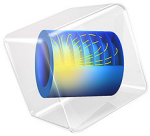

Thermionic Emission in a Planar Diode

Introduction

In this benchmark model, electrons are released via thermionic emission from a hot cathode in a plane parallel vacuum diode. Because the thermal electrons contribute to the space charge density in the region between the cathode and the anode, a potential barrier forms close to the cathode. This potential barrier retards the motion of electrons toward the anode so that electrons of lower energy are repelled back toward the cathode and only electrons with higher energy are transmitted. As a result, the transmitted current in the diode is only a fraction of the total thermionic current.

The Charged Particle Tracing interface is used to model thermionic emission from a cathode with a specified temperature and work function. A dedicated study for modeling bidirectionally coupled particle field interactions is used to include the contribution of the thermal electrons when computing the electric potential in the diode. The transmitted current and the potential in the diode are compared to the analytic solution of the Langmuir-Fry model.

The phenomenon of thermionic emission can be subdivided into different regimes based on the temperature and potential difference. In both regimes, a population of electrons following the classical Maxwell-Boltzmann energy distribution are emitted from a cathode at a fixed temperature. The emitted electrons have a velocity direction distribution following Lambert's cosine law. For a fixed temperature, as the electric potential difference between the cathode and anode is increased, the collected current at the anode increases and will eventually saturate. This special condition is called the *thermally limited regime*; the current at the anode depends only on the work function and temperature of the cathode and is unaffected by further increases in the potential difference. Before reaching this regime, at lower potential difference, the space charge in the region adjacent to the cathode creates a region of negative potential. This potential barrier repels some of the thermally emitted electrons back to the cathode surface, so the current at the anode is less than the emitted current at the cathode or *saturation current*. In this case, the electron emission is said to be in the *space charge limited regime*.

Space charge limited emission of thermal electrons in a plane parallel vacuum diode is one of the only problems in nonlaminar charged particle beam physics that has an exact analytic solution, making it a useful benchmarking tool. This solution is often called the Langmuir-Fry model, referring to the authors of two frequently cited early publications in this area (1,2).

Model Definition

The planar diode consists of two semi-infinite parallel electrodes separated by a distance $d = 1$ mm. The model geometry is three-dimensional but can be understood as quasi-1D because the potential and current are uniform in the x- and z-directions. The geometry of the diode and the functional form of the electric potential distribution in the space charge limited regime are illustrated in Figure 1. The cathode is grounded ($V_c = 0$) and the anode is maintained at a fixed potential of $V_a = 100$ V. The cathode is maintained at a uniform temperature of $T_c = 2500$ K and its work function is $\Phi_m = 4.5$ V.

Note that Figure 1 is not necessarily drawn to scale. The negative potential barrier is often extremely narrow compared to the diode width d.

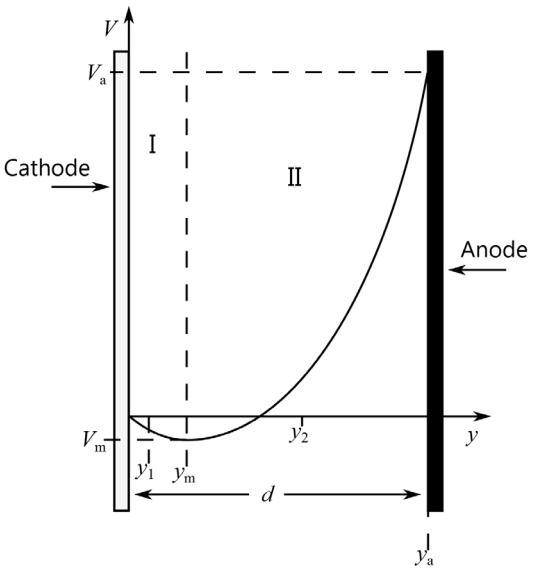

Figure 1: The planar diode in the space charge limited regime. The black solid curve shows the electric potential between the electrodes, which reaches a local minimum at the potential barrier before increasing closer to the anode.

The geometry is oriented so that the normal vector between the two parallel electrodes points in the positive y-direction. From the symmetry of the semi-infinite planar diode, the transverse electric field components are zero ($\boldsymbol{E}_x = \boldsymbol{E}_z = 0$), and the components of the electron velocity in these directions remain unchanged after they leave the cathode ($v_x = v_{x0}, v_z = v_{z0}$). For this reason, a **Swept** mesh is created with only a single element in the transverse directions.

This model uses the dedicated Particle Field Interaction, Non-Relativistic interface, which creates the following interfaces and couplings:

- An instance of the Electrostatics interface to compute the electric potential,
- An instance of the Charged Particle Tracing interface to exert forces on the electrons and compute their trajectories, and
- An **Electric Particle Field Interaction** Multiphysics coupling to compute the effect of the particles on the space charge density distribution within the modeling domain.

Although the electrons always exist at a number of discrete positions, the charge density must be represented as a field with finite values. The **Electric Particle Field Interaction** node defines a contribution from each model particle to the mesh element that the particle occupies, allowing their charge to be converted to a spatial density.

