A quantitative model for doping contrast in the scanning electron microscope using calculated potential distributions and Monte Carlo simulations

Augustus K. W. Chee, Ronald F. Broom, Colin J. Humphreys, and Eric G. T. Bosch

1Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, United Kingdom
2Department of Engineering, Electrical Engineering Division, Centre for Advanced Photonics and Electronics, University of Cambridge, 9 JJ Thompson Avenue, Cambridge CB3 0FA, United Kingdom
3FEI Electron Optics, FEI Company, Building AAE, Achtseweg Noord 5, Eindhoven 5651 GG, The Netherlands

(Received 24 May 2010; accepted 1 November 2010; published online 11 January 2011)

This paper describes the use of a Monte Carlo model incorporating a finite-element method computing the electrostatic fields inside and outside a semiconductor, plus a ray-tracing algorithm for determining the doping contrast observed in a scanning electron microscope (SEM). This combined numerical method also enables the effects on the doping contrast of surface band-bending to be distinguished from those of external patch fields outside the specimen, as well as any applied macroscopic external fields from the detection system in the SEM. Good agreement of our new theory with experiment is obtained. The contrast characteristics in energy-filtered secondary electron images are also explained. The results of this work lead to a more advanced understanding of the doping contrast mechanisms, thereby enabling quantitative dopant profiling using the SEM. © 2011 American Institute of Physics. [doi:10.1063/1.3524186]

I. INTRODUCTION

For the characterization of next generation semiconductor devices, the Semiconductor Industry Association has identified several important requirements. One of these includes dopant profiling at a resolution of sub-10 nm and detection sensitivity over a range of $10^{16}$–$10^{20}$ dopants cm$^{-3}$. Dopant profiling can be provided by secondary electron (SE) imaging using a scanning electron microscope (SEM). This is a rapid and contactless procedure which has shown promise among a number of competing alternatives, in characterizing dopants with sensitivity over the required range and resolution.

Experimentally, it is found that the SE intensity across a $p$-$n$ junction is higher from the $p$-side than the $n$-side (under standard imaging conditions), hence doping contrast can be used to determine the position of $p$-$n$ junctions. However, the general implementation of doping contrast mapping in industry has hitherto been inhibited by the lack of an accurate and robust quantification model, owing to an inadequate understanding of the contrast mechanisms.

Previous work had aimed at explaining why the intensity of SEs emitted from a semiconductor is a sensitive function of the doping. Castell et al., Perovic et al., and Howie suggested that this phenomenon is due to surface band-bending. Howie and Sealy et al. proposed that local external electric fields called patch fields are important for doping contrast. Patch fields can exist outside a semiconductor specimen due to charge variations on the surface. El-Gomati et al. have argued that doping contrast is due to a polymerized hydrocarbon contamination layer on the surface of samples in the SEM. However, this is not relevant to the present paper which concerns a freshly cleaved surface which is scanned only once in an SEM with a good, clean vacuum. Moreover, strong doping contrast can be observed upon low-pass energy-filtering of the SEs, collecting the lower energy SEs originating from deeper below the surface of the specimen, while spurious contributions from any surface oxides or contamination are eliminated. Howie has further proposed that differences in the inelastic mean free path and surface-barrier escape probability are also components of the doping contrast mechanism that should be accounted for.

The observed dependence of contrast on experimental parameters (e.g., working distance and extractor voltage) using an in-lens detector system has been attributed to the dissimilar angular characteristics of the SEs emitted from the different doped regions, caused by refraction effects occurring at the surface barrier and through any patch fields above the sample.

In this paper, we provide a more comprehensive understanding of the mechanisms for doping contrast which includes aspects of many of the explanations proposed earlier, by Castell et al., Perovic et al., Howie, and Sealy et al. The local electric fields that exist inside or outside the specimen, or both, constitute the basis for doping contrast. Additionally, we find that it is essential to include the effect of the detection system in the analysis to understand the observed doping contrast in experimental SEM images.

