Quantitative Z-contrast atomic resolution studies of semiconductor nanostructured materials

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Abstract. High angle annular dark field (HAADF) scanning transmission electron microscopy has demonstrated the capability to achieve sub-Angstrom resolution in the study of the structure of materials. Furthermore, the sensitivity of HAADF imaging to fine variations of the chemistry of the specimen allows one to derive the relevant chemical map from the intensity distribution in an image. Here, a general approach to calculate the HAADF image intensity for an alloy is derived and applied to experimental images to measure quantitatively the distribution of the chemical species. The calculations of HAADF image contrast have been performed by multi-slice methods in the framework of the frozen-phonon approximation by developing and using a parallel code to strongly reduce the computing time necessary to obtain a reliable simulation of realistic specimens. The parameters that influence the HAADF image contrast have been studied and their role has been quantified. Experimental examples of quantification of the chemistry of semiconducting heterostructures will be shown. Attention will be focused on the different parameters that influence the HAADF image contrast depending on the material system and on the specimen composition.

1. Introduction
Transmission Electron Microscopy (TEM) has been a main methodology for the study of the solid-state matter for more than half a century. The success of TEM is related to its capability to provide reliable information on the properties of the materials, at the highest spatial resolution, and to its flexibility to tackle a wide range of problems providing, over the years, different methods to solve old and new issues in the knowledge of solid state matter. Certainly, the capability of electron microscopy to provide images capable to show and measure important specimen properties is a big part of its success and popularity. The goal is to achieve knowledge of the crystal structure and perfection, chemistry, electronic structure and magnetic properties, at the highest spatial resolution. In the last years, high angle annular dark field (HAADF) imaging in scanning transmission electron microscopy (STEM) has played a big role in this direction. HAADF provides images of crystals, oriented in a given zone axis, achieving sub-Angstrom resolution [1]; the position of the atomic columns, projected on the observation plane, is visible as white dots for a relatively wide range of objective lens defoci and specimen thicknesses [2]. These features often make the interpretation of high resolution HAADF images much more straightforward compared to phase contrast high resolution TEM (HRTEM), where the distribution of the intensity in the image is a complex function of the interference of the Bloch waves, generated in the specimen by the primary electron beam, convoluted with the phase contrast transfer function of the objective lens. This latter image formation process gives results that are highly
sensitive even to small variation of lens defocus and specimen thickness and a simulation of the experimental results is needed to have reliable data [3]. On the contrary, in many cases basic information on specimen structure and perfection can be achieved by atomic resolution HAADF without image simulation. Nevertheless, more subtle information, as for example the kind of bond between the atoms in the specimen, can also be addressed by HAADF imaging but requires the modelling of the structure and the relevant image simulation [4]. One of the most desirable results for the nano-science, in particular in the field of semiconducting materials, would be to have an atomic resolution picture of both structure and chemistry of the specimen, especially at the interface between two materials, as the properties of materials and devices are strongly dependent on the structure and chemistry of their interfaces [5,6]. The HAADF image contrast is highly sensitive to the atomic number of the scattering species [7] and the proper choice of the experimental conditions allows one to obtain a direct high-resolution picture of the chemical distribution within the specimen [8], or to detect the presence of dopants within an atomic column [9] even without the computer simulation of the experimental results. Nevertheless, to quantify the chemistry it is necessary to simulate the Z-contrast image intensity [10,11]. Here we show how atomic resolution HAADF imaging coupled with multi-slice computer simulation allows one to obtain atomic resolution quantitative measurement of the chemistry of a specimen also in the case of an interface between two different materials. The studies performed on different semiconducting material systems emphasize how the parameters influencing the chemistry quantification are dependent on the compositions and on the kind of system considered.

