a projected component of the terminating Burgers vector amounting to $\mathbf{b}_{\text{proj}}/2$ with \mathbf{b}_{proj} denoting the closing vector of the entire defect when considering a projection to the $(1\bar{1}0)$ plane. Assuming a configuration build-up by 30° partials, characterized by $\mathbf{b}_{30^\circ\text{-A}} = a/6 [1\bar{2}1]$ as well as $\mathbf{b}_{30^\circ\text{-B}} = a/6 [\bar{2}11]$ and yielding $\mathbf{b}_{\text{proj},30^\circ\text{-A/B}} = a/12 [\bar{1}\bar{1}2]$, the associated total lattice displacement along the $[\bar{1}\bar{1}2]$ direction between the upper and the lower areas of the crystal far from the dislocation core should be $\Delta u_{\bar{1}\bar{1}2,30^\circ} = 2 \mathbf{b}_{\text{proj},30^\circ} = 231$ pm. This description is fully compatible with the definition of an extrinsic stacking fault bound by a 90° partial with $\mathbf{b}_{90^\circ} = \mathbf{b}_{\text{proj},90^\circ} = a/6 [\bar{1}\bar{1}2] = 231$ pm and a 30° partial with $\mathbf{b}_{\text{proj},30^\circ} = a/12 [\bar{1}\bar{1}2] = 115$ pm at the opposite core position. Both of these limiting partials are in fact again superpositions of 30° and 90° partials separated by two atomic layers [45] with the extrinsicity expressing in two adjacent ribbons of $\{111\}$ lattice planes with differently aligned atomic [liv].

To check the validity of this model hypothesis, the elastic displacement component $u_{\bar{1}\bar{1}2}$ along the $[\bar{1}\bar{1}2]$ direction has been evaluated from the $\Phi(\mathbf{r})$ image using geometrical phase analysis algorithms [lv]. Calculations have been performed applying Gaussian shaped masks with decay parameters $\sigma = |\mathbf{g}_{111}|/3$ centred around the \mathbf{g}_{111} beams thus averaging information over regions of about $r_{\text{dir}} \cdot 3 / (2 |\mathbf{g}_{111}|) \cdot 490$ pm in radius at most [lvi]. The correspondingly measured $u_{\bar{1}\bar{1}2}(\mathbf{r})$ distribution is displayed in

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5 Figure 4(e) together with a line profile $u_{\bar{1}\bar{1}\bar{1}}(\mathbf{r}_{\bar{1}\bar{1}\bar{1}})$ ex-
6 tracted from this distribution along the $[\bar{1}\bar{1}\bar{1}]$ direc-
7 tion, cf. Figure 4(e). For the latter, data values have
8 been averaged over a width of 1 nm, i. e. over the
9 width of the drawn-in dashed blue frame. The line pro-
10 file shows two conspicuous plateaus separated by an
11 abrupt discontinuity of $\cdot u_{\bar{1}\bar{1}\bar{1}} = 234 \text{ pm} \pm 60 \text{ pm}$. This
12 quantity is in excellent agreement with the closing
13 vector associated with the 90° partial of an extrinsic
14 stacking fault for which a total shift of lattice
15 planes of $\Delta u_{\bar{1}\bar{1}\bar{1}, 30^\circ} = 2 \mathbf{b}_{\text{proj}, 30^\circ - A/B} = 231 \text{ pm}$ is expected,
16 cf. above. We emphasize that the specified margin of
17 error in the $\cdot u_{\bar{1}\bar{1}\bar{1}}$ value rather reflects inhomogeneous
18 lattice distortions of the sample but not the fundamen-
19 tal accuracy to quantify atomic column positions which
20 may be measured to a precision of about a few picome-
21 tres [lvii, lviii].

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35 In Figure 4(d) single atomic columns, as allocated from
36 the determination of the polarity of the sample, are
37 superimposed to a magnified clipping of the phase im-
38 age. The global displacement of the upper and lower
39 crystal areas against each other is found to be medi-
40 ated by the local re-organization of the atomic columns
41 within those two (111) lattice planes forming the
42 faulted double ribbon. Hence, the associated disloca-
43 tion cores of both partials, indicated by red circles
44 in the figure, also lie on these very same (111)
45 planes. As these planes are narrowly spaced, the par-
46 tial dislocations are of glide set type. Both disloca-
47 tion cores are made up of gallium columns leading to a
48 so-called β dislocation [lix]. Moreover, the figure
49 also reveals a symmetrical six-fold structure of the
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5 overall dislocation core, which is in perfect agreement
6 with a 90° partial dislocation composed of two 30° par-
7 tials separated by two atomic layers [xlv].
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11 To put it a step further, we may also quantify local
12 distortions of the atomic dumbbells across the faulted
13 ribbon at some distance of the dislocation core. For
14 these purposes contrast dot positions have been meas-
15 ured from the $5.5 \text{ nm} \times 4.2 \text{ nm}$ phase image $\Phi(\mathbf{r})$ area
16 displayed in Figure 5(a), whose centre is 5.2 nm left
17 of the dislocation core. For these purposes a digital
18 image processing algorithm [lx] has been applied which
19 basically employs (i) dedicated image intensity thresh-
20 olding operations, (ii) a centre-of-mass analysis in-
21 side individual bright contrast dots supported by (iii)
22 adequate refining procedures as specified in [lxi,
23 lxii]. From the measured contrast dot positions, the
24 length and orientation of individual dumbbells have
25 been calculated and normalized to mean values associ-
26 ated with the lower (planes no. 0 - 3) and upper
27 (planes no. 11-13) areas of the $\Phi(\mathbf{r})$ image. For the im-
28 provement of statistics 15 data points have been aver-
29 aged along the $[\bar{1}\bar{1}2]$ direction and median values are
30 plotted in Figure 5(b) and (c) in dependence on spe-
31 cific (111) lattice plane positions.
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48 As can be seen from both plots, the dumbbells on either
49 side of the double ribbon rearrange roughly antisymmet-
50 ric in the vicinity of the faulted (111) planes. In
51 this context, the most conspicuous feature is that the
52 dumbbells of the bottommost lattice plane of the upper
53 crystal domain (plane no. 8) are compressed to a length
54 of $\langle d \rangle = 133 \text{ pm} \pm 4 \text{ pm}$ and turn towards the double rib-
55 bon with a misorientation angle $\langle \delta \rangle = 2.6^\circ \pm 1.3^\circ$ com-
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pared to the reference lattice planes. In contrast, the uppermost dumbbells of the lower crystal area (plane no. 5) are stretched to a length of $\langle d \rangle = 150 \text{ pm} \pm 4 \text{ pm}$ and bend away from the double ribbon at a misorientation angle of $\langle \delta \rangle = -4.9^\circ \pm 1.5^\circ$.

In order to gauge whether the observed antisymmetric distortions represent a genuine structural property or not, potential implications of scattering and imaging artefacts need to be ruled out. Since a hypothetical global misalignment of the sample cannot give rise to any local torsion and dilatation of projected atomic dumbbells we may disenfranchise from this explanation. An argument of the same kind holds true of the potential impact of not fully compensated aberrations as they would take effect on the entire image and, hence, would distort all atomic dumbbells of the same orientation equally. Strictly speaking any potential impact of both, on-axial and off-axial aberrations would need be evaluated separately. In practise this conceptual differentiation can, however, be neglected because of the rather limited field of view of the CCD detector and the semiamplanatic imaging properties of the double hexapole corrector [xiii]. Beyond electron-optical reasoning, a supposed strictly antisymmetric lattice distortion caused by a dedicated combination of higher order aberrations with the faulted ribbon incidentally acting as the symmetry plane, may be ruled out from a probability point of view because of an almost immense number of possible combinations which will not give raise to the observed distortion behaviour.

The observed alteration of atomic dumbbell lengths in the vicinity of stacking faults ribbons of about 10 pm

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5 is in fair agreement with recent measurements of lat-
6 tice distortions along intrinsic stacking faults rib-
7 bons in heavily beryllium doped GaAs. This analysis re-
8 vealed an average expansion of dumbbell lengths up to
9 158 pm in the faulted lattice plane which was explained
10 by the segregation of beryllium dopant atoms and the
11 subsequent formation of antisite defects inside of the
12 plane of the faulted ribbon [liii]. Additionally, lat-
13 tice displacements around the central stacking fault of
14 Z-shaped dipoles connecting two stair rod dislocations
15 in indium doped GaAs revealed the very same antisymmet-
16 ric distortion of dumbbell related contrast dots as
17 were observed in the present analysis. Lateral dis-
18 placements of gallium and arsenic atom pair related
19 contrast features along the $[\bar{1}\bar{1}2]$ direction were found
20 to be as much as 20 % to 50 % of the dumbbell length
21 [lxiii].
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35 As the specimen investigated in the present study was
36 undoped we may, in the first instance, rule out the
37 aforementioned explanations but only speculate about an
38 indium diffusion from the underlying $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ layer to
39 the GaAs layer along the faulted ribbon at most. As
40 long as an inhomogeneous incorporation of indium atoms
41 is not considered this approach, thus, cannot explain
42 the observed lattice distortions. Admittedly, the anti-
43 symmetric distortions become perspicuous when consider-
44 ing the elastic distortions associated with the 90°
45 partial dislocations which basically follow the meas-
46 ured characteristics of the dumbbell's measured expan-
47 sion and torsion but, alas, yield only alterations of
48 dumbbells lengths smaller than ± 3 pm and misorienta-
49 tion angles smaller than $\pm 0.4^\circ$ for the image area un-
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5 der investigation [liv]. Hence, a more likely explanation
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tion could be that the terminating partial dislocation biases the rearrangement of atomic columns in the vicinity of the faulted ribbons and that next but one neighbour interactions between different atomic species will indeed play an important role during this process.

6. ATOMIC STRUCTURE OF CHROMIUM IMPLANTATION INDUCED LATTICE DEFECTS IN GaN (1120)

As a finale example, we report on dislocations introduced by chromium implantation into GaN. Implantation of transition metals into semiconductors is a candidate process for the fabrication of diluted magnetic semiconductors for spintronic applications [lxiv]. A by-product of the implantation is the creation of ion-induced lattice defects: Extrinsic and intrinsic basal plane stacking faults, bounded by Frank partial or Shockley-Frank partial dislocations, are formed as the result of the precipitation of excess interstitials [liv, lxv].