The aim of this paper is to establish a quantitative model for doping contrast. In order to achieve this, we have developed from basic principles a numerical simulation tool comprising three integrated components. The first construct is a Monte Carlo model, capable of simulating the interaction of incident primary electrons with a specimen as well as the...
generation of secondaries. Second, a ray-tracing algorithm that traces SE trajectories onto a detector of finite size through electric fields existing both inside and outside the specimen, possibly including electromagnetic fields arising from the SEM detection system itself. Third, a finite-element model that computes the potential distributions inside and outside the specimen.

The model should be applicable to any semiconductor homojunction, but for illustration, a Si p-n junction is considered here, as an example. Following a description of this model, we report simulations computing the SE yields from a Si p-n junction for two limiting situations: with strong and weak surface band-bending due to surface states. The distinction is that in the former case all electrostatic potential gradients due to surface potentials are concentrated inside the sample while the patch fields are insignificant, whereas in the latter case these gradients occur outside the sample. In the former case, we can specify these surface states at a high density, inducing Fermi level pinning at the surface, resulting in an equipotential surface, and consequently no patch fields. Finally, we demonstrate good agreement of our model with experiment.

II. SIMULATION MODEL

To simulate the electron probe-specimen interactions, the Monte Carlo model described by Kieft and Bosch\textsuperscript{16} has been used. This model is based on the GEANT4 platform\textsuperscript{17} and includes a good description of low-energy (<50 eV) interactions of the energetic electrons with matter.

The tabulated angle- and energy-dependent Mott cross-section data from Czyzewski \textit{et al.}\textsuperscript{18} are used to compute elastic scattering for electrons having kinetic energies in the range of 100 eV to 30 keV, whereas for energies of less than 100 eV the elastic cross-section is modeled by the acoustic phonon scattering description\textsuperscript{19–21}. Inelastic scattering in the solid, including plasmon scattering, free electron, valence band, core level, and optical phonon excitations, is represented in terms of a dielectric response function $\varepsilon(q,\omega)$ for their equivalent energy loss functions via the dielectric theory approach. Ding and Shimizu\textsuperscript{22} have shown that the use of the dielectric function model accounting for inelastic scattering accurately simulates the energy and angular characteristics of SE emission. A quantum-mechanical model is used to describe reflection and refraction at the surface boundary of the solid.

Our detailed model provides a more accurate description of the physics of electron scattering by the crystal over a broad energy range, including low energies (<50 eV), than that of Dapor \textit{et al.}\textsuperscript{23} for example. Therefore, it is appropriate to use in the simulation study of the SE yield and energy spectra from semiconductor devices in the SEM (see Kieft and Bosch\textsuperscript{16}).

In order to focus on the effects of local electric fields, in this paper the optical dielectric constants and inner potentials of both $p$- and $n$-silicon are assumed to be of intrinsic silicon. Consequently, the generation rate of SEs in the $p$- and $n$-type regions is expected to be similar. The effects due to differences in inelastic mean free paths and surface-barrier escape probabilities as discussed by Howie\textsuperscript{13} are therefore effectively ruled out \textit{a priori} (see Chee \textit{et al.}\textsuperscript{4}). Based on the good agreement of our theory with experiment (see later) such effects are likely to be of second order, the main effects being due to the internal and external fields of the specimen coupled with a finite acceptance angular range for SE detection.

Ray-tracing is performed using the fourth order Runge-Kutta algorithm available on the GEANT4 platform. The required electric fields are imported from the finite-element model described below. A virtual detector is simulated at the sample surface, which detects all electron fluxes emitted from the specimen. This detector effectively has a potential that is equal to the locally existing surface potential of the specimen. A second virtual planar detector is defined parallel to the surface plane at a macroscopic distance ($z=0.5$ mm) above the sample, outside the effective range of the specimen microscopic patch fields (see Fig. 1). This virtual detector is centered on the junction and has dimensions of $1 \times 1$ mm$^2$ with zero potential relative to the specimen.

In order to calculate the electrostatic potential distributions, a simulation tool for semiconductor finite-element modeling\textsuperscript{24} is used to solve the Shockley equations of the sample, namely, Poisson’s equation, electron and hole continuity equations, for the electron and hole drift-diffusion current equations. The relevant physics, for example heavy doping effects, concentration- and field-dependent free carrier mobilities, and concentration-dependent free carrier lifetimes, are also incorporated into the calculations.

