Simulations of the electrostatic potential in a thin silicon specimen containing a *p-n* junction

P.K. Somodi[1], R.E. Dunin-Borkowski[1], A.C. Twitchett[1], C.H.W. Barnes[2] and P.A. Midgley[1]

1. Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, U.K.
2. Department of Physics, University of Cambridge, Madingley Road, Cambridge CB3 0HE, U.K.

pks26@cam.ac.uk
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Off-axis electron holography allows the phase shift, ϕ of the electron wave that has passed through a thin specimen to be recorded directly in the transmission electron microscope (TEM). The measured phase shift can be related to the electrostatic potential V in the specimen (projected in the electron beam direction) by making use of the equation

$$\phi(x,y) = C_E \int V(x,y,z)dz\,, \qquad (1)$$

where z is a direction parallel to the electron beam, x and y are perpendicular to the beam, and C_E is a sample-independent constant.

Previous electron holography studies have shown that built-in potentials across semiconductor *p-n* junctions in thin TEM specimens are usually lower than predicted. The concept of an electrically 'dead' layer, whose thickness has been measured to be between 25 and 100 nm on each specimen surface, has been used to describe this discrepancy [1-3]. The 'dead' layer thickness is highly dependent on the approach used to prepare the electron-transparent specimen, and is still poorly understood. In an attempt to understand these observations, we have performed simulations of the electrostatic potential in a thin silicon specimen that contains a single *p-n* junction. Our approach involves solving the non-linear second order differential equation that describes the potential in the specimen [4]

$$\nabla^2 V = -\frac{\rho(V)}{\varepsilon} \qquad (2)$$

where V is the potential (in this case the conduction band energy), ρ is the charge density and ε is the permittivity of the sample. An iterative finite element method [5] was used to solve Equation 2 numerically, starting from an initial guess for V. Figure 1 shows the specimen geometry and the directions along which the simulations were run. The results of the simulations are shown in Figures 2 and 3. For illustrative purposes, the surface state energy was assumed here to be 0.35 eV below the Fermi level [6]. However, the true value of this parameter must be found through comparisons of simulations with experimental data. The results show the expected built-in potential across the junction at the centre of the specimen (Figure 2) and additional depletion layers on the specimen surfaces on both sides of the junction (Figure 3). As a result of the presence of the depleted surface layers, the average potential difference across the junction is 0.77 V when projected through the thickness of the specimen, as compared with a value of 0.92V if surface states were neglected. The apparent 'dead' layer thickness in this specimen is then 38 nm on each specimen surface, which is comparable to values measured using electron holography. Work is now in progress on three-dimensional simulations of specimens of arbitrary geometry, with the aim of obtaining a full understanding of the effects of sample preparation on electrostatic potentials in doped semiconductor samples [7].

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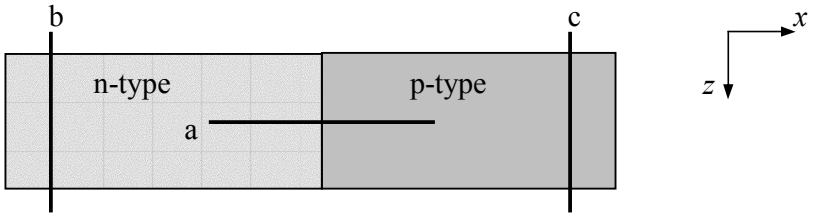

Figure 1. Schematic diagram showing the directions in which the simulations in Figures 2 and 3 were performed. The specimen thickness in the simulations is 400 nm.

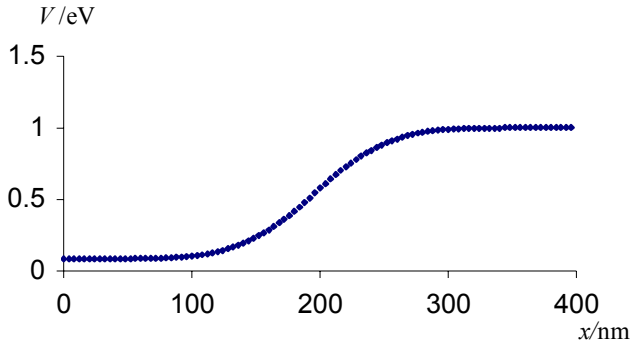

Figure 2. Conduction band energy (measured in electron volts above the Fermi level) along line 'a' in Figure 1. The dopant concentration is 10^{17} cm^{-3} for both the Sb-doped (*n*-type) and the B-doped (*p*-type) sides of the Si p-n junction.

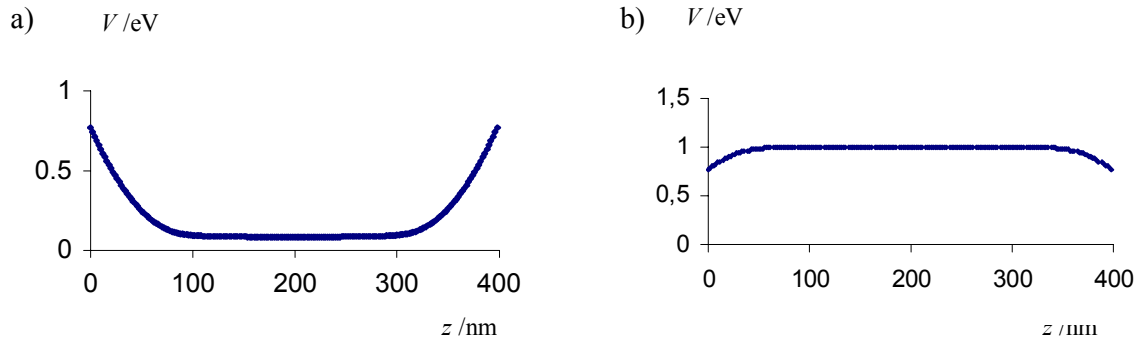

Figure 3. Simulated potential energy along a) line 'b' and b) line 'c' in Figure 1 (electron volts above the Fermi level), for a specimen of thickness 400nm.