The GaN films presented in this study were grown by metal organic chemical vapour deposition on (0001) oriented sapphire substrates under Si doping to a concentration of $2 \times 10^{17} \text{ cm}^{-3}$. Cr⁺ ions were implanted with an energy of 200 kV and a dose of $5 \times 10^{16} \text{ cm}^{-2}$ at a temperature of 350 °C to avoid amorphization in the as-implanted samples. A high density of basal plane stacking faults is observed besides spherical Cr-rich precipitates in surface near regions after chromium implantation and rapid thermal annealing at 700 °C for 5 min in N₂ atmosphere [lxvi].

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5 The majority of the basal plane stacking faults is ex-
6 trinsic bound by Frank partial dislocations with Bur-
7 gers vector $\mathbf{b} = 1/2 [0001]$. Figure 6 displays the am-
8 plitude image $A(\mathbf{r})$ and phase image $\Phi(\mathbf{r})$ of a perfect
9 nanometre sized interstitial loop in the end of range
10 depth of implantation. Gallium and nitrogen columns at
11 a dumbbell distance of 114 pm, considerably smaller
12 than the information limit of the instrument, are not
13 fully resolved. Nonetheless the N-polarity is unambigu-
14 ously visible from the directly interpretable bright
15 contrast in the phase image. The tetrahedral coordina-
16 tion across the faulted layer stacking is confirmed,
17 asserting that no foreign chromium-gallium alloy phase
18 is connected with the planar defects.

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30 A magnified view of the core of a Frank partial dislo-
31 cation at the terminating zone of a several 10 nm large
32 dislocation loop is shown in the Z_{opt} image and the $\Phi(\mathbf{r})$
33 image retrieved from a corresponding focal series dis-
34 played in Figure 7(a) and (b). Although the $I(\mathbf{r})$ and
35 $\Phi(\mathbf{r})$ appear very similar at a first glance, the im-
36 proved signal-to-noise ratio in the phase image en-
37 hances the visibility of the nitrogen positions and the
38 dumbbell orientation up to the core of the dislocation.
39 The phase image $\Phi(\mathbf{r})$ fortifies the presence of further
40 nitrogen atoms within the core surrounded by the cage
41 of the five marked gallium columns. The faint phase
42 shift in $\Phi(\mathbf{r})$, in which non-linear image components and
43 image delocalization are eliminated, indicates a nitro-
44 gen filled core in favour of a chromium or gallium rich
45 core.

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58 Based on these observations a tentative 5/7 ring con-
59 figuration for the core is presented in Figure 7(c).
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5 The nitrogen atoms shared by the 5- and 7-membered
6 rings are threefold coordinated with Ga and N. Due to
7 the wrong bond and the presence of unpaired electrons,
8 this structure is not expected to be the most stable
9 configuration. Since $\Phi(\mathbf{r})$ is retrieved from a focal se-
10 ries taken over a period of a few ten seconds, the im-
11 age conceivably reflects a transient state of the core
12 that gathers further interstitials during observation.
13 The Z_{opt} image level may therefore contain complementary
14 but not necessarily identical information when compared
15 to $\Phi(\mathbf{r})$. Indeed for the present case the Z_{opt} image with
16 its inferior noise level compared to $\Phi(\mathbf{r})$ also complies
17 an alternative structure which contains two wrong Ga-Ga
18 bonds connecting threefold coordinated Ga atoms at po-
19 sitions 1-5 and 2-3, respectively.
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34 7. CONCLUSIONS

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36 In summary, a combination of negative spherical aberration
37 imaging and the restoration of the exit-plane
38 wavefunction from a focal series of micrographs has
39 been applied for the investigation of lattice imperfec-
40 tions in semiconductor materials at atomic resolution
41 and, in particular, for the extraction of quantitative
42 information on local lattice distortions.
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49 It has been demonstrated that recent improvements in
50 the resolution power of transmission electron micro-
51 scopes enable the imaging of finest structure details
52 at directly interpretable contrast features also coming
53 along with a widely minimized image delocalization when
54 micrographs are taken under optimized imaging condi-
55 tions.
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5 Additionally, the numerical retrieval of the exit-plane
6 wavefunction allows for the elimination of artificial
7 contrast features still visible in micrographs taken
8 under optimized focusing conditions. Beyond its genu-
9 ine purpose, the retrieval of the exit-plane wavefunc-
10 tion was demonstrated to be a most suitable tool for
11 the measurement and numerical correction of residual
12 lens aberrations as well as for proper orientation of
13 specimens during operation of the electron microscope.
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17 Above and beyond the individual vantages coming along
18 with either technique their combined use allows for the
19 accurate identification of lattice imperfections in
20 semiconductor materials at hitherto unequalled imaging.
21 Experimental analyses conspicuously benefit from put-
22 ting to use aberration corrected input data, i.e. from
23 an increase of the instrumental information limit to-
24 gether with a decrease of image delocalization and a
25 pre-reduction of lens aberrations, as well as from the
26 complete elimination of residual aberrations by the nu-
27 merical retrieval of the exit-plane wavefunction, which
28 is also free from non-linear imaging artefacts and
29 yields images characterized by a decent signal-to-noise
30 ratio.
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34 By means of the deliberated combination of both tech-
35 niques, Lomer dislocation cores at $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ het-
36 erointerfaces have been imaged at atomic resolution and
37 directly identified as being composed of a mirror sym-
38 metric ten-atomic ring, thus rendering extensive image
39 simulations superfluous. The quantification of local
40 lattice distortions in the vicinity of a double stack-
41 ing fault ribbon in GaAs by means of the analysis of
42 experimental phase images $\Phi(\mathbf{r})$ brought clear evidence
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5 of an antisymmetric torsion and expansion of atomic
6 dumbbells with respect to the faulted ribbon. A similar
7 quantitative analysis focusing on lattice imperfections
8 in GaN at atomic resolution based on the synergetic
9 combination of negative spherical aberration corrected
10 imaging and the numerical retrieval of the exit-plane
11 wavefunction is presently merely hampered by the in-
12 strumental resolution but will come along with forth-
13 coming aberration corrected sub-Ångström resolution mi-
14 croscopes.
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31 ble specimen preparation work.
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5 **FIGURE CAPTIONS**
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10 **Figure 1:** Partially coherent contrast transfer function
11 (PC CTF) together with the coherent transfer function
12 (CTF) and the damping envelope (DE) assuming parameters
13 $\lambda = 2.51$ pm, $C_s = -40.6$ μm , $Z = 11.6$ nm as well as
14 0.2 mrad for the semi-angle of beam convergence and 6.4
15 nm for the half-width of the Gaussian spread of defo-
16 cus. Arrows indicate positions of crystalline reflec-
17 tions in GaAs.
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24 **Figure 2:** Analysis of a Lomer type dislocation with $\mathbf{b} =$
25 $a/2$ $[\bar{1}\bar{1}0]$ at an $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ heterointerface.
26 **a:** Optimum focus micrograph $\mathbf{I}(\mathbf{r})$ taken along the $[\bar{1}\bar{1}0]$
27 zone axis orientation of the sample. **b:** "Local" dif-
28 fraction pattern evaluated from the exit-plane wave-
29 function of the image area. **c:** Restored phase image
30 $\Phi(\mathbf{r})$ and **d:** amplitude image $A(\mathbf{r})$. **e:** Magnified clipping
31 of the GaAs related image area together with the asso-
32 ciated phase images $\Phi_{\text{unc}}(\mathbf{r})$ and $\Phi(\mathbf{r})$ obtained when ne-
33 glecting and considering measured residual lens aberrations,
34 respectively.
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44 **Figure 3:** Dislocation core models for symmetrical Lomer
45 dislocations. **a:** Model retrieved from the exit-plane
46 wavefunction displayed in Figure 2 together with **b:** the
47 symmetrical glide set type core model according to
48 Hornstra [xxxiv].
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53 **Figure 4:** Analysis of an extrinsic stacking fault in
54 GaAs bound by two adjacent 30° partial dislocations
55 with $\mathbf{b}_{\text{proj}} = [\bar{1}\bar{1}2]$ in total. **a:** High-resolution micrograph
56 $\mathbf{I}(\mathbf{r})$ taken under Z_{opt} conditions. **b:** Phase image $\Phi(\mathbf{r})$ and
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5 **c**: amplitude image $A(\mathbf{r})$ calculated from the associated
6 focal series of micrographs. **d**: Magnified clipping of
7 $\Phi(\mathbf{r})$ with the positions of atomic columns superimposed
8 and the dislocation core positions of 30° partials in-
9 dicated by red circles. **e**: Contour representation of
10 the lattice displacements along the $[\bar{1}\bar{1}2]$ direction with
11 reference to the dashed red framed area. **f**: Displace-
12 ment profile measured perpendicular to the faulted rib-
13 bon at the area indicated by the dashed blue frame.

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21 **Figure 5**: Locally inhomogeneous distortions of the
22 atomic dumbbells in the vicinity of the faulted double
23 ribbon. **a**: Clipping from the phase image displayed in
24 Figure 4(b) with atomic column positions superimposed
25 and dumbbell distortions indicated exemplarily in de-
26 pendence on specific positions along the $[111]$ direc-
27 tion. **b**: Average projected bond length $\langle d \rangle$ and **c**:
28 misorientation angle $\langle \delta \rangle$ of the dumbbells along the
29 (111) direction. The lattice planes belonging to the
30 double stacking fault ribbon are indicated in lighter
31 grey colour.

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41 **Figure 6**: Interstitial loop in Cr-implanted GaN viewed
42 along the $[11\bar{2}0]$ direction. **a**: Amplitude image $A(\mathbf{r})$ and
43 **b**: phase image $\Phi(\mathbf{r})$ calculated from a focal series of
44 micrographs. Simulated images of the periodic N-
45 polarity GaN structure assuming a sample thickness of
46 3.2 nm at a resolution of 7.5 nm^{-1} are superimposed in
47 the lower left part of the images. The stacking se-
48 quence is ABABCABAB, where the underlined part high-
49 lights sphalerite stacking.