The general physical structure being modeled is a Si–SiO$_2$–vacuum system, where the Si contains a p-n junction intersecting the surface perpendicularly. We include a SiO$_2$ layer because on a freshly cleaved Si crystal, a SiO$_2$ layer rapidly forms. All the equations are discretized on the simulation mesh using the box integration method, and the original continuum model is represented by an equivalent discrete nonlinear algebraic system. Along the bottom of the semiconductor bulk Dirichlet boundary conditions ($V=0$) are assumed. Along the noncontacted perimeter of the simulation structure we assume Neumann boundary conditions, where the normal component of the electric field is zero ($\mathbf{V} \cdot \mathbf{V} = 0$).

Since the calculated potential distributions are integrated
into the overall model, the vertical extent of the computation domain is defined large enough to ensure that the potential at the top of the vacuum region is sufficiently close to zero to allow embedding of the local grid in the simulations including the macroscopic detector. Furthermore, the two-dimensional potential model is assumed to extend indefinitely into the third (out of plane) dimension. As feature length scales vary considerably (e.g., nanometers for the oxide layer and depletion regions; microns for the whole structure), care has been taken to ensure that the computed solutions are independent of the finite-element mesh size.

When a crystal is terminated at the surface, the abrupt change in potential results in the formation of a surface dipole layer. For a semiconductor, the dipole layer is extended below the surface, giving rise to a surface depletion region and surface band-bending. The charges on a clean surface give rise to states, often in the band gap, called Tamm states. Surface states also arise from an oxide layer on the surface. Since SEs emitted from the specimen arise from near-surface regions, it is essential to calculate surface band-bending for quantitative doping contrast.

The main surface states on the Si are Si–SiO₂ interface states. To simulate the presence of these surface states, Poisson’s equation is modified to account for the trapped charges. Typical values of the electron and hole capture cross-section for the Si–SiO₂ interface states are $s_n = 10^{-15}$ cm$^2$ and $s_p = 10^{-16}$ cm$^2$, respectively. The capture cross-sections for the free carriers are treated as constant for all energies in a given band. It is assumed that the density and energy distribution of the surface states are independent of the local doping, as established by Fischer and Chung, and the spatial distribution of the interface states is considered to be uniform on the semiconductor surface.

The effect of the native oxide layer on the potential is generally irrelevant in the calculations since the electron probe in the SEM during operation completely penetrates the thin surface oxide layer of the freshly cleaved Si (~0.2–1 nm), modulating its conductivity such that the surface of the over-layer assumes the same potential as the semiconductor surface.

The measured intrinsic surface state density on in situ cleaved, atomically clean Si (111) surfaces under ultrahigh vacuum (UHV) conditions is $8 \times 10^{14}$ cm$^{-2}$, approximately the value of the surface atomic density (one dangling bond per surface atom is assumed). Surface state densities for freshly cleaved Si with a native oxide layer are of the order of $10^{12}$ cm$^{-2}$. Surface band-bending was simulated from donorlike monoenergetic levels of 0.38 eV above the top of the valence band for surface state densities of $10^{12}$ and $10^{14}$ cm$^{-2}$ on p-type Si having acceptor concentrations of $10^{16}$ and $10^{18}$ cm$^{-3}$. The result is shown in Fig. 2.

### III. SIMULATION RESULTS

The finite-element model for the calculation of potential distributions was integrated into the Monte Carlo model. This enables the effects of surface band-bending and external patch fields on doping contrast to be clearly distinguished. Calculations were performed for Si p-n junction specimens with negligible surface band-bending (i.e., a very low density of surface states), over a wide range of doping concentrations. In this hypothetical case, there are mainly external patch fields above the surface, so the effects of patch fields on doping contrast can be studied. In further simulations, phenomenological extrinsic surface state parameters were included. To understand the effects of surface band-bending, a high density of surface states was specified, inducing Fermi level pinning so that the surface is at an equipotential and no external patch fields could result.

The simulations used a focused probe of fast electrons of energy 1 keV, incident normally upon the sample, with $10^5$ electrons per pixel. This incident beam energy minimizes Si specimen charging and is within the optimal range for doping contrast imaging. The measured doping contrast can be a function of the incident beam current because the electron-hole pair generation has a negligible effect on the doping contrast except when high magnifications and low scan frequencies are used. In particular they have shown that at all magnifications and TV scan frequencies the effect of electron-hole pair generation on the contrast is negligible. Hence we do not need to include the effect of changes in beam current in our model, which is for standard SEM operating conditions for dopant profiling. The specified number of primary electrons per pixel in the simulations provides reasonable statistical accuracy to within about ±0.2% of the calculated SE yield.

