Simulations of the electrostatic potential distribution in a TEM sample of a semiconductor device

P K Somodi, R E Dunin-Borkowski, A C Twitchett, C H W Barnes and P A Midgley

Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, UK

ABSTRACT: Simulations of the electrostatic potential in a thin sample that contains a single Si p-n junction have been carried out in order to examine the effect of different boundary conditions at the sample surface on the potential within the sample. The calculations are compared with experimental electron holography results.

1. INTRODUCTION

The electrostatic potential in a transmission electron microscope (TEM) sample of doped semiconducting material can be mapped using off-axis electron holography. However, such measurements are known to be affected significantly by sample preparation. In particular, the electronic state of the sample surface will differ substantially from that in the bulk semiconductor and also from that of an atomically clean surface. This effect is expected to depend on the degree of implantation, oxidation, deposition and physical damage that occurs during sample preparation. The combined result of these processes on the electrical properties of the sample is usually described collectively, and imprecisely, as an electrically 'dead' or depleted layer on the sample surface. Experimental observations also show that the surface of an unbiased TEM sample that contains a doped semiconductor is always an equipotential, as revealed by the absence of electrostatic fringing fields outside the surface (Frabboni et al 1985, Twitchett et al 2002). Such fringing fields are only revealed when voltages are applied to some samples *in situ* in the TEM.

In order to address this issue, we have solved Poisson's equation iteratively to investigate the effect of a variety of possible surface states and dopant concentrations on the electrostatic potential in a Si TEM sample containing a single p-n junction. The simulations are compared with experimental electron holography results obtained from a sample prepared using focused ion beam (FIB) milling.

2. EXPERIMENTAL RESULTS

Off-axis electron holography allows the phase shift ϕ of an electron wave that has passed through a thin TEM sample to be measured directly. In a non-magnetic sample, the phase shift is proportional to the potential V in the sample integrated in the electron direction z, according to the equation

$$\phi(x,y) = C_E \int V(x,y,z)dz\,, \tag{1}$$

where x and y are directions perpendicular to the incident electron beam and C_E is a sample-independent constant that takes a value of 7.29×10^6 rad V^{-1} m^{-1} at a microscope accelerating voltage of 200 kV.

Fig. 1a shows a reconstructed electron holographic phase image acquired from an unbiased Si p-n junction that was prepared for TEM examination using FIB milling. This technique is known to result in a damaged sample surface containing implanted Ga. The nominal dopant concentration in the sample, whose crystalline thickness was measured to be 220 nm using convergent beam electron diffraction, is in excess of 10^{18}cm^{-3}. The measured phase shift across the junction is shown in Fig. 1b. On the assumption that the dead layer thickness is constant and that the built-in voltage across the junction is 0.9 V, the electrically active thickness of this sample is estimated to be approximately 90 nm. As the data are too noisy to allow the charge distribution in the depletion region to be inferred directly, an empirical model for the phase profile across the junction was fitted to the data, as shown in Fig. 1b. The charge density profile across the junction (Fig. 1c), which provides the most sensitive measure of the electrical state of the junction, was derived from the fitted phase profile rather than from the experimental data. Transition regions are evident at the edges of the junction depletion region, and the experimental charge density is lower than the nominal value for this sample.

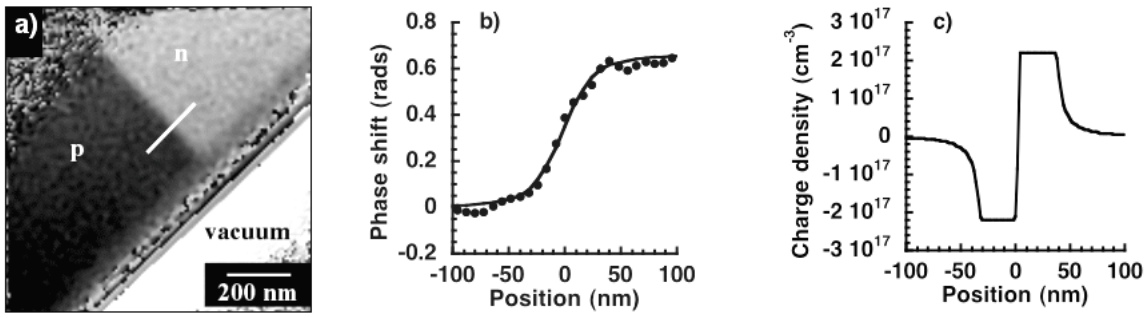

Fig. 1. a) Phase image of an unbiased Si p-n junction. b) Data points along the line marked in a), with the best-fitting profile to the data. c) Charge density across the junction derived from the line in b).

