Coordinates for Tip-Semiconductor System in SEMITIP VERSION 3

In SEMITIP VERSION 3 and higher, a new set of coordinates in the vacuum is used that are a generalization of the usual prolate spheroidal coordinates. The new coordinates \( \xi \) and \( \eta \) in the vacuum are related to the cylindrical coordinates \( r \) and \( z \) by

\[
\frac{r^2}{\xi^2 - 1} + \frac{(z - ac\eta)^2}{\xi^2} = a^2, \quad (1a)
\]
\[
- \frac{r^2}{1 - \eta^2} + \frac{(z - ac\eta)^2}{\eta^2} = a^2 \quad (1b)
\]

where \( c = z_0 / (a\eta_T) \) with \( \eta_T \) being the \( \eta \) value defining the hyperboloid that corresponds to the boundary of the probe tip and \( z_0 \) being the center point of this hyperboloid. The values of \( \eta \) thus run from 0 on the surface to \( \eta_T \) at the tip. The value of \( \xi \) is 1 on the central axis and increase with distance away from that axis. For \( z_0 = 0 \) these equations reduce to the standard definition of prolate spheroidal coordinates. With specified values for \( R \), \( b \), and \( s \) we have \( \eta_T = 1/\sqrt{1 + b^2} \), \( a = Rb^2 / \eta_T \), and \( z_0 = s - a\eta_T \). The inverse equations to (1a) and (1b) are

\[
z = a\xi\eta + ac\eta = a(\xi + c)\eta, \quad (2a)
\]
\[
r = a[(\xi^2 - 1)(1 - \eta^2)]^{1/2}. \quad (2b)
\]

Laplace's equation for the electrostatic potential energy \( \phi \) in the vacuum is found to be

\[
f_1(\xi, \eta) \frac{\partial^2 \phi}{\partial \xi^2} + f_2(\xi, \eta) \frac{\partial^2 \phi}{\partial \eta^2} + f_3(\xi, \eta) \frac{\partial^2 \phi}{\partial \theta^2} +
\]
\[
+ f_4(\xi, \eta) \frac{\partial^2 \phi}{\partial \xi \partial \eta} + f_5(\xi, \eta) \frac{\partial \phi}{\partial \xi} + f_6(\xi, \eta) \frac{\partial \phi}{\partial \eta} = 0 \quad (3a)
\]

where

\[
f_1(\xi, \eta) = \frac{(\xi^2 - 1)[(\xi + c)^2 - \eta^2(2c\xi + c^2 + 1)]}{\eta^2(c\xi + 1)} , \quad (3b)
\]
\[
f_2(\xi, \eta) = \frac{(1 - \eta^2)(\xi^2 - \eta^2)}{\xi(\xi + c) - \eta^2(c\xi + 1)} , \quad (3c)
\]
\[
f_3(\xi, \eta) = \frac{\xi(\xi + c) - \eta^2(c\xi + 1)}{(\xi^2 - 1)(1 - \eta^2)} , \quad (3d)
\]
\[
f_4(\xi, \eta) = \frac{-2c\eta(\xi^2 - 1)(1 - \eta^2)}{\xi(\xi + c) - \eta^2(c\xi + 1)} , \quad (3e)
\]
\[
f_5(\xi, \eta) = \frac{g_5(\xi, \eta)}{[\xi(\xi + c) - \eta^2(c\xi + 1)]^2} , \quad (3f)
\]

and

\[
f_6(\xi, \eta) = \frac{g_6(\xi, \eta)}{[\xi(\xi + c) - \eta^2(c\xi + 1)]^2} , \quad (3g)
\]

with
\[
g_5(\xi, \eta) = c^3 + 3c^2 \xi + c(2 + c^2) \xi^2 + 3c^2 \eta^3 + 4c\xi^4 + 2\xi^5 + \\
\eta^4[c^3 + (2 + 3c^2)\xi + c(6 + c^2)\xi^2 + 3c^2\xi^3] - \\
2\eta^2[c(c^2 - 1) + 3c^2\xi + c(6 + c^2)\xi^2 + (2 + 3c^2)\xi^3 + c\xi^4]
\] 
(3h)

and
\[
g_6(\xi, \eta) = -\eta \{c^2 + 4c\xi + c^2\xi^2 + 2\xi^4 + \eta^4[2 + c^2 + 4c\xi + c^2\xi^2] - \\
2\eta^2[c^2 + 4c\xi + (2 + c^2)\xi^2]\}.
\] 
(3i)

In VERSIONS 3, 4, and 5 there is not \(\theta\) dependence, so the second derivative with respect to \(\theta\) [third term of Eq. (3a)] is zero.

Grid points are labeled by \((i,j)\) with \(i\) referring to the radial direction and \(j\) referring to the direction perpendicular to the surface. In the new coordinate system for the vacuum the grid points are given by \((\xi, \eta)\). The spacing between the \(\eta\) values is chosen to be simply \(\Delta\eta = \eta_r / NV\), so that \(\eta_j = j(\eta_r / NV)\). The \(\xi\) values can be obtained by noting that the radial grid values at the surface are matched between the vacuum and the grid. Thus, using the \(R_i\) values output by the program and with \(j = 0\) referring to the surface, we have \(r_{i0} = R_i\). On the surface, \(\eta = 0\), so that \(r_{i0} = R_i = a(\xi_i^2 - 1)^{1/2}\) so that \(\xi_i = [1 + (R_i / a)^2]^{1/2}\). The particular values of \(r_{ij}\) and \(z_{ij}\) corresponding to the grid points can therefore be obtained by:

(i) for \(z_{ij}\) we have \(z_{ij} = a(\xi_i + c)\eta_j = ([a^2 + R_i^2]^{1/2} + ac) j \eta_r / NV\). The program defines \(DELV_i\) as \(([a^2 + R(1)^2]^{1/2} + ac) \eta_r / NV\), so that \(z_{ij} = j \times DELV_i\).

(ii) for the \(r_{ij}\) values, we again note that the radial values at the surface are \(R_i = a(\xi_i^2 - 1)^{1/2}\). Then, away from the surface we have \(r_{ij} = a[(\xi_i^2 - 1)(1 - \eta_j^2)]^{1/2} = R_i [1 - (j(\eta_r / NV))^2]^{1/2}\) with \(\eta_r = 1 / \sqrt{1 + b^{-2}}\) and where \(b\) is the user specified shank slope.