The simulated mean SE escape depth from the p-region is ~2.5–2.6 nm compared to ~2.1–2.3 nm from the n-region. These values are similar to those reported by Selzer for Si. SEs with sufficient energies to escape the surface potential barrier may originate from deeper below the surface in the p-type region compared to the n-type due to the internal surface band-bending fields.

#### A. Case 1: Low density of surface states

Simulations were performed for a Si p-n junction with a clean free surface and with a very low density of surface
states ($\sim 6 \times 10^8$–$2 \times 10^{10}$ cm$^{-2}$). This is the surface state density that results from solving Poisson’s equation for the step-function change in potential at the surface. An idealized step junction was modeled for simplicity. Potential variations result from the space-charge distribution across the junction. The calculated potential distributions across the junction, both in the specimen and in the vacuum region above the surface, are plotted two-dimensionally as shown in Fig. 3, for different doping concentrations ($10^{16}$ cm$^{-3}$ for both $p$ and $n$ and $10^{18}$ cm$^{-3}$ for both $p$ and $n$).

The width of the depletion region across the junction is greater for low doping than for high doping, as expected. Solutions of the Poisson equation for the semiconductor-vacuum system show that the locally varying surface potential gives rise to external electric fields (or patch fields) in the vacuum. These patch fields are of considerable significance for doping contrast as they can substantially influence the trajectories of low-energy SEs and hence the detected SE intensities from the doped regions (to be discussed below). Figure 3 shows strong patch fields above the specimen, that are larger for high doping than for low doping, as expected. Plots of the electric field distribution at various distances above the surface for low and high doping are shown in Fig. 4. The electric field increases with doping concentration and decreases with distance above the specimen surface. The transverse component of the field is large above the junction and decreases to zero away from it. The longitudinal field changes sign, being positive above the $n$-type region and negative above the $p$-type. Hence the SEs above the $n$-region experience an accelerating electrostatic force toward the specimen, whereas those above the $p$-region are accelerated away from the specimen. The longitudinal field extends for a considerable distance on each side of the junction.

**Fig. 3.** (Color) Two-dimensional potential distribution plots inside and outside the Si specimen, with a symmetric $p$-$n$ junction doping concentration of (a) $10^{16}$ and (b) $10^{18}$ cm$^{-3}$. The surface state density is $\sim 6 \times 10^8$–$2 \times 10^{10}$ cm$^{-2}$.

**Fig. 4.** (Color) The electric field at (a) 50 nm and (b) 200 nm above the surface of the Si $p$-$n$ junction, for low and high doping. The transverse component (solid curves) and the longitudinal component (dashed curves) of the electric fields are plotted.
The simulated energy and angular characteristics of the emitted SEs from the p-n junction specimen without extrinsic surface states are as shown in Fig. 5. The kinetic energy and angular characteristics at the surface are similar for the p- and the n-regions [see Figs. 5(a) and 5(b)]. These results stem from the assumption of an equivalent dielectric response and inner potential for the p- and the n-type material as mentioned earlier.

By comparing the theoretical plots in Figs. 5(a) and 5(b) obtained for the virtual detector at the surface and at z =0.5 mm, the effects of the patch fields and the finite detector size on the energy and shape of the SE energy distributions can be clearly observed. The angular acceptance range for the SEs is limited by the detector solid collection angle, which is determined by its dimensions and distance above the surface. Consequently the calculated angular distribution plots of the detected SEs in Fig. 5(b) exhibit a high-angle cutoff (at ~45°) for the detector at z=0.5 mm; note that the cutoff is not sharp but extends up to ~54.7° due to the square (rather than circular) geometry of the virtual detector. External surface fields modify the SE trajectories via refraction effects and return the lowest energy SEs emitted from the n-type region back to the specimen. By comparing the angular distribution plots at the surface and at z=0.5 mm, patch fields are seen to have enhanced the collection efficiency of the SEs for the p-type region and reduce that for the n-type within the angular acceptance limits. Emitted SEs approaching the detector are refracted by the patch fields to lower angles for the p-region (increasing the collection efficiency), and to higher angles for the n-region (reducing the collection efficiency). The doping contrast magnitude can be computed from the spectra in Fig. 5. Reducing the detector solid collection angle (e.g., a larger working distance) increases the doping contrast since the SEs emitted at higher angles contribute less to doping information [see Fig. 5(b)]. Therefore the doping contrast is a function of both the patch fields and the angular acceptance range for SE detection.