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57 **Figure 7**: Frank partial dislocation with the Burgers
58 vector $\mathbf{b} = 1/2 [0001]$ projected along the $[11\bar{2}0]$ direc-
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5 tion. **a**: Experimental micrograph $I(\mathbf{r})$ taken under Z_{opt}
6 conditions and **b**: correspondingly retrieved phase image
7 $\Phi(\mathbf{r})$. **c**: 5/7 ring configuration for the core of the
8 Frank partial dislocation.
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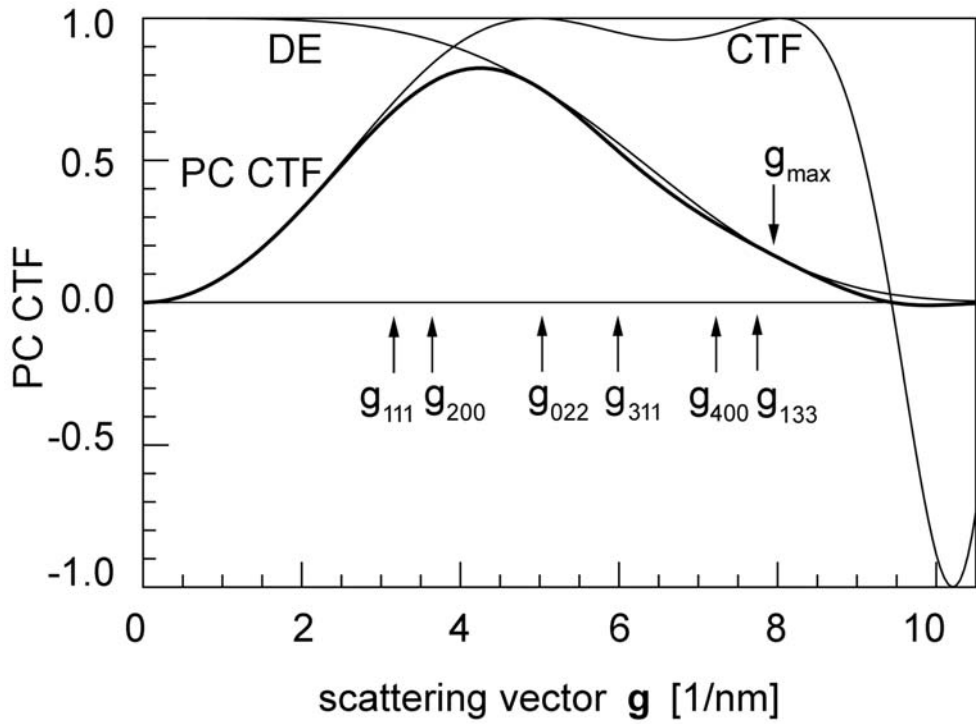
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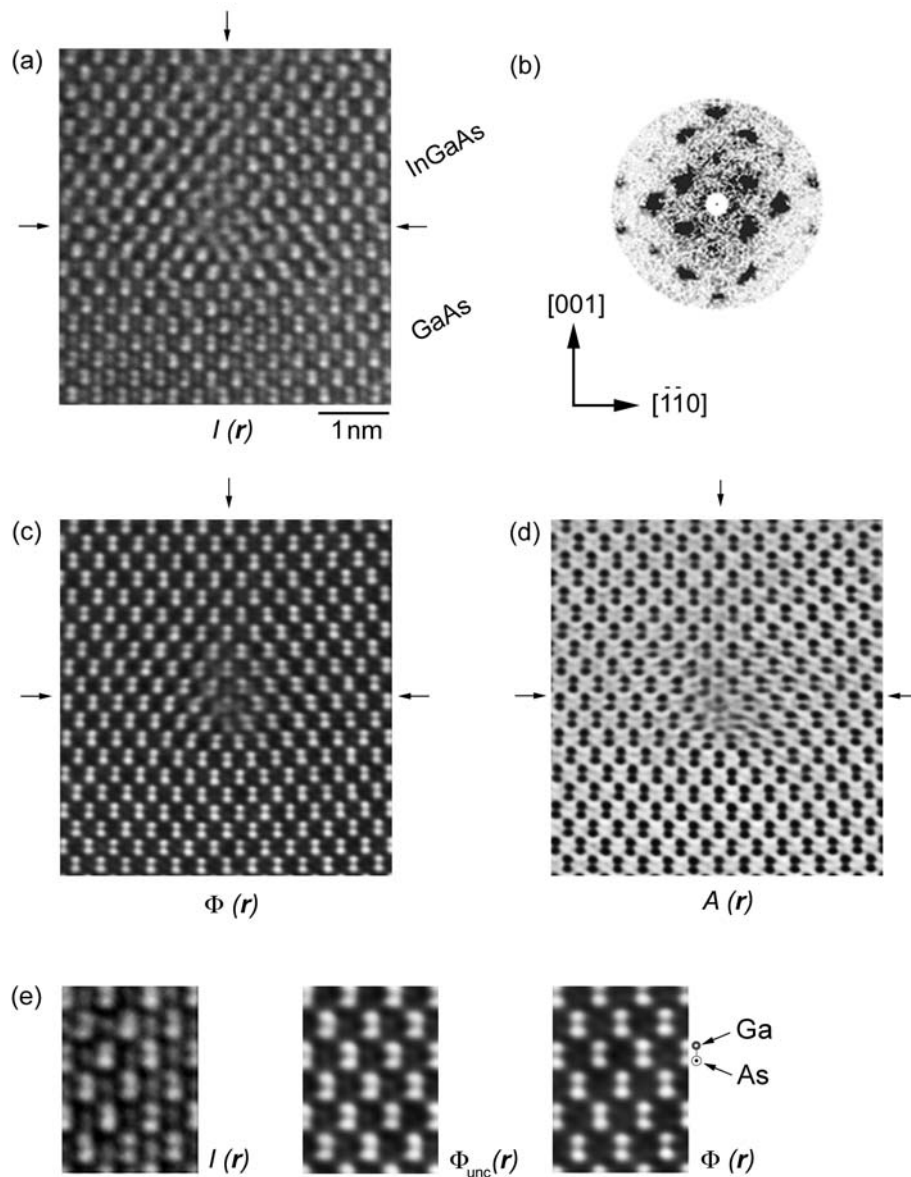
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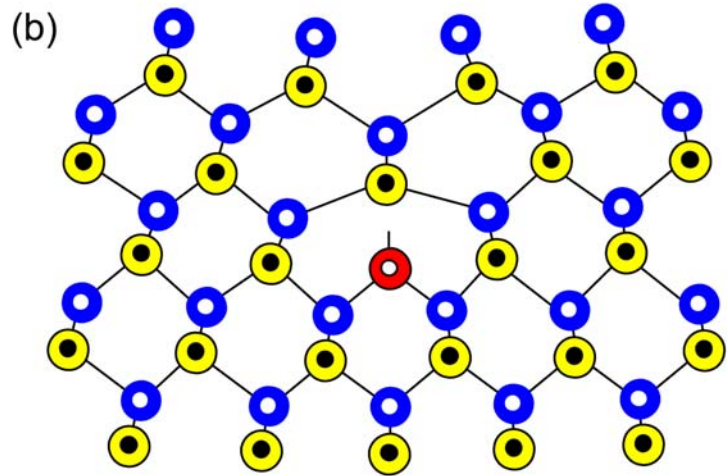
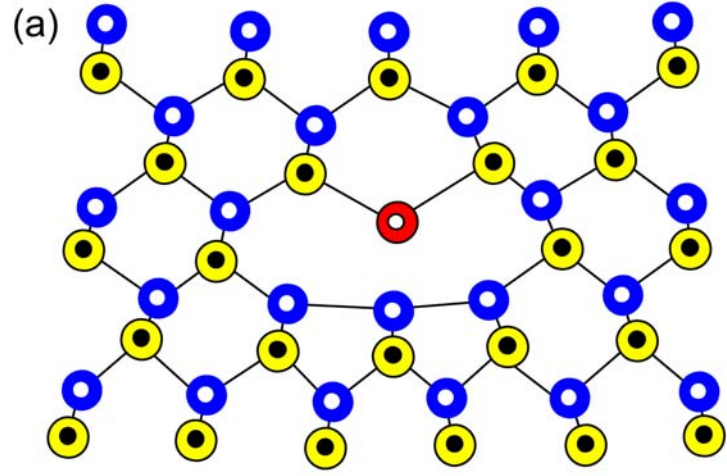
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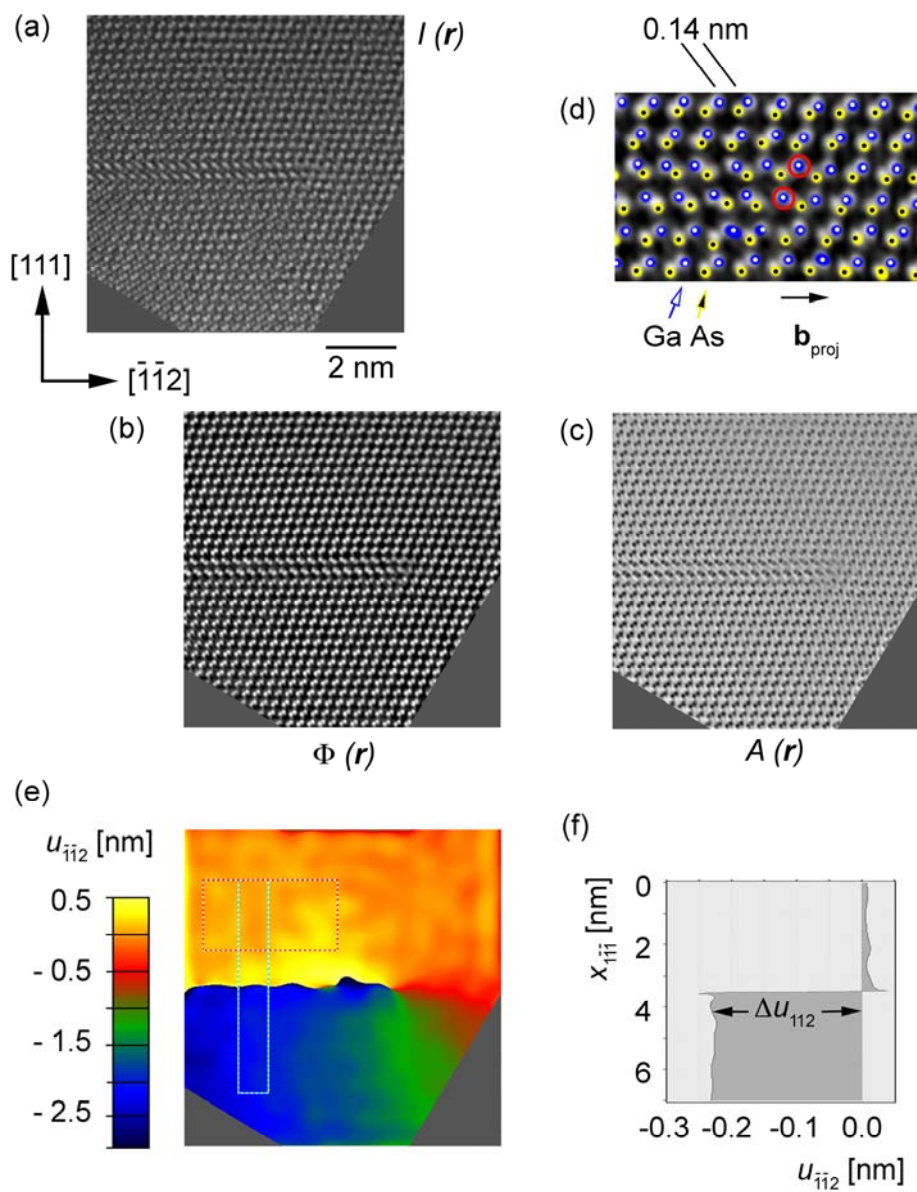
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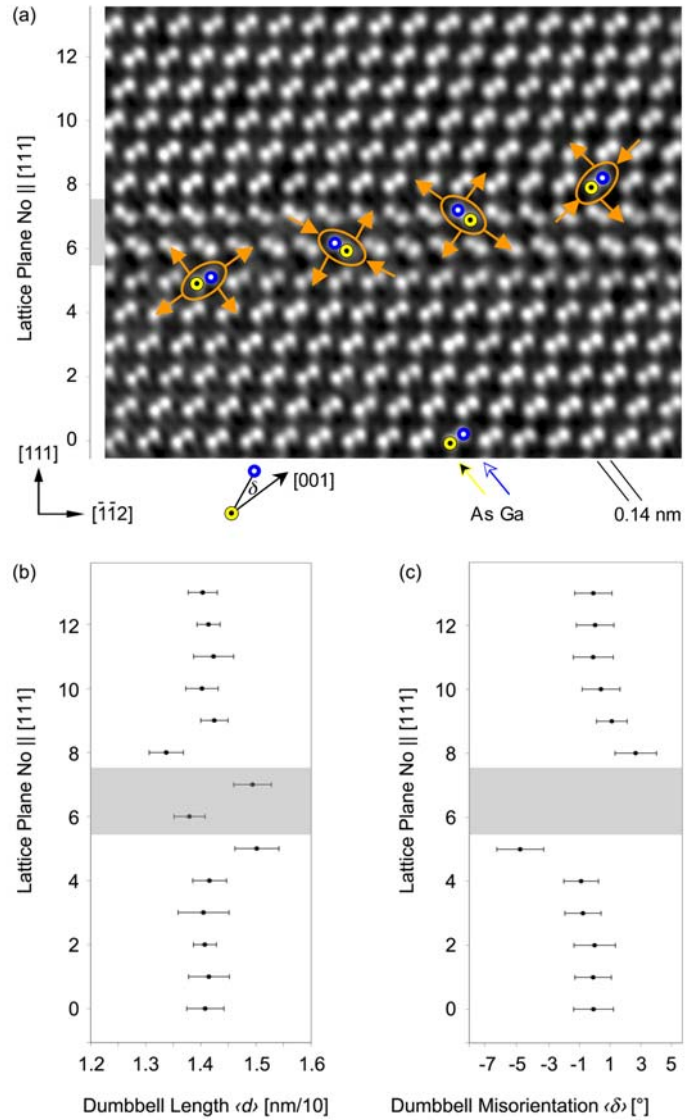