3. SIMULATION RESULTS

Simulations of the electrostatic potential across a p-n junction were obtained by solving Poisson's equation using a relaxation approach (Press 2002). The system of equations that must be solved is non-linear, as the charge in the sample depends on the band structure of the material, which depends, in turn, on the potential. An initial approximation for the potential is required, and the solution is then found iteratively. The directions in which simulations were performed in the present study are shown schematically in Fig. 2a. Figs 2b and c show room temperature conduction band and charge density profiles calculated along direction "1" (Fig. 2a) for a p-n junction of nominal dopant concentration 2.2×10^{17}cm^{-3} (the concentration measured experimentally in Fig. 1c) in both the p- and the n- type bulk semiconductor (assumed for the moment to be unaffected by sample preparation). Although the approximate form of the measured charge density (Fig. 1c) is reproduced in Fig. 2c, the difference between the measured and simulated depletion widths confirms that a detailed investigation of the effect of the electronic state of the sample surface on the potential distribution is required.

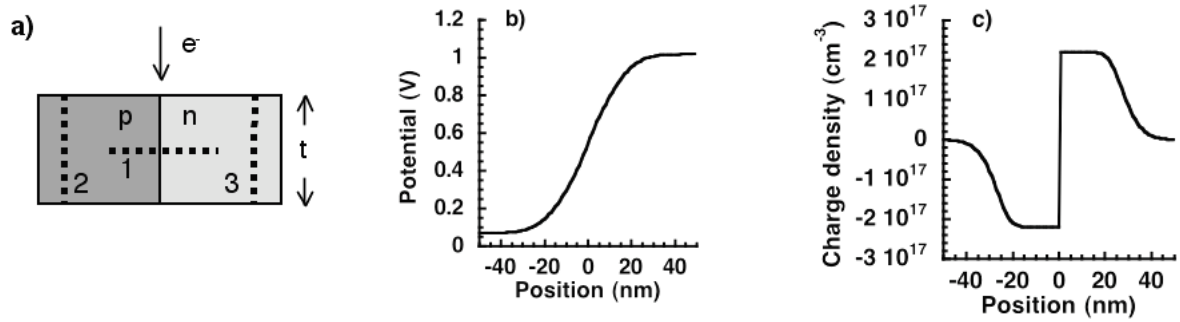

Fig. 2. a) Schematic cross-section of a TEM sample of thickness t containing a p-n junction. The numbers mark the directions in which simulations were performed in this paper. b) Simulated conduction band profile across a p-n junction, along direction "1" in a), for a dopant concentration on each side of the junction of 2.2×10^{17}cm^{-3}. c) Charge density across the junction inferred from b).

Equivalent simulations, which are shown in Figs. 3 and 4, were performed along directions "2" and "3" in Fig. 2a by setting the valence band energy E_V on the surface of the sample to a single, arbitrary value relative to the Fermi energy E_F. The parameter E_F-E_V was then varied to assess the effect of surface states of different energy on the depletion width at the surface of the sample, and hence on the measured phase shift across the junction. As an example of a typical value, E_F-E_V is known to be approximately 0.35 eV for one of the possible reconstructions of a clean Si {111} surface (Lüth 2001). This approach always results in an equipotential sample surface on which the Fermi level is pinned, as observed experimentally. The surface states in the p-type region behave similarly to donor levels, which are able to fully ionise the acceptors close to the surface of the bulk semiconductor, resulting in a negatively charged space charge layer close to the sample surface. The reverse happens in the n-type region. A surface charge density that has the same sign on both sides of the junction, as described by Beleggia et al (2003), cannot provide an equipotential surface using this approach.