2. Experimental

Two materials systems were considered in detail in this study: a Si monolayer buried in [001] GaAs substrate and InGaAs quantum wells, with different known In concentrations of 5%, 12% and 24% respectively, grown on [001] GaAs substrate. The samples were grown by molecular beam epitaxy following a procedure described in details in previous papers [8,12]. The choice of these case studies will make evident how the weight of the parameters involved in the HAADF image contrast formations are strongly dependent on the materials system and on the alloy concentration.

Specimen preparation for quantitative atomic resolution profiling of chemical species by STEM HAADF needs some special care as the surfaces of the thin sample play a basic role. Three points are of particular importance: (i) the specimen surfaces have to be smooth with no clustering, (ii) the amorphous layer due to the ion milling process has to be negligible and (iii) the eventual hydrocarbon contaminants should not have any influence during the image acquisition time with the highly focused electron probe necessary for atomic resolution HAADF imaging. STEM specimens for our studies were prepared in <110> cross section geometry. Milling conditions and geometry were chosen in order to minimize differential sputtering between substrate and epilayer [5]. In particular two ion-guns were used - one for each side of the STEM specimen - in order to avoid redeposition of sputtered material on the opposite surface. Furthermore, the use of a low milling angle and high Z-number ions reduces the dependence of the sputtering process on the specimen atomic number. In this case, the milling geometry was chosen in order to have the ion beam direction forming an angle of 4° relative to the {110} plane. Such precautions were employed together with a discontinuous milling process during rotation of the specimen holder. In particular, the guns were switched on only when the ion beams where within ± 30° of the direction normal to the substrate/epilayer interface. Hence, no sputtering was allowed when the ion beams were parallel to heterostructure interface, as such geometry is known to enhance preferential sputtering of the interface region. The milling procedure was performed by using Xe⁺ ions, with energy of 4.5 keV for the initial part of the milling process, and progressively reduced down to 2keV up to the formation of a small hole. Then, to remove the layers damaged by the high-energy ions, the specimens were ion milled by Xe⁺ ions by using hot cathode ion guns, specially designed to operate down to 200 V, with an incidence milling angle of 2°. Finally, the specimens and specimen holders were treated in low-energy, high frequency plasma of argon and oxygen to remove hydrocarbon contamination, prior to being inserted in the electron microscope vacuum.
HAADF experiments were performed at room temperature using a JEOL 2010F UHR TEM/STEM field-emission gun electron microscope, operating at 200 kV with a measured objective lens spherical aberration coefficient $C_s$ of 0.47±0.01 mm and interpretable resolution limit in HRTEM of 1.9 Å [3].

For Z-contrast imaging, the STEM attachment was equipped with a YAP HAADF detector. The resolution achievable in Z-contrast mode was 0.126 nm [13,14]. All Z-contrast micrographs were recorded digitally with a collection angle $84^\circ \leq 2\theta \leq 224$ mrad. The convergence angle, and hence the optimum aperture of the condenser lens, is related to the spherical aberration coefficient of the pre-field of the objective lens [15,16]. In our case a convergence angle of 14 mrad was chosen as the best compromise between the aperture cut-off of the detectable frequencies and the signal-to-noise ratio in the image. A much larger condenser aperture would produce a distorted image due to the spherical aberration, whereas a much smaller condenser aperture would reduce the highest frequencies in the images and therefore the visibility of the smallest lattice spacing. In between these two limits the choice of the aperture diameter was made taking into account the signal-to-noise ratio in the image. The use of an annular STEM detector with a collection angle larger than about 80 mrad allows acquisition of mainly incoherent electrons, since thermal diffuse scattering dominates at high scattering angles [17,18]. This choice significantly reduces the contribution to the image of the scattering due to a possible strain at the interfaces [15]. The simulations of the HAADF image contrast were performed according to these parameters of the microscope.