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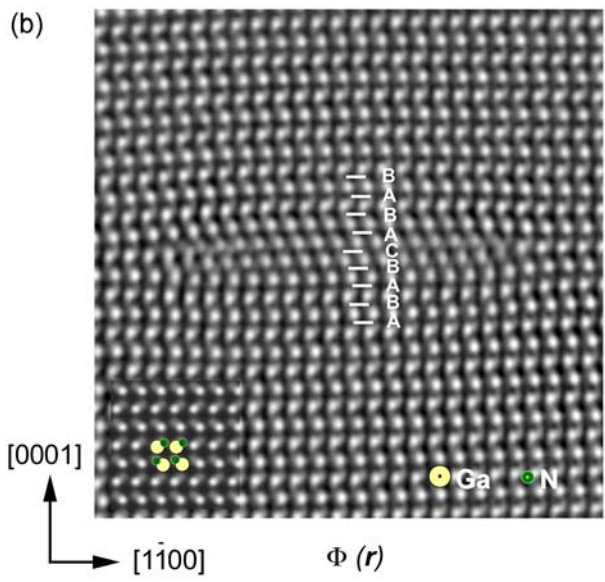
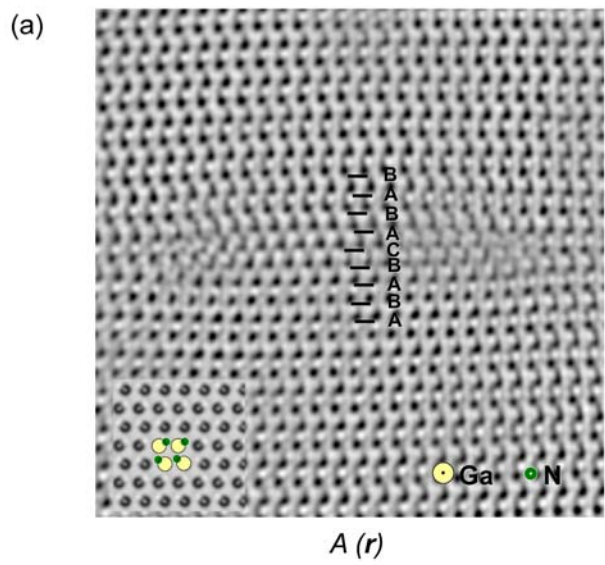
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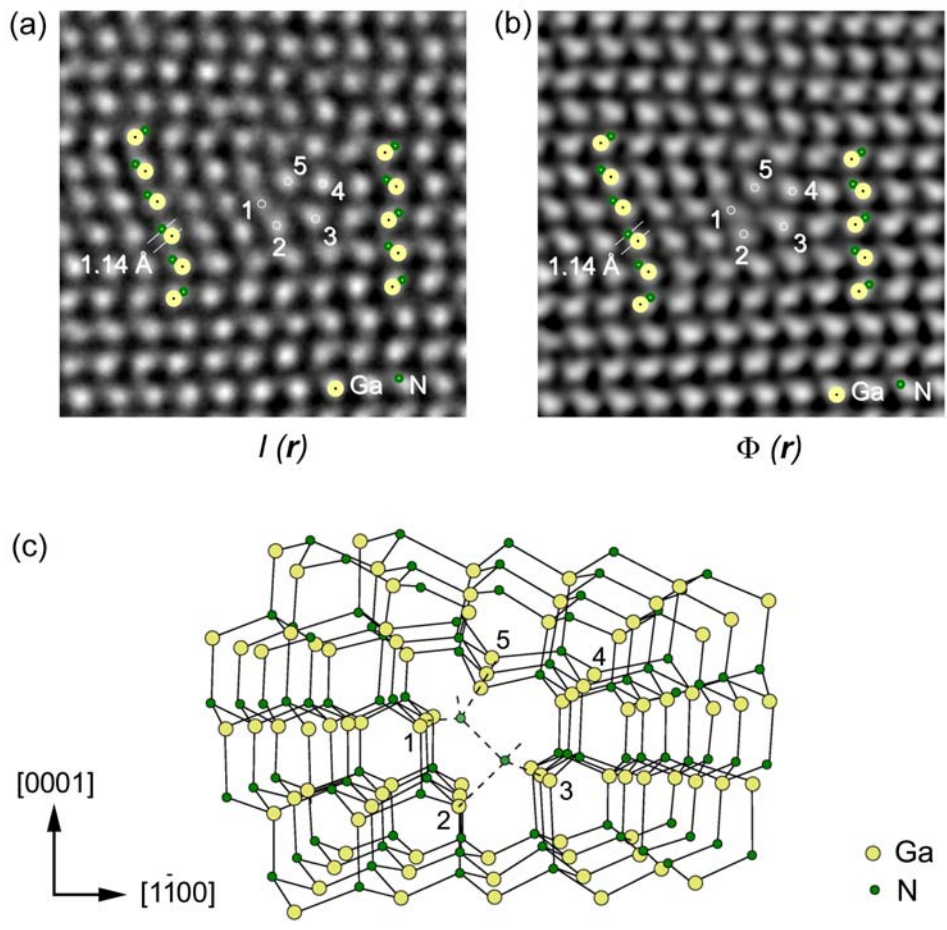
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ATOMIC-RESOLUTION IMAGING OF LATTICE IM-
PERFECTIONS IN SEMICONDUCTORS BY CON-
JOINED ABERRATION-CORRECTED HRTEM AND
EXIT-PLANE WAVEFUNCTION RETRIEVAL

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ABSTRACT

With the amelioration of the instrumental information limit and the simultaneous minimization of image delocalization, high-resolution transmission electron microscopy is presently enjoying exceeding popularity with respect to the atomic-scale imaging of lattice imperfections in solid state materials. In the present study the benefits derived from the deliberated combination of spherical aberration corrected imaging together with the numerical retrieval of the exit-plane wavefunction from a focal series of micrographs are illustrated by highlighting their combined use for the atomic-scale characterization of lattice defects frequently observed in common semiconductor materials. For these purposes, experimental analyses will review the core structure of Lomer dislocations at $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ -heterointerfaces and focus on atomic lattice displacements associated with extrinsic stacking faults in GaAs, as well as on the core structure of chromium implantation induced Frank partial dislocations in GaN at directly interpretable contrast features. Supplementary, practical advantages of the retrieval of the exit-plane wavefunction for the subsequent numerical elimination of residual lens aberrations are demonstrated.

