Progress towards quantitative dopant profiling in the SEM

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Abstract. Dopant contrast from secondary electron (SE) imaging is essentially determined by the local electronic band structure at the surface of the solid specimen being analysed in the scanning electron microscope (SEM). To study dopant contrast mechanisms on inhomogeneously doped semiconductors, we have developed a quantitative model by using a numerical method based on a combination of finite-element carrier and potential modelling and Monte Carlo simulation of SE emission and contrast detection. This combined model enables distinction between the effects of specimen internal fields (surface band-bending), microscopic external fields (patch fields) and any macroscopic external fields applied in the SEM.

1. Introduction
The quantification of dopant distributions directly from two-dimensional secondary electron (SE) contrast imaging is in principle a rapid and non-destructive \textit{in-situ} characterisation procedure. Scanning electron microscopy therefore provides a promising contactless technique to study dopant distributions in semiconductor samples with sensitivity over a wide dynamic range ($\sim 10^{16} - 10^{20}$ dopants cm$^{-3}$) and at sub-10 nanometre spatial resolution [1]. However, its general implementation in industry has thus far been inhibited by the lack of an accurate and robust quantification procedure. Although it is known that the dopant contrast observed across a p-n junction is a function of the built-in voltage across the junction, surface band-bending and external local fields (patch fields) above the specimen, the lack of understanding of the respective contributions from all of these factors have hampered accurate quantification. To analyse the problem, we have used detailed computer modelling to investigate the effects of surface states and doping concentrations on the surface band-bending and external patch fields from the specimen, as well as their effects on SE yields and detected contrast in the SEM. The aim of our work presented here is to describe from first principles, a solid quantitative model for dopant profiling in the SEM, and compare it with experimental observations.
2. Problem and solution approach
One obvious issue in SEM doping profiling quantification is that there is no simple analytical relation between the band-bending and trap states at the surface, which constitute a significant effect on dopant contrast [2]. To deal with this problem, numerical modelling was carried out using the finite-element method to calculate the surface charges as well as their effects on surface band-bending and external patch fields. Computations of the electrostatic fields were incorporated into a state-of-the-art Monte Carlo model which takes into account the physics of low energy electron scattering [3]. The Mott or acoustic phonon scattering cross section was used to describe (quasi)elastic interactions in the solid, and a dielectric formulation approach was adopted to determine inelastic scattering and SE generation. SE emission and contrast detection calculations were initially performed for p-n junction samples without surface band-bending (i.e. no surface states). In this case, there are no internal surface fields arising from surface states but only patch fields above the surface. Surface states were next included in the model to simulate their effects on dopant contrast.

3. Results and discussion
Iteratively converged solutions providing the equilibrium carrier and electrostatic field distributions were self-consistently obtained using the finite-element method; the semiconductor Poisson equation as well as the Laplace equation for a semiconductor-vacuum system was solved, including the coupled carrier continuity and drift-diffusion transport equations where applicable. A modified Shockley-Read-Hall (SRH) recombination model was applied to describe recombination effects at the specimen surface [4]. Fermi-Dirac statistics was used and bandgap narrowing effects were accounted for at high doping concentrations. When simulating typical surface band-bending effects, an amphoteric model for surface states was used, with a density of $4 \times 10^{12}$ cm$^{-2}$. The value of the surface state density was determined from finite-element analysis in combination with systematic measurements of surface band-bending effects [5], and was found to agree with typical experimental values for a Si-SiO$_2$ system [6]. The donor- and acceptor-like surface states were specified localised in the bandgap at 0.35 and 0.73 eV above the top of the valence band respectively, and the electron- and hole-capture cross sections for the surface traps are $\tau_n = 10^{-15}$ and $\tau_p = 10^{-16}$ cm$^2$, respectively. In the foregoing calculations, it was assumed that the surface state density and energy are an intrinsic property of the semiconductor, and they do not depend on the local doping concentration [7]. Moreover, the spatial distribution of the surface states was assumed to be uniform in the semiconductor plane. Where $\varepsilon_{Si}$ and $\varepsilon_{SiO_2}$ are the dielectric permittivities of the semiconductor and the native oxide respectively, surface band-bending was computed according to a boundary condition at the semiconductor-oxide interface as follows:

$$\hat{n}\varepsilon_{Si}\vec{E}_{Si} - \hat{n}\varepsilon_{SiO_2}\vec{E}_{SiO_2} = \rho_s$$

(1)

$\hat{n}$ is the unit vector normal to the surface. The difference between the normal components of the electric fields at the respective regions adjacent to the surface boundary must be equal to the sheet charge density $\rho_s$ (Gauss’ Law). This charge term includes both the mobile (carriers) and fixed (ionised dopants and ionised surface states) charges.