3. Simulations and Measurement of an alloy by HAADF imaging

The experimental measurement of the spatially resolved chemical composition of the specimen is based on the simulations of the HAADF image intensity for a model structure as a function of the concentration of the relevant chemical species [19]. To achieve a reliable calculation all the parameters that could influence the image contrast, such as specimen thickness, distortion of the lattice cell, microscope objective lens defocus or the atomic size effects in the alloys [20], should be considered. As will be shown in the examples below the physical values influencing the image contrast can vary depending on the materials’ system or on the concentration of the species to be measured. The images were simulated in [110] zone axis according to the experimental conditions used and the image intensities were measured on both experimental and simulated images with the same criteria, in particular the image intensity was averaged on a half projected unit cell [19]. Atomic resolution HAADF image contrast can be simulated by Bloch-waves [21] or multi-slice approaches [22]. The Bloch-waves based methods are relatively fast, and represent a good tool to understand basic and subtle details of the physics of the interactions involved in the HAADF image formation process. The influence of thermal diffuse scattering (TDS), which plays a basic role in the HAADF image formation [23], is not naturally included in the calculation based on Bloch-waves approaches and requires ad hoc solutions [24-26]. Furthermore, Bloch-wave methods are not convenient whenever a non-periodic object is considered, as for example in the case of the description of a defect, or an interface in the material. In this case the use of multi-slice methods has been recognized as more effective also for the HRTEM image simulation. TDS effect has been introduced in the multi-slice calculations by several authors [27-31]. Nevertheless, STEM HAADF image contrast simulation by multi-slice with the “frozen-phonon” model has proven to be the most accurate method reaching an accuracy better than 2%, in the simulations of the HAADF image contrast, by considering 20 atomic configurations [32,19]. This approach has been used for the calculations presented here. Unfortunately, the approach is extremely time-consuming and image simulation considering models with several atoms, as in the case of large supercells, or realistic STEM specimen thickness, becomes impractical as it could require hundreds of hours of computing time. Indeed, the structure of the calculation of the image contrast by multislice in the frozen-phonon approximation is naturally parallel and can be modified and rewritten for parallel computing reducing the computing time of orders of magnitude [33]. We caution the reader that the use of virtual crystal approximation [34] in the description of the alloy being simulated could produce the formation of artefacts in the image intensity.
In fact, the description of the alloy within the virtual crystal approximation considers a certain position inside the crystal cell as occupied by a combination of potentials weighted according to the concentration to be modelled. The crystal potential $V$ is given by

$$V = \sum_{i=\text{specie}} x_i V_i,$$

where $x_i$ is the partial occupation coefficient for the i-th species with potential $V_i$. In the frozen phonon approximation the effect of thermal diffuse scattering is simulated by offsetting the position of each atom by a small random amount and then performing the standard multislice calculations [30]. This procedure together with the virtual crystal approximation could produce an artificial splitting of the crystal potential and hence the formation of artefacts in the simulated HAADF image.

3.1. Measurement of the Ga(Si)As alloy composition

The intensity of the HAADF image is sensitively dependent on the order of the atoms in the atomic column, as shown in figure 1. These data were obtained by calculating the HAADF image intensity of a Ga(Si)As alloy, averaged over half a unit cell projected on the (110) plane, as a function of the position of the Si atoms within the atomic column. The calculations were performed by taking into account the tetragonal distortion of the unit cell due to the presence of the Si in the GaAs matrix [19], and for a STEM specimen thickness of 10 nm. In particular, the dots in figure 1 were obtained by considering Si atoms randomly distributed on Ga sites, the squares were obtained by considering the atoms on both Ga and As sites and the triangles were obtained by considering the Si atoms of the alloy all located at the beginning or at the end of the atomic column. The latest configuration produces a strong difference in the calculated intensity showing, from one side, the high sensitivity of HAADF to the presence of clusters within the crystalline matrix but, from the other side, raises concerns on the accuracy of the chemistry measurement by HAADF. In fact, the same concentration of Si could produce different intensities in the image.