Key words: High-resolution transmission electron microscopy, spherical aberration correction, exit-plane wavefunction reconstruction, lattice defects, dislocation core structure, stacking faults, semiconductors, GaAs, GaN

1. INTRODUCTION

Over the past fifty years, transmission electron microscopy has become the technique of choice whenever structural properties associated with lattice imperfections in solid state materials have been investigated experimentally. Even though enormous progress has been made in the characterization of dislocations, stacking faults and internal boundaries in these common semiconductor materials, there is still much to learn about the precise atomic configuration in the vicinity of these structural imperfections. Above and beyond purely scientific curiosity this task is also of technological interest as further improvements in applied semiconductor research stand in need of an amended understanding of the interaction between structural and electronic properties with advancing miniaturization [1, 2]. To put it another way, the detailed evaluation of electronic features induced by lattice imperfections and the elucidation of the atomic structure of these imperfections are interdependent [3, 4].

Recently of particular interest with high-resolution transmission electron microscopy is (i) the pursuit of sub-Ångström resolution at medium acceleration voltages [5, 6, 7] in close communion with (ii) the straightforward interpretability of micrographs [8, 9, 10] characterized by (iii) a rather low image delocalization in the vicinity of lattice imperfections [11, 12]. Two sophisticated techniques to accomplish all three of these objectives simultaneously, not within reach during operation of “traditional” medium voltage instruments equipped with field emission gun emitters, have attracted much interest in recent years.

On the one hand, double hexapole corrector elements enabling a compensation of detrimental lens aberrations are practically usable these days [13, 14]. As a result, the aberration coefficient C_s emerges as an additional parameter for extending the point resolution at phase contrast imaging conditions to the information limit together with the simultaneous maximization of phase contrast and the minimization of contrast delocalization [15]. Moreover, when employing a negative C_s value combined with a certain overfocus setting $Z_{\text{opt}} > 0$, not only a substantial contrast improvement is achieved but low-nuclear charge elements can also be imaged at bright atom contrast features in the vicinity of high-nuclear charge atoms [8, 9].

On the other hand, numerical techniques enable the restoration of the phase $\Phi(\mathbf{r})$ and the amplitude $\mathbf{A}(\mathbf{r})$ of the exit-plane wavefunction from a focal series [16, 17, 18] or an illumination tilt direction series [19, 20] of experimental micrographs. By this means, all spatial information up to (focal series) or even beyond (tilt direction series) the axial information limit of the instrument can be retrieved, also allowing for a subsequent elimination of residual lens aberrations still present in aberration corrected microscopy [21, 22, 23, 24].

The objective of the present contribution is to demonstrate the benefits accruing from the deliberated combination of both of these state-of-the-art techniques for the atomic scale imaging of structural imperfections in semiconductor materials. Special emphasize will be put on conceptual vantages for the characterization of lattice defects at atomic resolution and for the quantification of atomic column positions in the vicinity of lattice imperfections in semiconductor materials.

2. METHODOICAL BACKGROUND: NEGATIVE SPHERICAL-ABERRATION CORRECTED IMAGING IN TANDEM WITH THE NUMERICAL RETRIEVAL OF THE EXIT-PLANE WAVEFUNCTION

In aberration-corrected microscopy a high amount of negative phase contrast may be obtained simultaneously with a widely minimized image delocalization, when setting the constant of spherical aberration to an optimized value [9, 15]

$$C_S = -64/27 \lambda^{-3} g_{\max}^{-4} \quad (1)$$

and choosing an overfocus setting of the objective lens

$$Z_{\text{opt}} = 16/9 \lambda^{-1} g_{\max}^{-2} \quad (2)$$

with λ and $1/g_{\max}$ denoting the electron wavelength and information limit of the instrument, respectively. A corresponding set-up of the instrument yields direct interpretable high-resolution micrographs accompanied by a residual image delocalization of

$$R = 16/27 g_{\max}^{-1} \quad (3)$$

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5 Using an aberration corrected CM-200 FEG ST instrument, the aforementioned pa-
6 rameters amount to $Z_{\text{opt}} = 11.6$ nm, $C_S = -40.6$ μm and $R = 80$ pm when putting to
7 use an electron wavelength of $\lambda = 2.51$ pm and an information limit of $1/g_{\text{max}} =$
8 125 pm with the latter value measured from a Young's fringe analysis of images
9 taken with the microscope utilized in this study [15].

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14 The associated partially coherent phase contrast transfer function, displayed in
15 Figure 1, extends up to $1/g_{\text{max}}$ and is characterized by a broad pass-band with a phase
16 deviation close to $\pi/2$. Simplifying the imaging process to linear theory, a weak
17 phase object is then imaged under bright atom contrast conditions [25] and a sub-
18 stantial contrast improvement is achieved since the linear phase contrast and the
19 nonlinear dark field signal add rather than subtract as is usual when applying "tradi-
20 tional" high-resolution imaging modes [26]. In the strict sense Eqns. (1) to (3) base
21 upon a first order expansion of the aberration function, thus neglecting any detri-
22 mental impact of higher order lens aberrations. As the hexapole corrector of the
23 CM-200 FEG ST allows for a sufficient correction of aberrations up to the third or-
24 der [27] and higher order aberrations will become relevant not until $1/g_{\text{max}}$ becomes
25 smaller than 100 pm [28, 29], these aberrations do not need to be considered for the
26 instrument under consideration.

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37 The numerical retrieval of the exit-plane wavefunction $\Psi(\mathbf{r})$ from a focal series of mi-
38 crographs provides auxiliary improvements as it is basically free from nonlinear imag-
39 ing artifacts and the impact of the low frequency gap in information transfer is con-
40 siderably reduced by the combination of many images taken at different foci. As im-
41 provements of the instrumental resolution limit still gather pace, this aspect is of
42 special importance when imaging common semiconductors at atomic resolution
43 since the structural information is predominantly carried by the low-frequency {111}
44 reflections. Furthermore, by extracting information from about $N = 20 \dots 30$ images,
45 the signal-to-noise ratio at high spatial frequencies can be substantially increased.
46 Even the application of small C_S values, which is a prerequisite to obtain phase con-
47 trast, induces a parasitic delocalization whereas $\Psi(\mathbf{r})$ is ideally free from any delocali-
48 zation induced artifacts.
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Moreover, the availability of $\Psi(\mathbf{r})$ allows for the numerical *a posteriori* measurement of residual lens aberrations. This aspect is of special practical importance as experience shows that not all aberrations of the microscope are sufficiently constant over the period of operation or cannot be determined before the experiment with sufficient accuracy. In detail, the measurement of even aberrations, i. e. the defocus Z and the twofold astigmatism A_1 , may be carried out by processing the weak signal originating from amorphous overlayers [21] while odd aberrations, i. e. the axial coma B_2 and the threefold astigmatism A_2 , may be determined by sampling a variety of discrete aberration azimuths and magnitudes up to twice their arguable limits according to [27] followed by handpicking those aberrations at which the symmetry properties of the corresponding $\Phi(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ images correlate best with the supposed lattice structure [22]. Irrespective of this procedure even more sophisticated approaches are available to tackle the problem of measurement of odd aberrations [30].

Finally, since $\Psi(\mathbf{r})$ is complex-valued, we may evaluate “local” diffraction patterns from specimen areas as small as desired. When evaluated during operation of the microscope, the judgement of the symmetry properties of these “local” diffraction patterns is a most convenient tool for the proper orientation of specimen areas under investigation. By this means, a proper zone axis alignment of the samples with an accuracy below 3 mrad is ensured while the vast majority of samples aligned by “traditional” procedures demonstrates off-zone-axis orientations above 10 mrad [31].

To set aright the common fallacy that the aforementioned benefits coming along with the restoration of the exit-plane wavefunction do not necessitate the use of spherical aberration corrected instrumentation but rather suggest an increase of the instrumental resolution solely, e. g. by monochromatisation of the electron source, it is emphasized that the *a posteriori* measurement of residual lens aberrations requires a sufficient pre-reduction of the very same aberrations. Moreover, image delocalization in a non-corrected instrument will generally not be less than [11]

$$R_L = C_S / 4 \lambda^3 g_{\max}^3 \quad (4)$$

and only to be within reach at Lichte's defocus of least confusion

$$Z_L = -3/4 C_S \lambda^2 g_{\max}^2 \quad (5)$$

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5 which, alas, comes along with the great disadvantage that the phase contrast transfer
6 function exhibits a large number of rapid contrast oscillations at medium spatial fre-
7 quencies, and the corresponding contrast reversals make the resulting image quite
8 difficult to interpret. Moreover, image delocalization according to Eqn. (4) does not
9 only have a detrimental effect on the spread out of structural information in the vi-
10 cinity of lattice imperfections but also to data acquisition at marginal areas of the
11 recording medium. In other words, the rather large image delocalization of uncor-
12 rected instruments represents a serious limitation for the usable field of view of the
13 charge-coupled device (CCD) camera detector.
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24 3. EXPERIMENTAL SETUP

