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

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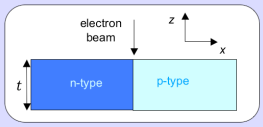
Introduction

- Off-axis electron holography allows the phase shift of a high-energy electron wave to be recorded in a transmission electron microscope (TEM).
- In non-magnetic specimens the phase shift, _, is proportional to the electrostatic potential in the thin (<1_m) specimen projected in the electron beam direction, according to the equation

$$\varphi(x,y) = C_E \int V(x,y,z)dz.$$

where *x*, y are co-ordinates in the projected plane, *z* is a co-ordinate perpendicular to the plane and C_E is a constant that depends on the microscope accelerating voltage.

- Electron holography is increasingly being employed as a technique for the measurement of electrostatic fields in semiconductor devices[1,2].



Schematic diagram showing the direction of the electron beam relative to a parallel-sided TEM sample.

Quantitative interpretation of results

Although electron holography has been applied to the characterisation of dopant potentials in *p-n* junctions, the measured variation in potential is often found to be less than the value predicted by simple theory[3]. The reasons for this discrepancy are not understood but are thought to result from several factors, including

• Sample preparation artefacts, for example the implantation of gallium or argon atoms on the sample surface during ion beam milling.

• Oxidation of the sample surface.

• Charging of the sample surface in the microscope.

A key observation is that TEM samples almost never show electrostatic fringing fields outside their surfaces close to the positions of *p-n* junctions, indicating that the potential on the surface of a TEM sample can be regarded as constant for the present calculations. The actual value of the surface potential is unknown as it will depend heavily on the sample preparation. For a clean surface of silicon the surface energy is approximately 0.35eV below the conduction band energy of the bulk material.[4]

Here we solve the semi-classical equations for a parallel sided sample containing a *p-n* junction. We show that the reduction in the measured potential compared to the expected value is consistent with the presence of surface sates, which act to pin the Fermi levels on the specimen surface.

Numerical Method

The total charge density at a given point within a sample containing *p-n* junction is given by

$$\rho = N_D - N_A + p_A + p_v - n_D - n_C$$

Charge density

N_D: Density of donors

N_A: Density of acceptors

p_A: Density of holes in the acceptor levels

p_v: Density of holes in the valence band

n_D: Density of electrons in the donor levels

n_C: Density of electrons in the conduction band

All of these quantities can be found using the standard semi-conductor equations.[5]

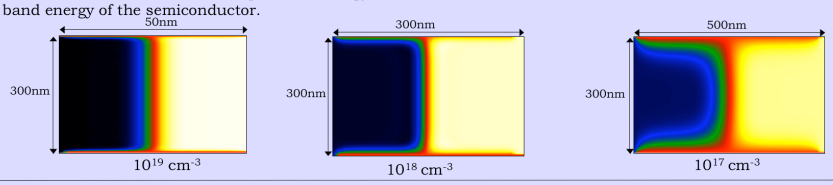
The potential, V, within a specimen of permittivity _ is then calculated using Poisson's equation

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

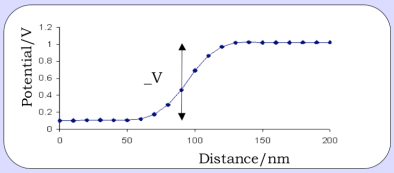
This system of equations is non-linear and must be solved using numerical methods. Here, a finite element method (FEM), based on the Diffpack[6] FEM package, is used to solve the equations iteratively for a *p-n* junction in a parallel-sided TEM specimen.

Results

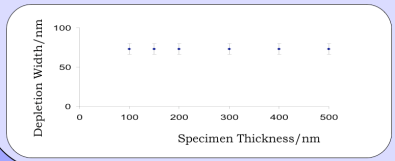
Simulations were run for an abrupt Si *p-n* junction containing Sb (*n*-type) and B (*p*-type) dopants of various concentrations. The value of the potential energy on the surface was taken to be 0.35eV below the conduction band energy of the semiconductor.



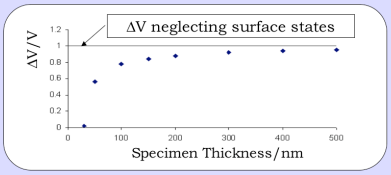
The change in potential across the junction is found by averaging the potential in the direction of the electron beam. The diagram shown below is an average projection through the middle image above.



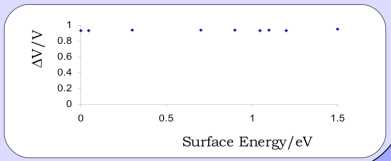
The depletion width (taken to be the distance between the two points where the second derivative of the potential falls to zero) is found to be independent of sample thickness, however this could be due to the poor sampling density used in the calculation. This is shown for the same parameters as the image above.



The variation in the apparent step in voltage, ΔV, for various sample thickness is shown below for a dopant concentration of 10^{18} cm^{-3} and a surface energy of 0.35eV.



The apparent step in potential is approximately independent of the surface energy, as can be seen below for a sample thickness of 300nm and dopant concentration of 10^{18} cm^{-3}.



Conclusions

- The reduction in the variation in potential across a *p-n* junction measured using electron holography can be partially accounted for by the presence of surface states.
- If the sample surface is an equipotential then the measure variation in potential will always be less than that predicted from a knowledge of the dopant concentrations and sample thickness.
- The asymmetry between the *p-* and *n-* sides of the junction observed using electron holography is also observed in these calculation when the surface states are included.
- For small sample thicknesses and low dopant concentrations the built-in voltage is reduced significantly from that expected by simple theory.
- The variation in potential is approximately independent of the surface state energy assumed in the calculation.

References

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