To simulate electron beam-specimen interactions, a focussed probe consisting of $10^5$ particles per pixel incident on the sample was defined with an accelerating voltage of 1 kV. The number of primary electrons per pixel used in the simulations provides reasonable statistical accuracy to within about $\pm 0.3\%$ of the calculated SE yield. The simulated primary electron beam energy is within the optimal range for dopant contrast imaging, allowing direct comparison with experimental data. The incident electrons are tracked inside the crystal, which generate further cascades of SEs. All particles are traced through any local electric fields, both inside and outside the solid. When computing the ratio and angular distribution of the emitted SEs, a quantum-mechanical model for transmission and refraction or reflection at a potential transition was employed based on the formulation referred to in
[8] to describe electron scattering at the surface boundary. A planar detector was defined directly on the surface plane, which virtually detects all particles that are emitted from the specimen. Note that this detector effectively has a potential that is equal to the locally existing surface potential of the specimen. A second virtual planar detector parallel to the surface plane was defined, centred on the metallurgical junction at a macroscopic distance above the sample ($z = 0.5 \text{ mm}$) - which was outside the effective range of the specimen's microscopic patch fields. This virtual detector was specified with dimensions of $1 \times 1 \text{ mm}^2$ and with zero potential relative to the specimen. Therefore in general, particles having emission angles less than approximately $45^\circ$ measured from the optical axis are collected, and those with larger emission angles are considered to be undetected. The theoretical absolute values for contrast were calculated using the following formula:

$$C_{\text{cal}} = \frac{\Delta N}{N_p} = \frac{N_p - N_n}{N_p}$$

(2)

where $N_p$ and $N_n$ are the number of calculated SEs from the p- and the n-type regions respectively.

The computed contrast values as at the surface over a wide range of doping concentrations are shown in Fig. 1. When no surface band-bending in the specimen is present, no systematic variation could be observed of the calculated number of SEs emitted from the p- and n-type regions. This is an expected result a priori because of the following reasons. When deriving the differential inelastic cross sections, the optical data for the semiconductor were equivalently applied to the p- and the n-type material, and therefore the calculated generation rate of SEs in the p- and the n-type region is expected to be similar. The inner potential parameters for the p- and the n-type regions were also treated as equal, assuming that these values are not significantly dependent on doping. Hence, the surface boundary transmission probabilities at the respective doped regions are equivalent. The computed contrast varies systematically with doping concentration on the output of the virtual detector at 0.5 mm above the surface (see Fig. 1).

**Figure 1.** Theoretical calculations of dopant contrast (in %) for Si specimens containing a p-n junction with and without surface band-bending. Experimental values of contrast are included for comparison.

**Figure 2.** (a) A simulated SE image as on the surface, a simulated (b) BSE and (c) SE image as on the output of the virtual detector at 0.5 mm above the surface, and (d) a corresponding experimental SE image.
When surface band-bending effects are accounted for, there is a monotonic rise of the calculated contrast with acceptor concentration of up to about $10^{18}$ cm$^{-3}$. For higher doping concentrations, the calculated surface depletion width reduces and becomes comparable or even smaller than the inelastic mean free path for the SEs [9]. Experimental contrast data were also included in Fig. 1 for comparison. These experimental values were obtained on the FEI XL30 sFEG SEM using a through-the-lens detector (TLD) with an extractor voltage of 20 V. The collection angle of this TLD for the operating conditions used is around 45° for a working distance of ~ 6 mm, and the results are therefore directly comparable with the computed output of the virtual detector at $z = 0.5$ mm. It is clear from this comparison that, for the examples chosen, there is quite a convincing agreement between the experimental data and the theoretical plots including surface band-bending effects. BSE and SE images were numerically generated using $10^3$ primary electrons per pixel for an electron probe incident normally on the surface with a landing energy of 1 keV. The plural scattering approach was adopted here in order to accelerate the computation speed. A numerical scan on the sample was performed over an area of 200×100 pixels$^2$. Comparison with a corresponding experimental SE image is provided as shown in Fig. 2. These images were obtained from a Si specimen consisting of a symmetric p-n junction, having a net acceptor and donor concentration of ~ $5 \times 10^{18}$ cm$^{-3}$ in the p- and the n-type regions respectively. Typical surface band-bending characteristics were assumed on this specimen. No significant dopant contrast is observable from the numerical BSE image as expected. Dopant contrast from the simulated SE image as at the surface was found to be too low, but that from the output of the virtual detector above the surface was comparable to the experimental SE image. Numerical accuracy for the simulated image is expected to improve further when using a primary electron count of a few orders of magnitude higher, but such simulations will take much longer to complete.

4. Conclusion
A rigorous quantitative model for SEM dopant profiling has been developed from basic principles and compared with experimental observations. To calculate dopant contrast, the combined numerical model has to account for both the effects of internal surface band-bending and external patch fields from inhomogenously doped specimens. Simulation results show close agreement with experimental data for the chosen modelling parameters, at least within the limits of experimental uncertainty. The results of this work lead to a deeper understanding of the physical mechanisms underpinning dopant contrast, thereby enabling the future development of a quantitative procedure for dopant profiling of semiconductors in the SEM.

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References
[1] Elliott SL, Broom RF and Humphreys CJ 2002 J. Appl. Phys. 91, 9116
[2] Chee KWA, Rodenburg C and Humphreys CJ 2008 MRS Symp. Proc. C04-02, 1026
[3] Kieft E and Bosch EGT 2008 J. Phys. D: Appl. Phys. 41, 215310
[4] Roulston DJ, Arora ND and Chamberlain SG 1982 IEEE Trans. Elec. Dev. 29, 284
[5] Chee KWA, Rodenburg C and Humphreys CJ 2007 J. Phys. Conf. Ser. 120, 407
[6] Stesmans A and Van Gorp G 1990 Phys. Rev. B. 42, 3765
[7] Chung MF 1971 J. Phys. Chem. Solids 32, 475
[8] Cohen-Tannoudji C, Diu B and Laloe F 1977 Quantum Mechanics (Hermann, Paris)
[9] Chee KWA, Bosch EGT and Humphreys CJ to be published