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26 This study utilizes a Philips CM-200 FEG instrument equipped with a computer-
27 controlled electromagnetic hexapole system for the correction of the spherical aber-
28 ration of the objective lens [27]. An optical coarse adjustment of the hexapole correc-
29 tor elements was performed by analysing Zemlin tableaux taken from amorphous
30 specimen areas with an incident electron beam tilted up to 20 mrad from the optical
31 axis [32] thus yielding an initial estimate on the quality of higher-order aberration
32 corrections. Setting down an optimized negative $C_s = -40 \mu\text{m}$ the magnitudes of re-
33 sidual aberration coefficients were limited to $A_1 \leq 2.0 \text{ nm}$ for the two-fold astigma-
34 tism, to $A_2 \leq 170 \text{ nm}$ for the three-fold astigmatism and to $B_2 \leq 55 \text{ nm}$ for the axial
35 coma [27].
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44 Focal series of about $N = 20 \dots 30$ images were recorded using a 1k x 1k CCD cam-
45 era system at a sampling rate of about 20 pm per picture element. This corresponds
46 to an image discretization well below the Nyquist frequency with respect to half of
47 the instrumental information limit $1/(2 g_{\text{max}}) = 65 \text{ pm}$ and represents an adequate
48 sampling to tap the full potential of the instrument facing that the modulation trans-
49 fer function of many CCD cameras is known to exhibit a rather poor transfer at
50 higher spatial frequencies. The focal range of each series included the focus setting
51 with $Z_{\text{opt}} = 11.6 \text{ nm}$ for optimized phase contrast. From these series the exit-plane
52 wavefunction was retrieved for the frequency band between 1 nm^{-1} and 8 nm^{-1} apply-
53 ing a doughnut-shaped restoration filter.
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4. ATOMIC RESOLUTION IMAGING AT A DECENT SIGNAL-TO-NOISE RATIO: CORE STRUCTURE OF MISFIT DISLOCATIONS AT $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ /GaAs HET- EROINTERFACES

As a first materials science example of use, we report on the core structure of Lomer type pure edge dislocations [33] at the heterointerfaces between lattice-mismatched sphalerite semiconductors. In view of the multiplicity of conceivable lattice positions of the pulled out half-plane's terminal point, numerous core models have been proposed for this type dislocations [34, 35] but owing to the hitherto insufficient instrumental resolution previous high-resolution analyses required elaborate support by numerical image simulations merely to draw indirect conclusions on the corresponding dislocation core structures [36, 37, 38].

In the present analysis we focus on an $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayer with a thickness of 35 nm that was grown by molecular beam epitaxy on a GaAs(001) substrate and subsequently overgrown with a GaAs capping layer of 55 nm in thickness whereby growth conditions were chosen as specified in a previous analysis [39].

Figure 2(a) displays an optimum focus micrograph $I(\mathbf{r})$ of a Lomer dislocation with a Burgers circuit yielding a projected closing vector $\mathbf{b} = a/2 [\bar{1}\bar{1}0]$ in the proximity of the interface between the $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayer and the GaAs(001) substrate viewed with a $[1\bar{1}0]$ zone axis orientation of the sample. Far-off the dislocation core, the image contrast is dominated by clearly separated pairs of contrast dots constituting atomic dumbbells at distances of $a/4 \approx 141$ pm with $a = 565$ pm denoting the lattice parameter of the substrate material.

However, two conspicuous contrast artifacts become evident from close inspection of the Z_{opt} micrograph of the GaAs matrix displayed in Figure 2(e). Firstly, non-structure related spurious intensity peaks are observed in between the atomic column positions which are due to an expended transfer of low spatial frequencies at severe phase offsets, especially of the strongly excited $\{111\}$ beam amplitudes [26]. Secondly, a kidney-shaped distortion of the dumbbells is observed. As can be shown from quantitative measurements on the associated "local" diffraction pattern dis-

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5 played in Figure 2(b), these distortions are not due to any potential misorientation of
6 the sample but instead result from parasitic lens aberrations amounting to
7 $A_1 = 2.2 \text{ nm}$ (83°), $B_2 = 110 \text{ nm}$ (83°), and $A_2 = 150 \text{ nm}$ (43°) with the values in pa-
8 rentheses indicating the respective azimuth angles inclined with the [001] direction
9 [31]. For that reason, the phase $\Phi_{\text{unc}}(\mathbf{r})$ of exit-plane wavefunction retrieved from a
10 focal series of $N = 30$ micrographs and displayed in Figure 2(e) still shows distortions
11 of the contrast dumbbells as long as these residual aberrations are not considered
12 during the initial step of the reconstruction process. By contrast, the phase image
13 $\Phi(\mathbf{r})$ is free of any distortions after the above specified aberrations A_i and B_i have
14 been eliminated [31].
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23 Above and beyond this, the phase image is also richer in contrast compared to the
24 Z_{opt} micrograph since there are practically no limitations with respect to the temporal
25 and spatial coherence, thus providing a superior signal-to-noise ratio at high frequen-
26 cies up to the information limit. Additionally, the retrieved phase benefits from the
27 averaging of information from a complete series of micrographs. When quantifying
28 the signal-to-noise-ratios σ_Φ and σ_I of the $\Phi(\mathbf{r})$ and $I(\mathbf{r})$ images, respectively, by apply-
29 ing analysis procedures outlined in [40] an improvement through the restoration of
30 the exit-plane wavefunction by a factor of $(\sigma_\Phi/\sigma_I)_{\text{exp}} = 4.1$ is obtained. This value is in
31 excellent agreement with the ideal factor of $(\sigma_\Phi/\sigma_I)_{\text{th}} = \sqrt{N}/2 = \sqrt{30}/2 = 3.9$ to be
32 expected for information retrieval from a focal series of $N = 30$ micrographs.
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41 When also determining the polarity of the sample by the evaluation of a set of rele-
42 vant reciprocal-space amplitudes from the “local” diffraction pattern and the subse-
43 quent trimming of simulated data, individual bright contrast dots in the $\Phi(\mathbf{r})$ image
44 may be directly associated with gallium and arsenic columns [31]. Corresponding
45 atomic species are indicated in Figure 2(e).
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50 The essential benefit of the combined use of the numerical retrieval of the exit-plane
51 wavefunction with aberration-corrected imaging, however, becomes evident when
52 having a closer look at the atomic structure of the dislocation core, which is basically
53 not resolved in the single optimum focus image $I(\mathbf{r})$ but only in the amplitude and
54 phase images, respectively. Both, $A(\mathbf{r})$ and $\Phi(\mathbf{r})$, show the atomic arrangement down
55 to the dislocation core and reveal a detached atomic column at the point of intersec-
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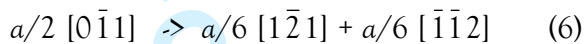
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5 tion of extrapolated line positions indicated by the horizontal and vertical arrows.
6 Relevant contrast features show mirror symmetry with respect to the medial ($\bar{1}\bar{1}0$)
7 lattice plane indicated by the upright arrows. This global symmetry behaviour ranges
8 down to the dislocation core.
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12 From the exit-plane wavefunction a core structure model according to Figure 3(a)
13 can be deduced as contrast features are intuitively interpretable. The dislocation
14 core shows some similarity to the glide set type model of a Lomer dislocation origi-
15 nally proposed by Hornstra [34] which is displayed in Figure 3(b) and characterized
16 by an eight-atomic inner ring. The present analysis, however, reveals a less compact
17 core, which is build up of a ten-sided polygon also traversing the detached atomic
18 column with a coordination different from the surrounding matrix. This structure
19 also deviates from rather complex mirror symmetric configurations observed at
20 GaAs/Si interfaces [36, 41] and in Ge/Si heterosystems [38]. As surface effects in the
21 vicinity of the highly strained dislocation core are likely to occur in thin electron mi-
22 croscopy specimens, the retrieved core structure may certainly deviate from that of a
23 dislocation core embedded in bulk material. This problem, however, exists in any
24 high-resolution analysis concerned with lattice defects raising rather strong lattice
25 distortions.
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37 Referring to a detailed discussion of the matter [31] we briefly summarize the causal
38 connections impeding the resolvability of the dislocation core in the Z_{opt} image but
39 evidently not in the retrieved exit-plane wavefunction. Numerical image calculations
40 give clear evidence that this non-resolvability in the single $\mathbf{I}(\mathbf{r})$ image will neither be
41 due to (i) the residual image delocalization or (ii) a decreased sample thickness in the
42 vicinity of the dislocation core. Moreover, a potential impact of (iii) a locally inho-
43 mogeneous strain relaxation of the thin specimen may be ruled out since, otherwise,
44 the $\mathbf{A}(\mathbf{r})$ and $\Phi(\mathbf{r})$ images would similarly be affected. Instead, the practically im-
45 proved resolution of the amplitude and phase images will be rather due to (iv) an
46 increased resistibility against time-dependant electron beam induced degeneration of
47 the sample. While numerical retrieval techniques purge information from intrinsi-
48 cally unstable amorphous overlayers by averaging, a single Z_{opt} micrograph simply
49 represents merely a snap-shot of a sample under illumination with a certain probab-
50 ility of an adverse atomic overlayer assembly during the time of exposure [31].
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5. GEOMETRIC LINEARITY AT HIGH-LEVEL PRECESSION: LATTICE DISTORTIONS ASSOCIATED WITH DISSOCIATED 60° DISLOCATIONS IN GAAS (110)

In sphalerite materials 60° dislocations with a Burgers vectors of type $\mathbf{b} = a/2 \langle 0\bar{1}1 \rangle$ may dissociate into two partials bounding either an intrinsic or an extrinsic stacking fault [42, 43, 44, 45]. The dissociation reaction is:



with the Burgers vectors of both partials inclining angles of 30° and 90° with the dislocation line along the $[1\bar{1}0]$ direction, respectively. While most analyses at the outset of quantitative high-resolution microscopy were primarily concerned with distinguishing glide and shuffle set dislocations, i. e. discriminating whether dislocations cores lie on the narrowly or widely spaced $\{111\}$ planes, by interpreting characteristic contrast features in the vicinity of the dislocations cores [46, 47, 48], it is only recently that efforts have been put forth to investigate the core structure of 30° and 90° partials, both theoretically applying *ab initio* calculations [49, 50, 51] and experimentally employing advanced electron microscopy techniques [52, 53].