Figure 5(c) shows the SE yield (or cumulative energy distributions) from the p- and n-regions. Due to the finite size of the detector at z=0.5 mm, in conjunction with patch field effects, the total number of SEs collected from the n-region is larger than that from the p-region for energies below ~4 eV and the situation is the opposite for higher SE energies. Contrast reversal (bright n-type contrast and dark p-type contrast) will therefore be observable in the SE image under energy-filtering when SEs of all energies up to a specific level are collected from the sample; normal doping contrast (p brighter than n) will otherwise be observed.3

B. Case 2: Higher density of surface states

Finite-element calculations were performed to evaluate the effect of a higher surface state density (i.e., typical surface state density for freshly cleaved Si with a native oxide layer). The calculated potential distributions, both in the specimen and in the vacuum region above the surface, are shown in Fig. 6, for different doping concentrations (10^{16} cm^{-3} for both p and n and 10^{18} cm^{-3} for both p and n). The surface states are specified to have a density of 10^{12} cm^{-2} and amphoteric energy levels localized in the Si band gap of 0.38 eV from the band edges. Figure 6 shows both patch fields above the specimen and internal surface

![Energy and angular characteristics of the emitted SEs](image-url)
band-bending fields inside the specimen, which are greater for high doping than for low doping, as expected.

Simulations were also performed for p-n junctions having a boron concentration ranging from $10^{16}$ to $10^{20}$ cm$^{-3}$ in the p-type region and an arsenic concentration of $5 \times 10^{18}$ cm$^{-3}$ in the n-type. Figure 7 shows the junction built-in potential at a depth of 1 nm below the Si surface. For a very low density of surface states ($\sim 6 \times 10^8$ to $2 \times 10^{10}$ cm$^{-2}$), the built-in potential 1 nm below the surface has a linear-logarithmic dependence on the doping concentration, comparable to bulk material, whereas this relation is more complicated in the presence of a higher density of extrinsic surface states ($4 \times 10^{12}$ cm$^{-2}$).

The effect of surface states on the external patch fields is next illustrated. The doping concentration for the p-n junction sample in the p- and n-regions is $10^{18}$ cm$^{-3}$, and surface states with densities $10^{12}$ and $10^{14}$ cm$^{-2}$ have been considered (having amphoteric energies as noted above). The patch fields across the junction at various distances above the surface for the two different surface state densities are shown in Fig. 8.

To identify the effects of surface band-bending on SE emission, a high density of surface states was modeled, i.e., $8 \times 10^{18}$ cm$^{-2}$. These states induce Fermi level pinning, resulting in an equipotential surface, and consequently no patch fields are present (see Fig. 9). This approach therefore enables surface band-bending effects on doping contrast to be distinguished from that of the patch fields. The simulated energy and angular characteristics of SE emission as well as the SEs detected on the finite virtual detector at $z=0.5$ mm are shown in Fig. 10.

Comparing Figs. 5 and 10, surface band-bending effects on the energy and angular characteristics of the emitted SEs are evident. The general shape of the SE spectra detected 0.5 mm above the surface is largely the same as at the surface [see Fig. 10(a)]. SEs in the surface region of the p-type semiconductor gain additional kinetic energy from the surface band-bending fields prior to escaping the sample. Conversely, the SEs in the surface region of the n-type semiconductor lose kinetic energy when approaching the surface.

As emphasized by Shimizu and Ding, reflection and refraction effects due to scattering at the surface boundary must be carefully accounted for using a transmission function (see Kieft and Bosch). Since the average kinetic energy of the SEs in the p-type surface region is higher than that in the n-type, a greater proportion of SEs can escape the p-type surface compared to that from the n-type over the entire angular range [see Fig. 10(b)]. The trajectories of the
SEs are not further modified by any refraction effects above the surface because virtually no patch fields are present in this case.