**Figure 1.** Calculated HAADF image intensity for Ga(Si)As alloy as a function of the atomic species distribution within the atomic column.
The more straightforward way to tackle this problem is to average the intensity $I$ within the atomic column on all the possible atomic configurations, for each Si content, and to calculate $\bar{I} = \frac{\sum_{\text{config}} I_i}{N_{\text{config}}}$.

This averaging introduces an intrinsic uncertainty, of about 2%, in the measurement of the concentration of Si in Ga(Si)As from HAADF imaging, calculated as the standard deviation of each intensity value from the mean value.

The HAADF experiments indicate that, in most of the cases, the images are acquired for a specimen thickness between 10 nm and 40 nm. Figure 2 shows the calculation of the HAADF image intensity for Ga(Si)As alloy, as a function of Si concentration, for four STEM specimen thicknesses.

![Figure 2](image)

**Figure 2.** Calculated HAADF image intensity for Ga(Si)As alloy as a function of Si concentration and STEM specimen thickness.

It should be noted that for each thickness the image intensity varies nearly linearly with the Si concentration. This is not a general behaviour but it is peculiar of this material system. A similar behaviour was also reported for GaAlAs system [10]. If we define the maximum contrast as: $C_{100\%} = \frac{I_{\text{GaAs}} - I_{\text{SiAs}}}{I_{\text{GaAs}}}$, this value varies from 0.30 to 0.26 going from a specimen thickness of 10 nm to 40 nm, resulting in a relatively small role of the specimen thickness on the quantification of the composition of the alloy by HAADF imaging.

It is now worthwhile to remark that, experimentally, the atomic resolution HAADF images in scanning transmission electron microscope, not equipped with correctors for spherical aberration, are obtained with a defocus value relatively close to the optimum defocus [35]. Experiments and simulations of atomic resolution HAADF images have shown that the role of the variation of the objective lens focus value, in an interval of some tens of nm around the optimum defocus, has a negligible influence on the quantification of the chemistry by HAADF imaging [35]. Another aspect that should be considered in the simulation of the HAADF image contrast of an alloy is related to the influence of the static atomic displacements (SDs) due to atomic size effects in alloys with atoms having different covalent or ionic radii. The calculation performed on Ga(Si)As system in a range of...
concentrations of Si below 15% has shown an influence smaller than 1% [20]. This aspect will be discussed in more detail below.

Figure 3 shows a) an experimental HAADF image of a nominal one monolayer of Si atoms buried in a GaAs matrix with b) the relevant quantification of the Ga(Si)As alloy as derived from the measure of the image intensity. The HAADF image gives an immediate and intuitive picture of the formation of a Ga(Si)As region within the GaAs matrix. In fact, the formation of the Ga(Si)As alloy is evidenced by the dark region, in the middle of figure 3a, due to the smaller scattering factor of Si atoms compared to Ga and As atoms. A close inspection to the high-resolution image shows the well known cation-anion dumbbells of the sphalerite structure seen in [110] projection and spaced by 0.14 nm. The inset in figure 3a is the experimental intensity profile, averaged over the opaque marked region to increase the signal to noise ratio. The average along the direction of the interface reduces the resolution to 0.28 nm.

![Figure 3](image_url)

**Figure 3.** a) HAADF image of a nominal 1ML of Si buried in GaAs matrix. The inset of a) is the image intensity line profile averaged on the 5 nm region parallel to the interface sketched in the figure; b) Si concentration profile as measured by HAADF and X-STM