A further advantage of using a **Swept** mesh with only one element in each cross-section parallel to the *xz*-plane is that there is no possibility of non-physical transverse electric field components arising from discretization of the charge density and discrete sampling of the electrons in velocity space.

THE THERMIONIC EMISSION FEATURE

In this example, electrons are released from the cathode using the dedicated **Thermionic Emission** release feature. This feature pseudorandomly samples the initial velocity components of the emitted electrons so that they follow a Maxwell-Boltzmann energy distribution and a Lambertian distribution of release angles with respect to the surface normal.

The initial particle velocity components are

$$v_{t1} = |\mathbf{v}| \sin\theta \cos\phi$$

$$v_{t2} = |\mathbf{v}| \sin\theta \sin\phi$$

$$v_{n} = |\mathbf{v}| \cos\theta$$

where v_n is the velocity component normal to the cathode surface and v_{t1} and v_{t2} are the two orthogonal velocity components parallel to the surface. The azimuthal angle ϕ (SI unit: rad) and the polar angle θ (SI unit: rad) follow the probability distribution function

$$f(\theta, \phi) = \frac{1}{\pi} \sin\theta \cos\theta$$

That is, ϕ has a uniform probability in the interval $[0, 2\pi]$ and θ has a Lambertian probability distribution in the interval $[0, \pi/2]$.

The velocity magnitude follows a probability distribution function

$$f(W) = W\exp(-W)$$

where W (dimensionless) is the normalized particle kinetic energy, defined as

$$W = \frac{m_e}{2k_B T_c}|\mathbf{v}|^2$$

where

- $m_e = 9.10938188 \times 10^{-31}$ kg is the electron mass,
- $k_B = 1.3806488 \times 10^{-23}$ J/K is the Boltzmann constant, and
- T_c (SI unit: K) is the cathode temperature.

For details on how the initial particle velocity components are sampled from these distributions, see the *Particle Tracing Module User's Guide*.

BIDIRECTIONALLY COUPLED PARTICLES AND FIELDS

Just as the electrons contribute to the space charge density which affects the electric potential, changes in the potential modify the electron trajectories. In this way the particle trajectories and field are bidirectionally coupled. Computing a self-consistent solution, in which the effects of each part of the solution on the other are taken into account, requires the following steps:

1. Compute the particle trajectories, assuming no space charge effects are present, using a **Time-Dependent Solver**. From these trajectories, compute the space charge density using the **Electric Particle Field Interaction** node. Because there is no potential barrier during the first iteration, all of the particles should reach the anode and the transmitted current should equal the thermionic current at the cathode.
2. Compute the electric potential due to the space charge density of electrons in the diode, using a **Stationary Solver**. The boundary conditions for the Electrostatics interface are the specified potentials at the cathode and the anode.
3. Use the electric potential calculated in step 2 to compute the perturbed particle trajectories. Recalculate the space charge density using these perturbed trajectories.
4. Repeat steps 2 and 3 until either a specified number of iterations has been reached or until the change in the transmitted thermionic current between successive iterations is less than a specified tolerance.

This iterative procedure is automatically set up when using the **Bidirectionally Coupled Particle Tracing** study step, a specialized study step intended specifically for modeling bidirectional couplings between time-dependent particle positions and stationary fields.

The Langmuir-Fry Model

The following analytic solution for the electric potential in a plane parallel vacuum diode in the space charge limited regime is based on Ref. 3.

The maximum total current density J_{th} (SI unit: $\mathrm{A/m^2}$) that can be drawn from a cathode has been predicted theoretically and shown experimentally to follow the Richardson equation,

$$J_{\mathrm{th}} = A^* T_{\mathrm{c}}^2 \exp\left(-\frac{e\Phi}{k_{\mathrm{B}} T_{\mathrm{c}}}\right) \tag{1}$$

where

- A^* (SI unit: $\mathrm{A/(m^2K^2)}$) is the effective Richardson constant,
- T_{c} (SI unit: K) is the cathode temperature,
- $e = 1.602176565 \times 10^{-19}$ C is the fundamental charge, and
- $k_{\mathrm{B}} = 1.3806488 \times 10^{-23}$ J/K is the Boltzmann constant, and
- Φ (SI unit: V) is the cathode work function.

J_{th} is also called the saturation current. If the voltage saturation has not been reached, and thus the current at the anode is less than J_{th}, then there must be a potential minimum between the cathode and anode that repels electrons of low energy back toward the cathode as illustrated in Figure 1.

It is convenient to express the charge density and current density in terms of the number density of particles in 6-dimensional phase space $n(\mathbf{x},\mathbf{v})$ (SI unit: $\mathrm{s^3/m^6}$), where $\mathbf{x}$ (SI unit: m) is the position vector with components x, y, and z; and $\mathbf{v}$ (SI unit: m/s) is the velocity vector with components v_x, v_y, and v_z.

