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 ξ and η in the vacuum are related to the cylindrical coordinates r and z by

$$\frac{r^2}{\xi^2-1}+\frac{(z-ac\eta)^2}{\xi^2}=a^2\,, \tag{1a}$$

$$-\frac{r^2}{1-\eta^2}+\frac{(z-ac\eta)^2}{\eta^2}=a^2 \tag{1b}$$

where $c\equiv z_0/(a\eta_T)$ with η_T being the η 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 η thus run from 0 on the surface to η_T at the tip. The value of ξ 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

$$z=a\xi\eta+ac\eta=a(\xi+c)\eta\,, \tag{2a}$$

$$r=a[(\xi^2-1)(1-\eta^2)]^{1/2}\,. \tag{2b}$$

Laplace's equation for the electrostatic potential energy ϕ in the vacuum is found to be

$$\begin{aligned} &f_1(\xi,\eta)\frac{\partial^2\phi}{\partial\xi^2}+f_2(\xi,\eta)\frac{\partial^2\phi}{\partial\eta^2}+f_3(\xi,\eta)\frac{\partial^2\phi}{\partial\theta^2}+\\ &\quad+f_4(\xi,\eta)\frac{\partial^2\phi}{\partial\xi\partial\eta}+f_5(\xi,\eta)\frac{\partial\phi}{\partial\xi}+f_6(\xi,\eta)\frac{\partial\phi}{\partial\eta}=0 \end{aligned} \tag{3a}$$

where

$$f_1(\xi,\eta)=\frac{(\xi^2-1)[(\xi+c)^2-\eta^2(2c\xi+c^2+1)]}{\xi(\xi+c)-\eta^2(c\xi+1)}\,, \tag{3b}$$

$$f_2(\xi,\eta)=\frac{(1-\eta^2)(\xi^2-\eta^2)}{\xi(\xi+c)-\eta^2(c\xi+1)}\,, \tag{3c}$$

$$f_3(\xi,\eta)=\frac{\xi(\xi+c)-\eta^2(c\xi+1)}{(\xi^2-1)(1-\eta^2)}\,, \tag{3d}$$

$$f_4(\xi,\eta)=\frac{-2c\eta(\xi^2-1)(1-\eta^2)}{\xi(\xi+c)-\eta^2(c\xi+1)}\,, \tag{3e}$$

$$f_5(\xi,\eta)=\frac{g_5(\xi,\eta)}{[\xi(\xi+c)-\eta^2(c\xi+1)]^2}\,, \tag{3f}$$

and

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

with

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

and

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

In VERSIONS 3, 4, and 5 there is not θ dependence, so the second derivative with respect to θ [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 (ξ_i, η_j). The spacing between the η_j values is chosen to be simply $\Delta\eta = \eta_T / \mathrm{NV}$, so that $\eta_j = j(\eta_T / \mathrm{NV})$. The ξ_i 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 $r_{i0} = \mathrm{R}_i$. On the surface, $\eta = 0$, so that $r_{i0} = \mathrm{R}_i = a(\xi_i^2 - 1)^{1/2}$ so that $\xi_i = \{1 + [\mathrm{R}_i / a]^2\}^{1/2}$. 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 $z_{ij} = a(\xi_i + c)\eta_j = ([a^2 + \mathrm{R}_i^2]^{1/2} + ac)\, j\eta_T / \mathrm{NV}$. The program defines DELV_i as $([a^2 + \mathrm{R(I)}^2]^{1/2} + ac)\eta_T / \mathrm{NV}$, so that $z_{ij} = j \times \mathrm{DELV}_i$.

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