It is worthwhile to remark that in the calculated images the intensity it is also averaged over half a unit cell, removing the need of the intensity subtraction, reported by other authors [36] and due to the delocalised scattering in the specimen and to the electron and mechanical instabilities of the instrumentation. To evaluate the Ga(Si)As experimental image contrast, the high angle annular dark field detector background has been subtracted and the Ga(Si)As intensity value has been normalized to the GaAs regions on both sides of the dark Ga(Si)As region. Indeed, the experimental images should be acquired close to a hole in the specimen to adjust the HAADF detector gain to have zero counts, or the lowest value of counts, in the hole as a high value of the dark counts could produce the formation of artefacts in the image intensity [37]. Figure 3b shows the Si concentration profile as measured from figure 3a, together with the Si concentration measurement performed by cross-sectional scanning tunnelling microscopy (XSTM) on the same specimen [8]. The total amount of Si in the alloy corresponds to about two monolayers, instead of the nominal one monolayer, and results in the formation of an alloy distributed over about 3 nm. The error bar reported in the figure 3b could be a bit overestimated and it was calculated considering the sum of the uncertainties in the calculations (2%).
the intensity averaging over all the possible atomic configurations (2%) and the uncertainty on the STEM specimen thickness (2%).

3.2. Measurement of InGaAs alloy composition

As will be seen in the following, the features of HAADF images for InGaAs are rather different with respect to what has been reported so far for Ga(Si)As. To study the InGaAs system, specimens with three different concentrations of In were considered: (5±1)%, (12±1)% and (24±1)% respectively, as measured by photoluminescence (PL) and, in-situ during the molecular beam epitaxy growth, by X-ray photoelectron spectroscopy (XPS). Figure 4 shows the simulated HAADF image intensity ratio for an alloy of InGaAs, calculated as a function of the In concentration, taking into account the effect of the static atomic displacements, \( I_{SD} \), or without the effect of static atomic displacements, \( I_0 \), for two specimen thicknesses of 10 nm and 40 nm respectively. The supercells with SDs were calculated by Valence Force Field (VFF) model [38-41] which reproduces accurately the SD field in semiconductor alloys [38]. The supercells were then used to calculate the atomic resolution HAADF image contrast following a procedure described in a previous paper [20]. The \( \frac{I_{SD}}{I_0} \) gives an evaluation of the weight of the SD effect on the simulation of the HAADF image intensity of InGaAs. From figure 4 it can be seen that the effect of static displacements is highest for In concentrations of 50%, as expected, and has a parabolic behaviour, as can be seen from the solid line obtained by fitting the simulated data with a parabola whose fitting parameters are also shown in figure 4. It should be noted that the SDs and the corrections to the structure factors due to the SDs also follow a parabolic law as a function of the In concentration [41-44]. Hence, SDs in the case of InGaAs play a role that cannot be neglected if the chemistry of the specimen is derived from HAADF image.

![Figure 4. Ratio of the HAADF intensities for InGaAs, calculated with and without taking into consideration the effect of the atomic static displacements, as a function of the In content and for two specimen thicknesses of 10nm and 40nm.](image-url)
Figure 5a is a low magnification high resolution image, in [110] zone axis of InGaAs QWs/GaAs (001), and has been acquired by achieving the condition for atomic resolution, with objective lens focus close to Scherzer’s value, and then decreasing the magnification to show all the QWs of InGaAs, and adjusting the detector gain to optimize the visibility of all the features of interest: the three QWs, the GaAs barriers and the black level in the hole of the specimen to evaluate the dark count of the detector to be subtracted for the image intensity quantification. The intensity profile in figure 5a immediately reveals the kind of In concentration in the three QWs as the high angle scattering increases with increasing the In content in the alloy. The ratios $\frac{I_{\text{InGaAs}}}{I_{\text{GaAs}}}$ between the HAADF image intensity of InGaAs QWs and the relevant intensity of the GaAs barriers have been measured for different thickness of the STEM specimen and are reported, as squares, in figure 5b, together with the relevant experimental errors, for the different In concentrations. The calculated HAADF image intensities for the three wells, taking into account the effect of SDs (solid lines) and without the effect of SDs (dotted lines), as a function of the STEM specimen thickness are also reported in figure 5b. The figure 5b demonstrates that the image intensity is strongly dependent on the specimen thickness, showing a pronounced dip in its value around a thickness of 10 nm, and hence a reliable quantification of the chemistry in the InGaAs alloy requires an accurate measurement of the specimen thickness.