As before, the doping contrast value may be computed from Fig. 10. In this case, the doping contrast is a function of the surface band-bending and the angular acceptance range for the SEs. As shown in Fig. 10, the intensity of the SEs from the p-type region is generally higher than that from the n-type over the entire energy range. Therefore, brighter p-type contrast (more SEs) and darker n-type contrast (fewer SEs) will be observed across the p-n junction. Unlike in Fig. 5(c), contrast reversal is not expected to occur under any energy-filtering.

IV. COMPARISON WITH EXPERIMENT

The contrast profile across the cross-section of a specially designed resolution test Si structure was simulated and compared with experimental data, as shown in Fig. 11. SE imaging was performed under standard imaging conditions, using a through-the-lens detector, with a tube bias of 250 V and a working distance of 3 mm, for a 1 keV primary beam. The homoepitaxial structure comprises six boron-doped (p-type) layers, each having a target p-type doping concentration of $10^{19}$ cm$^{-3}$ and target layer widths of 1, 2, 3, 5, 10, and 30 nm, chemical-vapor deposition grown on an n-substrate antimony-doped to $10^{18}$ cm$^{-3}$ (see Chee et al. $^{37}$). The capping layer and the spacer layers (100 nm thick) between the thin p-layers were nominally undoped.

Line profiles across the regions of interest were row-averaged over at least 100 pixels perpendicular to the scan direction to yield experimental contrast profiles. The doping contrast value $C$ was determined by normalizing the SE intensity from the layer of interest (doped or nominally undoped) to that from the doped substrate using the formula as follows (adapted from Goldstein et al. $^{38}$):

$$C = \begin{cases} \frac{\Delta I}{I_d} = \frac{I_d - \overline{I}_{sub}}{I_d - I_0} & \text{if } I_d > \overline{I}_{sub}, \\ \frac{\Delta I}{I_{sub}} = \frac{I_d - \overline{I}_{sub}}{I_{sub} - I_0} & \text{if } \overline{I}_{sub} > I_d. \end{cases}$$

$I_d$ is the column-averaged SE intensity from the layer of interest, $\overline{I}_{sub}$ is the mean SE intensity from the uniformly doped substrate, and $I_0$ is the extraneous background intensity obtained by blanking out the primary electron beam. $\Delta I = I_d - \overline{I}_{sub}$ is the absolute intensity difference and $I_d$ or $\overline{I}_{sub}$ is the absolute intensity from the respective semiconductor.

FIG. 8. (Color) The electric field distribution at (a) 50 nm and (b) 200 nm above the surface of the Si p-n junction sample for two different surface state densities as a parameter. The transverse component (solid curves) and the longitudinal component (dashed curves) of the electric fields are plotted.

FIG. 9. (Color) Potential distribution plots inside and outside the Si specimen with a symmetric p-n junction doping concentration of $5 \times 10^{18}$ cm$^{-3}$ for a surface state density of $8 \times 10^{18}$ cm$^{-2}$. 
regions. The contrast value is constrained to within the range $-1 \leq C \leq 1$ using Eq. (1). The case $C=1$ or $C=-1$ indicates absolute zero yield from the substrate ($I_{sub}=0$) or the layer of interest ($I_d=0$), respectively. Therefore, the absolute contrast value is independent of the microscope display contrast and brightness settings on the control console.

Good agreement is observed between the numerical and experimental line profiles. It should be noted that doped layers of width down to 1 nm can be detected, but that their image width is considerably greater. The simulations reproduce both the observed image widths, and the observed image intensities, to a good approximation.