Fig. 3 shows the simulated charge densities and conduction band energies on both sides of the junction as a function of position from one surface of a 200-nm-thick sample to the other, for two different surface state energies and for a single dopant concentration of 2.2×10^{17} cm^{-3}. The surface depletion width is typically different on the p and n sides of the junction, and can extend by several tens of nm from the surface, as observed experimentally. The presence of the surface depletion layers results in an apparent decrease in the measured change in potential across the junction, as shown in Fig. 4a for nominal dopant concentrations of 2.2×10^{17}, 5×10^{17} and 1×10^{18} cm^{-3}, for which the expected built-in potentials are 0.94, 0.97 and 1.0 V, respectively. The electrically dead layer thicknesses that would be inferred from Fig. 4a are shown in Fig. 4b, and the widths of the surface depletion layers on both sides of the junction are shown in Figs. 4c and d. It is significant to note that, within the present approximation used to model the electronic states on the surface of a TEM sample, the apparent change in potential across the junction is *always* smaller than expected. For a given surface state energy, the surface depletion width increases with decreasing dopant concentration.

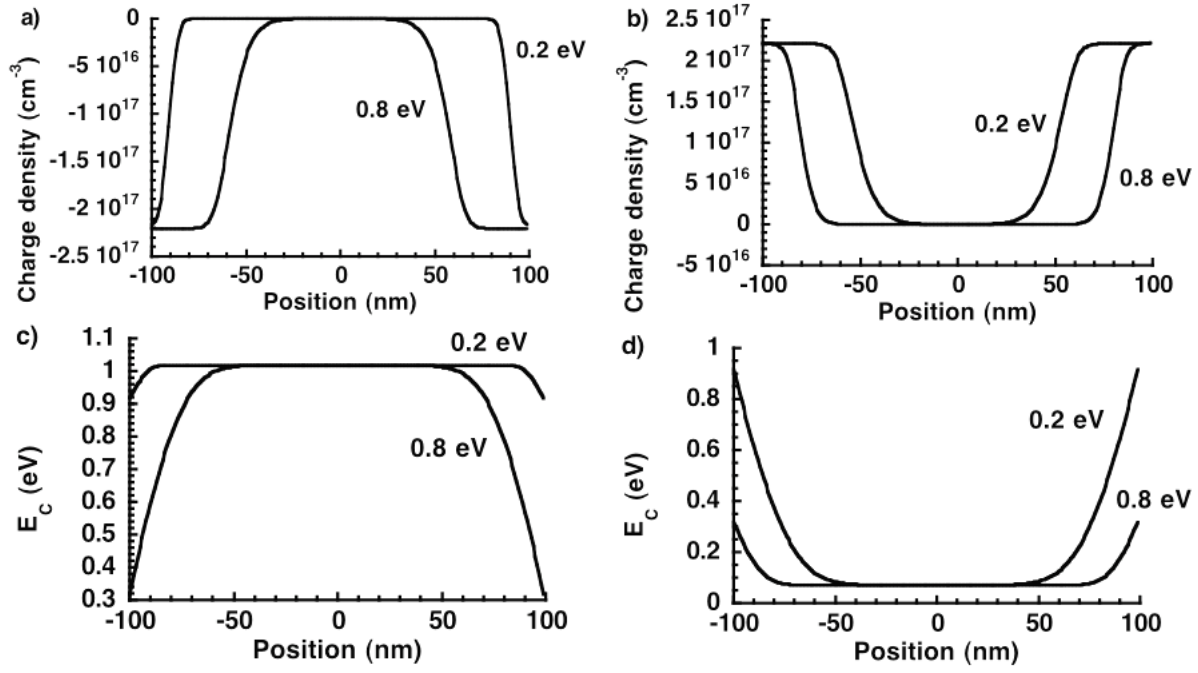

Fig. 3. Simulated charge density profiles between one surface of a sample of thickness 200 nm and the other surface, showing surface depletion on a) the p-side of the junction (direction "2"), and b) the n-side of the junction (direction "3"), for two different surface state energies E_F-E_V (marked) and a single dopant concentration of 2.2×10^{17} cm^{-3}. The corresponding conduction band profiles are shown in c) and d), respectively.