In the following we shall focus on a dissociated 60° dislocation bounding a double stacking fault ribbon. Figure 4(a) displays an optimum micrograph $I(\mathbf{r})$ of the terminating zone of such an extended dislocation in GaAs viewed along the crystallographic $[1\bar{1}0]$ direction. The image has been taken from the same specimen investigated in the previous section focusing on the GaAs capping layer in this case. The associated phase $\Phi(\mathbf{r})$ and amplitude $A(\mathbf{r})$ images displayed in Figure 4(b) and (c) allow for an accurate identification of the atomic arrangement of the stacking fault ribbons and, especially, the core structure of the dislocation terminating the defect.

As the overall lattice defect is composed of two adjacent (111) lattice planes showing similar misorientations of the atomic dumbbells, it appears inceptively reasonable to describe the entire defect as a sequence of two adjoining likewise congenerous faulted fault ribbons. Both ribbons need then to be characterized by a projected component of the terminating Burgers vector amounting to $\mathbf{b}_{\text{proj}}/2$ with \mathbf{b}_{proj} denoting the closing vector of the entire defect when considering a projection to the $(1\bar{1}0)$

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5 plane. Assuming a configuration build-up by 30° partials, characterized by $\mathbf{b}_{30^\circ-A} =$
6 $a/6 [1\bar{2}1]$ as well as $\mathbf{b}_{30^\circ-B} = a/6 [\bar{2}11]$ and yielding $\mathbf{b}_{\text{proj},30^\circ-A/B} = a/12 [\bar{1}\bar{1}2]$, the as-
7 sociated total lattice displacement along the $[\bar{1}\bar{1}2]$ direction between the upper and
8 the lower areas of the crystal far from the dislocation core should be $\Delta u_{\bar{1}\bar{1}2,30^\circ} =$
9 $2 \mathbf{b}_{\text{proj},30^\circ} = 231$ pm. This description is fully compatible with the definition of an ex-
10 trinsic stacking fault bound by a 90° partial with $\mathbf{b}_{90^\circ} = \mathbf{b}_{\text{proj},90^\circ} = a/6 [\bar{1}\bar{1}2] = 231$ pm
11 and a 30° partial with $\mathbf{b}_{\text{proj},30^\circ} = a/12 [\bar{1}\bar{1}2] = 115$ pm at the opposite core position.
12 Both of these limiting partials are in fact again superpositions of 30° and 90° partials
13 separated by two atomic layers [45] with the extrinsicity expressing in two adjacent
14 ribbons of $\{111\}$ lattice planes with differently aligned atomic [54].
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23 To check the validity of this model hypothesis, the elastic displacement component
24 $u_{\bar{1}\bar{1}2}$ along the $[\bar{1}\bar{1}2]$ direction has been evaluated from the $\Phi(\mathbf{r})$ image using geomet-
25 rical phase analysis algorithms [55]. Calculations have been performed applying
26 Gaussian shaped masks with decay parameters $\sigma = |\mathbf{g}_{111}|/3$ centred around the \mathbf{g}_{111}
27 beams thus averaging information over regions of about $r_{\text{dir}} \approx 3 / (2 |\mathbf{g}_{111}|) \approx 490$ pm
28 in radius at most [56]. The correspondingly measured $u_{\bar{1}\bar{1}2}(\mathbf{r})$ distribution is displayed
29 in Figure 4(e) together with a line profile $u_{\bar{1}\bar{1}2}(\mathbf{r}_{\bar{1}\bar{1}\bar{1}})$ extracted from this distribution
30 along the $[\bar{1}\bar{1}\bar{1}]$ direction, cf. Figure 4(e). For the latter, data values have been aver-
31 aged over a width of 1 nm, i. e. over the width of the drawn-in dashed blue frame.
32 The line profile shows two conspicuous plateaus separated by an abrupt discontinu-
33 ity of $\Delta u_{\bar{1}\bar{1}2} = 234$ pm \pm 60 pm. This quantity is in excellent agreement with the clos-
34 ing vector associated with the 90° partial of an extrinsic stacking fault for which a
35 total shift of lattice planes of $\Delta u_{\bar{1}\bar{1}2,30^\circ} = 2 \mathbf{b}_{\text{proj},30^\circ-A/B} = 231$ pm is expected, cf. above.
36 We emphasize that the specified margin of error in the $\Delta u_{\bar{1}\bar{1}2}$ value rather reflects in-
37 homogeneous lattice distortions of the sample but not the fundamental accuracy to
38 quantify atomic column positions which may be measured to a precision of about a
39 few picometres [57, 58].
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53 In Figure 4(d) single atomic columns, as allocated from the determination of the po-
54 larity of the sample, are superimposed to a magnified clipping of the phase image.
55 The global displacement of the upper and lower crystal areas against each other is
56 found to be mediated by the local re-organization of the atomic columns within
57 those two (111) lattice planes forming the faulted double ribbon. Hence, the associ-
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ated dislocation cores of both partials, indicated by red circles in the figure, also lie on these very same (111) planes. As these planes are narrowly spaced, the partial dislocations are of glide set type. Both dislocation cores are made up of gallium columns leading to a so-called β dislocation [59]. Moreover, the figure also reveals a symmetrical six-fold structure of the overall dislocation core, which is in perfect agreement with a 90° partial dislocation composed of two 30° partials separated by two atomic layers [45].

To put it a step further, we may also quantify local distortions of the atomic dumbbells across the faulted ribbon at some distance of the dislocation core. For these purposes contrast dot positions have been measured from the $5.5 \text{ nm} \times 4.2 \text{ nm}$ phase image $\Phi(\mathbf{r})$ area displayed in Figure 5(a), whose centre is 5.2 nm left of the dislocation core. For these purposes a digital image processing algorithm [60] has been applied which basically employs (i) dedicated image intensity thresholding operations, (ii) a centre-of-mass analysis inside individual bright contrast dots supported by (iii) adequate refining procedures as specified in [61, 62]. From the measured contrast dot positions, the length and orientation of individual dumbbells have been calculated and normalized to mean values associated with the lower (planes no. 0 - 3) and upper (planes no. 11-13) areas of the $\Phi(\mathbf{r})$ image. For the improvement of statistics 15 data points have been averaged along the $[\bar{1}\bar{1}2]$ direction and median values are plotted in Figure 5(b) and (c) in dependence on specific (111) lattice plane positions.

As can be seen from both plots, the dumbbells on either side of the double ribbon rearrange roughly antisymmetric in the vicinity of the faulted (111) planes. In this context, the most conspicuous feature is that the dumbbells of the bottommost lattice plane of the upper crystal domain (plane no. 8) are compressed to a length of $\langle d \rangle = 133 \text{ pm} \pm 4 \text{ pm}$ and turn towards the double ribbon with a misorientation angle $\langle \delta \rangle \approx 2.6^\circ \pm 1.3^\circ$ compared to the reference lattice planes. In contrast, the uppermost dumbbells of the lower crystal area (plane no. 5) are stretched to a length of $\langle d \rangle = 150 \text{ pm} \pm 4 \text{ pm}$ and bend away from the double ribbon at a misorientation angle of $\langle \delta \rangle \approx -4.9^\circ \pm 1.5^\circ$.

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5 In order to gauge whether the observed antisymmetric distortions represent a genu-
6 ine structural property or not, potential implications of scattering and imaging arte-
7 facts need to be ruled out. Since a hypothetic global misalignment of the sample
8 cannot give rise to any local torsion and dilatation of projected atomic dumbbells we
9 may disenfranchise from this explanation. An argument of the same kind holds true
10 of the potential impact of not fully compensated aberrations as they would take ef-
11 fect on the entire image and, hence, would distort all atomic dumbbells of the same
12 orientation equally. Strictly speaking any potential impact of both, on-axial and off-
13 axial aberrations would need be evaluated separately. In practise this conceptional
14 differentiation can, however, be neglected because of the rather limited field of view
15 of the CCD detector and the semiamplanatic imaging properties of the double
16 hexapole corrector [13]. Beyond electron-optical reasoning, a supposed strictly anti-
17 symmetric lattice distortion caused by a dedicated combination of higher order aber-
18 rations with the faulted ribbon incidentally acting as the symmetry plane, may be
19 ruled out from a probability point of view because of an almost immense number of
20 possible combinations which will not give raise to the observed distortion behaviour.
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33 The observed alteration of atomic dumbbell lengths in the vicinity of stacking faults
34 ribbons of about 10 pm is in fair agreement with recent measurements of lattice dis-
35 tortions along intrinsic stacking faults ribbons in heavily beryllium doped GaAs.
36 This analysis revealed an average expansion of dumbbell lengths up to 158 pm in the
37 faulted lattice plane which was explained by the segregation of beryllium dopant at-
38 oms and the subsequent formation of antisite defects inside of the plane of the
39 faulted ribbon [53]. Additionally, lattice displacements around the central stacking
40 fault of Z-shaped dipoles connecting two stair rod dislocations in indium doped
41 GaAs revealed the very same antisymmetric distortion of dumbbell related contrast
42 dots as were observed in the present analysis. Lateral displacements of gallium and
43 arsenic atom pair related contrast features along the $[\bar{1}\bar{1}2]$ direction were found to
44 be as much as 20 % to 50 % of the dumbbell length [63].
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54 As the specimen investigated in the present study was undoped we may, in the first
55 instance, rule out the aforementioned explanations but only speculate about an in-
56 dium diffusion from the underlying $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ layer to the GaAs layer along the
57 faulted ribbon at most. As long as an inhomogeneous incorporation of indium at-
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oms is not considered this approach, thus, cannot explain the observed lattice distortions. Admittedly, the antisymmetric distortions become perspicuous when considering the elastic distortions associated with the 90° partial dislocations which basically follow the measured characteristics of the dumbbell's measured expansion and torsion but, alas, yield only alterations of dumbbells lengths smaller than ± 3 pm and misorientation angles smaller than $\pm 0.4^\circ$ for the image area under investigation [54]. Hence, a more likely explanation could be that the terminating partial dislocation biases the rearrangement of atomic columns in the vicinity of the faulted ribbons and that next but one neighbour interactions between different atomic species will indeed play an important role during this process.

