THE IMPORTANCE OF THE FRINGING FIELD SURROUNDING A TEM FOIL TO THE QUANTIFICATION OF PHASE CONTRAST AT A P-N JUNCTION

R.E. DUNIN-BORKOWSKI, W.O. SAXTON
Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, UK, red10@cam.ac.uk

ABSTRACT

The space charge contribution to the electrostatic potential both inside and outside a dielectric slab containing a p-n junction is calculated using classical electrostatics, with particular reference to the use of phase contrast techniques in transmission electron microscopy for the characterisation of the carrier distributions present at such layers.

INTRODUCTION

Phase contrast techniques such as electron holography\(^1\) and Fresnel contrast analysis\(^2\) are routinely used to measure variations in electrostatic potential across interfaces in cross-sectional specimens in the transmission electron microscope (TEM). The application of the same techniques to the determination of the electrical activities of p-n junctions and interfacial space charge layers has been considered both theoretically\(^3\)-\(^5\) and experimentally\(^6\)-\(^7\). However, the interpretation of measured potential profiles is complicated by the fact that there are many possible contributions to the variation in specimen potential across an interface. These include changes in composition, density and bonding character, as well as the presence of dipole layers on the specimen surfaces\(^8\) and fringing (or leakage) fields which result from the fact that a TEM foil has a finite thickness. If experimentally measured potential profiles are to be interpreted quantitatively, then calculations that incorporate accurate models for the predicted variations in potential must be used.

Here, we present a new method for calculating the contribution to the potential from fringing fields. These are associated with the fact that the finite thickness of TEM foil requires the presence of polarisation charges on the specimen surfaces in order to satisfy boundary conditions for Maxwell's equations at the specimen/vacuum interfaces. Not only is the potential within the specimen altered from the profile that it would have if the finite specimen thickness were not taken into account, but a non-zero potential outside the specimen is also predicted. Calculations of the contrast must then be extended to take account of variations in potential in regions outside the specimen. Ultimately, it will be of interest to determine the importance of such surface polarisation effects for a wide range of materials problems that involve the analysis of cross-sectional layers; however, here we restrict ourselves to the consideration of fringing fields which are associated with charge distributions that vary over distances much larger than atomic dimensions. We will illustrate our approach through the calculation of the potential of a specimen containing a p-n junction, as the presence of a wide depletion layer and a consequent long-range variation in specimen potential will maximise both the extent and the magnitude of the fringing field. It will be of interest both to determine the experimental conditions under which this contribution to the potential dominates the contrast so that it can be minimised experimentally or included in simulations correctly, and to assess whether measurements of phase shifts occurring outside the specimen can themselves be used to provide information about charge redistribution within the material.

Our method for calculating the contribution to the potential from fringing fields is based on the use of classical image charge theory, and relies on the premise that high energy electron diffraction depends only on variations in the Coulomb potential within the material. For the purpose of the following calculations, we will model a TEM specimen as an isotropic dielectric
Fig. 1. Schematic diagram showing the orientation of an interface such as a p-n junction (shaded) in a foil of finite specimen thickness $t$, when viewed in cross-section in the TEM.

slab, which has thickness $t$ in the incident beam direction $z$ and relative permittivity $\varepsilon_r$ (assumed not to vary within the specimen), as shown schematically in Fig.1. The charge density $\rho(x)$ in the material will be assumed to vary only in the $x$ direction.

CALCULATION DETAILS

Existing calculations of fringing fields$^3,4$ have relied on the assumptions that the potential within the specimen is unaffected by the finite thickness of the foil, and have resulted in expressions that are independent of the relative permittivity of the specimen. The image charge system that we use here does not rely on these assumptions, and is obtained by reflecting each element of line charge making up the charge distribution $\rho(x)$ in the two specimen/vacuum interfaces in turn. This results in expressions of the form

$$V_{in}(x,z) = \left( \frac{-1}{2\pi \varepsilon_0 \varepsilon_r} \right) \int_{x'=-\infty}^{x'=-\frac{1}{2}} \int_{z'=-\frac{1}{2}}^{z'=-\frac{1}{2}} \sum_{i=0}^{i=\infty} \rho(x') \left[ \beta^{2i} \ln \left( (x'-x)^2 + (z'-z - 2it)^2 \right) \right]^{\frac{1}{2}} dz' dx'$$

$$V_{out}(x,z) = \left( \frac{-\alpha}{2\pi \varepsilon_0 \varepsilon_r} \right) \int_{x'=-\infty}^{x'=-\frac{1}{2}} \int_{z'=-\frac{1}{2}}^{z'=-\frac{1}{2}} \sum_{i=0}^{i=\infty} \rho(x') \left[ \beta^{2i} \ln \left( (x'-x)^2 + (z'-z - (2i-1)t)^2 \right) \right]^{\frac{1}{2}} dz' dx'$$

for the potentials inside and outside the specimen respectively, where $\varepsilon_0$ is the permittivity of free space. The boundary conditions at each of the two interfaces (continuity of the $x$-component of the electric field $E_x$ and the $z$-component of the electric flux density $D_z = \varepsilon_0 \varepsilon_r E_z$) are satisfied when the coefficients $\alpha$ and $\beta$ take values of
Fig. 2. Schematic diagrams showing the variation in charge density and electrostatic potential at a p-n junction, for a specimen of infinite thickness.

\[
\frac{2\varepsilon_r}{\varepsilon_r + 1} \quad \text{and} \quad \frac{\varepsilon_r - 1}{\varepsilon_r + 1}
\]

respectively, and the uniqueness theorem justifies the validity of the solution.

