

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

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

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

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

$$z = a\xi\eta + ac\eta = a(\xi + c)\eta, \quad (2a)$$

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

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 $\Delta\eta = \eta_T / NV$, so that $\eta_j = j(\eta_T / NV)$. 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 $r_{i0} = R_i$. 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 $z_{ij} = a(\xi_i + c)\eta_j = ([a^2 + R_i^2]^{1/2} + ac)j\eta_T / NV$. The program defines $DELV_i$ as $([a^2 + R_i^2]^{1/2} + ac)\eta_T / NV$, 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 $r_{ij} = a[(\xi_i^2 - 1)(1 - \eta_j^2)]^{1/2} = R_i \{1 - [j(\eta_T / NV)]^2\}^{1/2}$ with $\eta_T = 1/\sqrt{1+b^{-2}}$ and where b is the user specified shank slope.