6. ATOMIC STRUCTURE OF CHROMIUM IMPLANTATION INDUCED LATTICE DEFECTS IN GAN (1120)

As a finale example, we report on dislocations introduced by chromium implantation into GaN. Implantation of transition metals into semiconductors is a candidate process for the fabrication of diluted magnetic semiconductors for spintronic applications [64]. A by-product of the implantation is the creation of ion-induced lattice defects: Extrinsic and intrinsic basal plane stacking faults, bounded by Frank partial or Shockley-Frank partial dislocations, are formed as the result of the precipitation of excess interstitials [54, 65].

The GaN films presented in this study were grown by metal organic chemical vapour deposition on (0001) oriented sapphire substrates under Si doping to a concentration of $2 \times 10^{17} \text{ cm}^{-3}$. Cr^+ ions were implanted with an energy of 200 kV and a dose of $5 \times 10^{16} \text{ cm}^{-2}$ at a temperature of 350°C to avoid amorphization in the as-implanted samples. A high density of basal plane stacking faults is observed besides spherical Cr-rich precipitates in surface near regions after chromium implantation and rapid thermal annealing at 700°C for 5 min in N_2 atmosphere [66].

The majority of the basal plane stacking faults is extrinsic bound by Frank partial dislocations with Burgers vector $\mathbf{b} = 1/2 [0001]$. Figure 6 displays the amplitude image $A(\mathbf{r})$ and phase image $\Phi(\mathbf{r})$ of a perfect nanometre sized interstitial loop in the

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5 end of range depth of implantation. Gallium and nitrogen columns at a dumbbell
6 distance of 114 pm, considerably smaller than the information limit of the instru-
7 ment, are not fully resolved. Nonetheless the N-polarity is unambiguously visible
8 from the directly interpretable bright contrast in the phase image. The tetrahedral
9 coordination across the faulted layer stacking is confirmed, asserting that no foreign
10 chromium-gallium alloy phase is connected with the planar defects.
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16 A magnified view of the core of a Frank partial dislocation at the terminating zone of
17 a several 10 nm large dislocation loop is shown in the Z_{opt} image and the $\Phi(\mathbf{r})$ image
18 retrieved from a corresponding focal series displayed in Figure 7(a) and (b). Although
19 the $I(\mathbf{r})$ and $\Phi(\mathbf{r})$ appear very similar at a first glance, the improved signal-to-noise
20 ratio in the phase image enhances the visibility of the nitrogen positions and the
21 dumbbell orientation up to the core of the dislocation. The phase image $\Phi(\mathbf{r})$ forti-
22 fies the presence of further nitrogen atoms within the core surrounded by the cage of
23 the five marked gallium columns. The faint phase shift in $\Phi(\mathbf{r})$, in which non-linear
24 image components and image delocalization are eliminated, indicates a nitrogen
25 filled core in favour of a chromium or gallium rich core.
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34 Based on these observations a tentative 5/7 ring configuration for the core is pre-
35 sented in Figure 7(c). The nitrogen atoms shared by the 5- and 7-membered rings are
36 threefold coordinated with Ga and N. Due to the wrong bond and the presence of
37 unpaired electrons, this structure is not expected to be the most stable configuration.
38 Since $\Phi(\mathbf{r})$ is retrieved from a focal series taken over a period of a few ten seconds,
39 the image conceivably reflects a transient state of the core that gathers further inter-
40 stitials during observation. The Z_{opt} image level may therefore contain complemen-
41 tary but not necessarily identical information when compared to $\Phi(\mathbf{r})$. Indeed for the
42 present case the Z_{opt} image with its inferior noise level compared to $\Phi(\mathbf{r})$ also com-
43 plies an alternative structure which contains two wrong Ga-Ga bonds connecting
44 threefold coordinated Ga atoms at positions 1-5 and 2-3, respectively.
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56 7. CONCLUSIONS

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In summary, a combination of negative spherical aberration imaging and the restoration of the exit-plane wavefunction from a focal series of micrographs has been applied for the investigation of lattice imperfections in semiconductor materials at atomic resolution and, in particular, for the extraction of quantitative information on local lattice distortions.

It has been demonstrated that recent improvements in the resolution power of transmission electron microscopes enable the imaging of finest structure details at directly interpretable contrast features also coming along with a widely minimized image delocalization when micrographs are taken under optimized imaging conditions.

Additionally, the numerical retrieval of the exit-plane wavefunction allows for the elimination of artificial contrast features still visible in micrographs taken under optimized focusing conditions. Beyond its genuine purpose, the retrieval of the exit-plane wavefunction was demonstrated to be a most suitable tool for the measurement and numerical correction of residual lens aberrations as well as for proper orientation of specimens during operation of the electron microscope.

Above and beyond the individual advantages coming along with either technique their combined use allows for the accurate identification of lattice imperfections in semiconductor materials at hitherto unequalled imaging. Experimental analyses conspicuously benefit from putting to use aberration corrected input data, i.e. from an increase of the instrumental information limit together with a decrease of image delocalization and a pre-reduction of lens aberrations, as well as from the complete elimination of residual aberrations by the numerical retrieval of the exit-plane wavefunction, which is also free from non-linear imaging artefacts and yields images characterized by a decent signal-to-noise ratio.

By means of the deliberated combination of both techniques, Lomer dislocation cores at $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ heterointerfaces have been imaged at atomic resolution and directly identified as being composed of a mirror symmetric ten-atomic ring, thus rendering extensive image simulations superfluous. The quantification of local lattice distortions in the vicinity of a double stacking fault ribbon in GaAs by means of the analysis of experimental phase images $\Phi(\mathbf{r})$ brought clear evidence of an anti-

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5 symmetric torsion and expansion of atomic dumbbells with respect to the faulted
6 ribbon. A similar quantitative analysis focusing on lattice imperfections in GaN at
7 atomic resolution based on the synergetic combination of negative spherical aberration
8 corrected imaging and the numerical retrieval of the exit-plane wavefunction is
9 presently merely hampered by the instrumental resolution but will come along with
10 forthcoming aberration corrected sub-Ångström resolution microscopes.
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15 16 17 18 19 **ACKNOWLEDGEMENTS**

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22 the samples investigated in this study as well as Doris Meertens for indefatigable
23 specimen preparation work.
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FIGURE CAPTIONS

Figure 1: Partially coherent contrast transfer function (PC CTF) together with the coherent transfer function (CTF) and the damping envelope (DE) assuming parameters $\lambda = 2.51$ pm, $C_s = -40.6$ μm , $Z = 11.6$ nm as well as 0.2 mrad for the semi-angle of beam convergence and 6.4 nm for the half-width of the Gaussian spread of defocus. Arrows indicate positions of crystalline reflections in GaAs.

Figure 2: Analysis of a Lomer type dislocation with $\mathbf{b} = a/2 [\bar{1}\bar{1}0]$ at an $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$ heterointerface. **a:** Optimum focus micrograph $\mathbf{I}(\mathbf{r})$ taken along the $[\bar{1}\bar{1}0]$ zone axis orientation of the sample. **b:** “Local” diffraction pattern evaluated from the exit-plane wavefunction of the image area. **c:** Restored phase image $\Phi(\mathbf{r})$ and **d:** amplitude image $\mathbf{A}(\mathbf{r})$. **e:** Magnified clipping of the GaAs related image area together with the associated phase images $\Phi_{\text{unc}}(\mathbf{r})$ and $\Phi(\mathbf{r})$ obtained when neglecting and considering measured residual lens aberrations, respectively.

Figure 3: Dislocation core models for symmetrical Lomer dislocations. **a:** Model retrieved from the exit-plane wavefunction displayed in Figure 2 together with **b:** the symmetrical glide set type core model according to Hornstra [34].

Figure 4: Analysis of an extrinsic stacking fault in GaAs bound by two adjacent 30° partial dislocations with $\mathbf{b}_{\text{proj}} = [\bar{1}\bar{1}2]$ in total. **a:** High-resolution micrograph $\mathbf{I}(\mathbf{r})$ taken under Z_{opt} conditions. **b:** Phase image $\Phi(\mathbf{r})$ and **c:** amplitude image $\mathbf{A}(\mathbf{r})$ calculated from the associated focal series of micrographs. **d:** Magnified clipping of $\Phi(\mathbf{r})$ with the positions of atomic columns superimposed and the dislocation core positions of 30° partials indicated by red circles. **e:** Contour representation of the lattice displacements along the $[\bar{1}\bar{1}2]$ direction with reference to the dashed red framed area. **f:** Displacement profile measured perpendicular to the faulted ribbon at the area indicated by the dashed blue frame.

Figure 5: Locally inhomogeneous distortions of the atomic dumbbells in the vicinity of the faulted double ribbon. **a:** Clipping from the phase image displayed in Figure 4(b) with atomic column positions superimposed and dumbbell distortions indicated exemplarily in dependence on specific positions along the $[111]$ direction.

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5 **b**: Average projected bond length $\langle d \rangle$ and **c**: misorientation angle $\langle \delta \rangle$ of the dumbbells
6 along the (111) direction. The lattice planes belonging to the double stacking fault
7 ribbon are indicated in lighter grey colour.
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11 **Figure 6:** Interstitial loop in Cr-implanted GaN viewed along the $[11\bar{2}0]$ direction.
12 **a**: Amplitude image $A(\mathbf{r})$ and **b**: phase image $\Phi(\mathbf{r})$ calculated from a focal series of
13 micrographs. Simulated images of the periodic N-polarity GaN structure assuming a
14 sample thickness of 3.2 nm at a resolution of 7.5 nm^{-1} are superimposed in the lower
15 left part of the images. The stacking sequence is ABABCABAB, where the under-
16 lined part highlights sphalerite stacking.
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22 **Figure 7:** Frank partial dislocation with the Burgers vector $\mathbf{b} = 1/2 [0001]$ projected
23 along the $[11\bar{2}0]$ direction. **a**: Experimental micrograph $I(\mathbf{r})$ taken under Z_{opt} condi-
24 tions and **b**: correspondingly retrieved phase image $\Phi(\mathbf{r})$. **c**: 5/7 ring configuration
25 for the core of the Frank partial dislocation.
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