![Figure 5a](image)

**Figure 5.** a) low magnification high resolution [110] zone axis HAADF image of three quantum wells of InGaAs, with In content of (5±1)%, (12±1)% and (24±1%) respectively, as measured by photoluminescence and in-situ photoemission spectroscopy; b) intensity ratio $\frac{I_{\text{InGaAs}}}{I_{\text{GaAs}}}$ measured on the experimental images (square dots) for each QW, and calculated with the effect of SDs (solid lines) and without SDs (dotted lines).

Furthermore, the role of the SDs cannot be neglected as, for example in the case of the well with 24% of In, it could produce an error of 10% in the absolute measurement of the In concentration. The figure 5b demonstrates that taking into account the SDs produces a good agreement between simulated and experimental curves. The results of the experiments and simulations also indicate that, for reliable quantification of the InGaAs alloy composition, STEM specimen thicknesses larger than 20 nm should be preferred.

The examples shown so far demonstrate how the specimen thickness plays a subtle role in the quantification of the specimen chemistry by HAADF. In fact, from one side the precise knowledge of the specimen thickness is not very important for the quantification of Si in Ga(Si)As, for the Si concentrations here considered, and hence thin specimen could be preferred to maximize the incoherent component of the HAADF image [24]; on the other side, chemistry quantification for other
materials system, like InGaAs or SiGe [45,46], needs larger specimen thickness to avoid non-monotonic behaviour of image contrast as a function of thickness, observed for small sample thicknesses.

4. Conclusions

HAADF images contain detailed chemical information that can be quantified thus providing, at the same time, structural and chemical information at atomic resolution. The chemistry of the specimen can be measured within an accuracy of few percent if the parameters influencing the HAADF image contrast have been properly addressed and simulated by reliable calculations. In particular, in the modelling of the alloy, the use of virtual crystal approximation can produce the formation of artefacts in the images. Furthermore, it has been observed that different atom positions within atomic columns, with the same overall composition, can produce different image intensity and hence limit the intrinsic accuracy of the chemistry measurement by HAADF imaging. The parameters influencing the measurement are: the STEM specimen thickness, the crystal cell distortion induced, for example, by the presence of a guest species in a host matrix, or by the mismatch at the interface between the substrate and the epilayer, and the influence of the static atomic displacements due to atomic size effects in alloy with atoms having different covalent or ionic radii. These parameters have different weight in the accuracy of the measurement depending on the material system considered and, within the same system, also as a function of the chemical species concentration. The results reported here show that for Ga(Si)As alloy, with a maximum Si content of 15%, an accuracy of few percent in the chemistry quantification can be achieved with an uncertainty on the specimen thickness between 10 nm and 40 nm and neglecting the role of SDs. On the other side the example of InGaAs demonstrates that completely unreliable chemistry quantification can be done neglecting the role of SDs and without an accurate STEM specimen thickness measure. The amount of uncertainty depends on the In concentration: for example for a specimen thickness of 30 nm, neglecting the SDs produces an absolute error on the In concentration of 10% in an alloy containing 24% of In whereas, for the same specimen thickness, it produces an absolute error of 1% in the alloy containing 5% of In. In all the cases, an uncertainty on the specimen thickness in the range between 10nm and 40nm produces completely unreliable determination of the chemistry of the InGaAs alloy. The simulations of the HAADF image intensity suggest the strategy to be used for STEM experiments as they allow one to derive the specimen thickness necessary to obtain quantitative analytical information from HAADF images. Finally, atomic resolution HAADF provides in an image a reliable and well reproducible quantitative description of the structure and chemistry of the specimen and represents a further powerful tool, now available also on standard field emission gun TEM/STEM microscopes, to study in a direct way the properties of the solid-state matter at the highest spatial resolution.

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