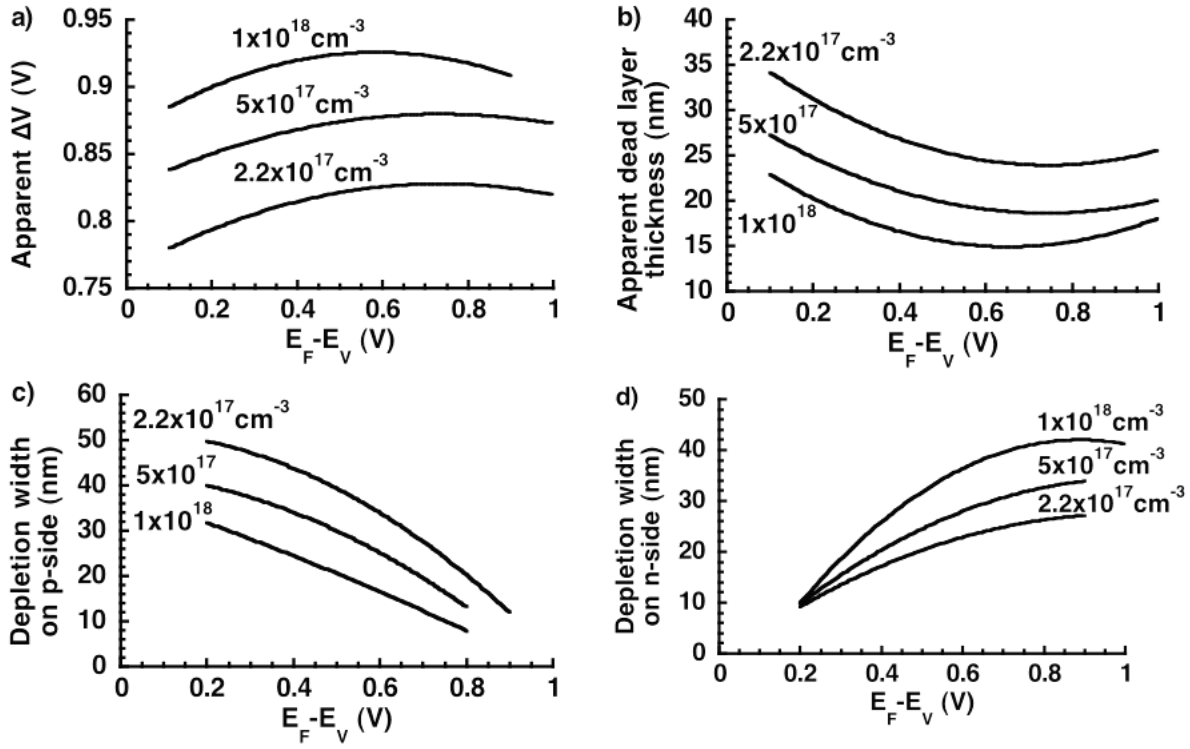

Fig. 4. a) The step in potential across a p-n junction in a sample of thickness 200 nm, inferred from simulations that include the effects of surface depletion, plotted as a function of surface state energy for three different dopant concentrations in the sample. b) The combined electrically 'dead' layer thickness on both sample surfaces inferred from a). The surface depletion width is plotted in c) on the p-side of the junction, and in d) for the n-side of the junction.

4. DISCUSSION AND CONCLUSIONS

The simulated surface depletion widths shown in Figs 3 and 4 are smaller than the electrically dead layer thickness typically measured for FIB milled samples, suggesting that this method of sample preparation affects the electronic structure of the TEM sample well below the sample surface, possibly as a result of Ga implantation or physical damage to the sample. In addition, the present simulations cannot account for the fact that TEM samples made by wedge polishing, limited Ar ion milling and subsequent C coating have been reported to show no surface depletion (McCartney et al 2002). Full three-dimensional simulations are now required to model the effect of the sample surface on the potential in the immediate vicinity of the p-n junction. Future simulations should also take into account the effects of implantation, damage and doping significantly below the sample surface.

We are grateful to Beata Kardynal for valuable discussions, and to the EPSRC, Newnham College and the Royal Society for financial support.

REFERENCES

Beleggia M, Fazzini PF, Merli PG and Pozzi G 2003 Phys. Rev. B **67** 045328

Frabboni S, Matteucci G, Pozzi G and Vanzi M 1985 Phys. Rev. Lett. **55** 2196

Lüth H 2001 Solid Surfaces Interfaces and Thin Films (New York, Springer) p 348

McCartney MR, Gribelyuk MA, Li J, Ronsheim P, McMurray JS and Smith DJ 2002 Appl. Phys. Lett. 80 3213

Press WH, Teukolsky SA, Vettering WT and Flannery BP 2002 Numerical Recipes in C++ (Cambridge, CUP) ch 17

Twitchett A C, Dunin-Borkowski R E and Midgley P A 2002 Phys. Rev. Lett. **88** 238302