V. CONCLUSIONS

We have presented a quantitative numerical model for doping contrast in the SEM, which is suitable for any geometry, and allows direct comparison with experiment. This model provides a detailed understanding of doping contrast from first principles. The simulations are based on a Monte Carlo model, a ray-tracing algorithm for SEs traversing in the electric fields inside and outside the specimen, and a semiconductor-oxide-vacuum finite-element model for calculating these fields. This comprehensive model minimizes the number of unknown parameters in contrast to other functionally different models, e.g., Dapor et al.\textsuperscript{23} or Volotsenko et al.\textsuperscript{39}

Surface band-bending due to surface states is accounted for, and the effects of patch fields outside the specimen have been calculated. An accurate estimate of the doping contrast can be obtained given the density of surface states. We have used the model to distinguish between the effects on doping contrast of the internal and external electric fields of the specimen. A high density of surface states was specified inducing Fermi level pinning at the surface, which suppresses the patch fields and isolates surface band-bending effects on doping contrast; on the other hand, a low density of surface states was specified on a free surface (without extrinsic surface states) in order to observe the effects of patch fields on doping contrast. Our results demonstrate the influence of the
patch fields on the trajectory of the emitted SEs, thereby
determining their energy and angular characteristics. Above
the p-type (n-type) region, the SEs are accelerated away
from (toward) the specimen, hence increasing the collection
efficiency of the SEs from the p-type region and reducing it
from the n-type. Our results also demonstrate the effects of
surface band-bending on the emission rate and angular char-
acteristics at the p- and n-type regions.

When a realistic finite collection angle is defined, it can
be seen in the simulations that the patch fields are respon-
sible for a contrast reversal effect (i.e., the p-type region is
dark and the n-type region bright), also experimentally ob-
serveable in an SE image using energy-filtering, where SEs of
the lowest energies are collected from the specimen. The
finite collection angle of the detector sets the angular accep-
tance range for the SEs, thereby determining the doping con-
trast value. We have demonstrated an excellent agreement of
our theory with experiment. The results of this work lead to
a deeper understanding of the physical mechanisms under-
pinning doping contrast, enabling the future development of
a quantitative procedure using an SEM for dopant profiling.

ACKNOWLEDGMENTS

A. K. W. Chee acknowledges financial sponsorship from the Overseas Research Studentship Award Scheme (ORS-
SAS), the Cambridge Commonwealth Trust, the Trinity Hall
Brockhouse Engineering Studentship and FEI company. The
authors are grateful to Silvaco company for access to their
program source code and CERN for their open-source simul-
tation toolkit. The authors also thank Gerard Van Veen and
Seyno Sluyterman (FEI company) for initiating the Image
Contrast and Detection (ICD) European consortium program
to facilitate this work.

1The International Technology Roadmap for Semiconductors, www.itrs.net,
2S. L. Elliott, R. F. Broom, and C. J. Humphreys, J. Appl. Phys. 91, 9116
(2002).
209, 012054 (2010).
7D. D. Perovic, R. Turan, and M. R. Castell, Proceedings of the Interna-
687, edited by A. Kirkland and P. D. Brown (IOM Comunications Ltd.,
9C. P. Sealy, M. R. Castell, and P. R. Wilshaw, J. Electron Microsc. 49, 311
(2000).
11M. M. El-Gomati, T. C. R. Wells, I. Mullerova, L. Frank, and H. Jayakody,
15C. Schönjahn, R. F. Broom, C. J. Humphreys, A. Howie, and S. A. M.
17S. Agostinelli, J. Allison, K. Amako, J. Apostolakis, H. Araujo, P. Arce,
20H. J. Fitting, E. Schreiber, and I. A. Glavatskikh, Microsc. Microanal. 10,
21E. Schreiber and H. J. Fitting, J. Electron Spectrosc. Relat. Phenom. 124,
25 (2002).
23M. Dapor, B. J. Inkson, C. Rodenburg, and J. M. Rodenburg, EPL 82,
30006 (2008).
24Silvaco Company, ATLAS Device Simulation Software User Manual,
25E. H. Nicollain and J. R. Brews, MOS Physics and Technology (Wiley-
Interscience, New York, 1982).
Chem. 100, 1801 (1996).
(1964).
31E. H. Poin dexter, G. J. Gerardi, M. E. Rueckel, P. J. Caplan, N. M.
34P. Kazemian, C. Rodenburg, and C. J. Humphreys, Microelectron. Eng.
126, 012033 (2008).
Sawyer, and J. Michael, Scanning Electron Microscopy and X-Ray Mi-
39I. Volotsenko, M. Molotskii, Z. Barkay, J. Marczewski, P. Grabiec, B.
Phys. 107, 014510 (2010).