The form of the phase contrast visible at a charged layer is governed most directly by the total phase shift experienced by an electron as it passes through the specimen in the z-direction, with respect to that of an electron passing through an identical region that does not contain a layer. This can be expressed in the form

\[
\phi(x) = k \left( \frac{E + E_0}{E(E + 2E_0)} \right) \left( \int_{|z| \leq \frac{1}{2}} V_{\text{in}}(x,z) dz + \int_{|z| > \frac{1}{2}} V_{\text{out}}(x,z) dz \right),
\]

where \( k \) is the wavevector, \( E \) the kinetic energy and \( E_0 \) the rest energy of the incident electron.

Fig. 2 shows schematic diagrams of the charge density and the electrostatic potential at an abrupt p-n junction, as would be assumed for an infinite specimen thickness. The above expressions for \( V_{\text{in}}, V_{\text{out}} \) and \( \phi(x) \), which are described in more detail elsewhere, will now be used to assess the degree to which the effect of a finite specimen thickness changes both the potential and the phase contrast in a TEM foil containing a p-n junction in Si (\( \varepsilon_r = 11.9 \)).

RESULTS AND DISCUSSION

The parameters used for the calculations are summarised in Table I. Specimen thicknesses of 5 and 50 nm were chosen, with dopant densities on each side of the junction of \( 10^{24} \text{m}^{-3} \) and a reverse bias of 2 V. Temperatures of 300 K and 100 K were included in the calculations in the form of incomplete electrical activation of the dopants, allowing the effect of a change in the charge density distribution to be assessed. Fig. 3 shows a montage of two-dimensional potential
Fig. 3. Calculations of two-dimensional electrostatic potentials at a p-n junction in Si, together with the phase shift $\phi(x)$ experienced by an electron as it passes through the specimen in the $z$-direction with respect to that of an electron passing through an identical region that does not contain a layer. Thirty evenly-spaced equipotential contours have been overlayed onto each of the calculated potentials.

a) $T=300K$, $t=5nm$; b) $T=300K$, $t=50nm$; c) $T=100K$, $t=5nm$; d) $T=100K$, $t=50nm$.

total phase shift (radians) --- ; contribution from ...... inside and ----- outside specimen.
Table I. Parameters used for the calculations presented here.

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>300</th>
<th>100</th>
</tr>
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<tr>
<td>Nominal ( n_a ) (m(^{-3}))</td>
<td>1.0\times10^{24}</td>
<td>1.0\times10^{24}</td>
</tr>
<tr>
<td>Electrically active ( n_a ) (m(^{-3}))</td>
<td>7.7\times10^{23}</td>
<td>7.5\times10^{22}</td>
</tr>
<tr>
<td>( x_p ) (nm)</td>
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<td>718</td>
</tr>
<tr>
<td>Nominal ( n_d ) (m(^{-3}))</td>
<td>1.0\times10^{24}</td>
<td>1.0\times10^{24}</td>
</tr>
<tr>
<td>Electrically active ( n_d ) (m(^{-3}))</td>
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<td>8.0\times10^{21}</td>
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<tr>
<td>( x_n ) (nm)</td>
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<td>6756</td>
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<tr>
<td>Built-in voltage (V)</td>
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<td>1.06</td>
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distributions calculated using equations (1) and (2), with equipotential contours marked at equally spaced intervals. The corresponding phase shifts \( \phi(x) \) are also plotted, with the contributions from inside and outside the specimen given separately. In order to clarify the form of the potential distributions shown in Fig.3, the contour plot in Fig.3d is redrawn in three dimensions in Fig.4, alongside the corresponding potential that would be obtained if fringing fields were not taken into account. Several points are apparent from Figures 3 and 4:

- Most importantly, a finite specimen thickness has a very large effect on both the magnitudes and the forms of the potential profiles. The equipotential plots resemble line dipoles more than they do the potentials that would normally be included in calculations if the finite specimen thickness were not taken into account. Fig.4 illustrates the fact that the potential now decays smoothly from the specimen surface into the vacuum. Such effects must therefore always be included in simulations of phase contrast at p-n junctions if experimental TEM data are to be interpreted quantitatively.

- The total phase shift is dominated by the contribution from outside the specimen for all of the specimen thicknesses examined here. The proportion of the phase shift occurring outside the specimen is always much larger than would be predicted if the fringing field were neglected, but decreases with increasing specimen thickness. As the specimen thickness increases, the phase shift varies over a much larger lateral distance across the specimen than the width of the depletion region (see Table I).

- The results of our calculations differ substantially from those reported by previous authors\(^3\), which has serious implications for any quantitative inferences drawn from experimental data. A full comparison of our calculations with those obtained using complementary approaches will be presented elsewhere\(^1\).

- Our conclusions are in partial agreement with the experimental results of McCartney et al.\(^6\), who measured the phase shift across a p-n junction in Si and found it to be larger than would be expected on the basis of a calculation that did not take the finite specimen thickness into account. However, in contradiction to the present calculations they did not find that the phase shift changed over a distance that was much larger than the depletion width. This may result from the fact that a significant proportion of the external phase shift in our calculations occurs at values of \( z \) that are very large when compared with the specimen thickness, and so its contribution to experimental images may depend on the optics of the microscope used.

- The potential distribution both inside and outside the specimen clearly varies with both specimen thickness and the form of the charge distribution within the material, as indicated by the plots shown for two different temperatures in Fig.3. It may therefore be possible to quantify the variation in charge density within a material from the phase change occurring outside the TEM foil, or alternatively from the manner in which the electrically active carrier concentration changes as a function of temperature.
Fig. 4. A comparison of a) the potential (vertical scale) shown in Fig. 3d for a specimen thickness of 50nm and a temperature of 100K with b) a corresponding calculation that does not take the effects of finite specimen thickness into account.

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REFERENCES