The electric potential V (SI unit: V) in the vacuum diode follows Poisson's equation,

$$\nabla^2 V = -\frac{\rho}{\varepsilon_0} \tag{2}$$

where $\varepsilon_0 = 8.854187817 \times 10^{-12}$ F/m is the permittivity of vacuum and ρ (SI unit: $\mathrm{C/m^3}$) is the charge density of the electrons. In terms of the phase space number density, the charge density is

$$\rho = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} -en\,dv_x dv_y dv_z \tag{3}$$

In terms of the phase space number density, the current density of electrons emitted at the cathode is

$$J_{\text{th}} = \int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{-\infty}^{\infty} ev_y n\,dv_x dv_y dv_z \tag{4}$$

Note that the range of integration starts from 0 in the y-direction since the velocity of the electrons escaping the cathode can only be positive in this direction.

Also note that the sign conventions have been chosen here so that J_{th} is positive for the electron emission, even though the net flow of charge is in the -y-direction. This is consistent with the sign convention used in Equation 1 for the saturation current.

The phase space number density is assumed to follow a Gaussian distribution in velocity space,

$$n = C\exp[-F^2(v_x^2 + v_y^2 + v_z^2)] \tag{5}$$

where the coefficient F (SI unit: s/m) is given by

$$F = \sqrt{\frac{m_{\text{e}}}{2k_{\text{B}}T_{\text{c}}}}$$

and where $m_{\text{e}} = 9.10938188 \times 10^{-31}$ kg is the electron mass.

The constant C (SI unit: s^3/m^6) can be expressed in terms of the saturation current by substituting Equation 5 into Equation 4 and integrating, which yields

$$J_{\text{th}} = eC\frac{\pi}{2F^4}$$

or alternatively

$$C = \frac{2J_{\text{th}}F^4}{\pi e}$$

Thus, in terms of the saturation current the phase space number density is

$$n = \frac{2J_{\text{th}}F^4}{\pi e}\exp[-F^2(v_x^2 + v_y^2 + v_z^2)] \tag{6}$$

Liouville's theorem states that the phase space density is invariant along a particle's trajectory,

$$n(\mathbf{x}_0, \mathbf{v}_0) = n(\mathbf{x}_1, \mathbf{v}_1)$$

where the subscripts 0 and 1 indicate the particle's coordinates in phase space at two different times. Due to the symmetry of the planar diode, the phase space density is uniform in the x- and z-directions, so these arguments can be dropped. Furthermore, since the electric potential in the semi-infinite planar diode only varies in the y-direction, the transverse velocity components are constant along the particle's phase space trajectory. Thus, Liouville's theorem can be simplified to

$$n(y_0;v_{0x}, v_{0y}, v_{0z}) = n(y_1;v_{0x}, v_{1y}, v_{0z})$$

Taking $\mathbf{x}_0$ and $\mathbf{v}_0$ to be the phase space coordinates at the cathode where $y = 0$, this can be further simplified to

$$n(y;v_{0x}, v_y, v_{0z}) = n(0;v_{0x}, v_{0y}, v_{0z})$$

Substituting this result into Equation 5 yields an expression for the phase space number density at the cathode in terms of the initial velocity components at the cathode v_{0x}, v_{0y}, and v_{0z},

$$n(0;v_{0x}, v_{0y}, v_{0z}) = \frac{2J_{\text{th}}F^4}{\pi e}\exp[-F^2(v_{0x}^2 + v_{0y}^2 + v_{0z}^2)]$$

In the space charge limited regime, electrons are either transmitted to the anode or repelled back to the cathode depending on whether they have sufficiently high velocity in the y-direction to bypass the negative potential barrier close to the cathode. From conservation of energy for nonrelativistic electrons, the y-component of the velocity at any point along an electron's trajectory is a function of the electric potential V at that point and the electron's initial velocity in the y-direction,

$$v_y^2 - v_{0y}^2 = -2\eta V \tag{7}$$

where η is the charge-to-mass ratio of the electrons,

$$\eta = -\frac{e}{m_e}$$

The electric potential is measured with respect to the cathode; that is, $V_c = 0$. The electric potential reaches a minimum value at $y = y_m$ ($0 < y_m < d$, where d (SI unit: m) is the distance from the cathode to the anode) where the following conditions apply:

$$\begin{aligned} V &= V_m \\ E_y &= 0 \end{aligned} \tag{8}$$

Because $V = 0$ at the cathode and the electrons are negatively charged, V_m must be negative. The normal component of the electric field E_y is positive between the cathode and the semi-infinite plane located at $y = y_m$ (region I in Figure 1). This positive electric field in region I decelerates the electrons. For $y > y_m$ (region II in Figure 1), E_y is negative and the electrons are accelerated toward the anode. In order to enter region II, the emitted electrons must have sufficiently high velocity in the y-direction to bypass the potential barrier at y_m. Substituting $v_y = 0$ and $V = V_m$ into Equation 7 yields the minimum initial electron velocity needed to reach the location of the minimum potential,

$$v_{0my} = \sqrt{2\eta V_m} \tag{9}$$

In region I, electrons can move in both the positive and negative y-directions. An electron will cross a plane at y ($0 < y < y_m$) with electric potential V ($0 > V > V_m$) exactly once (going in the positive y-direction only) if and only if

$$v_{0y} \geq \sqrt{2\eta V_m}$$

since the electron then has sufficient energy to bypass the barrier and doesn't return to the cathode.

An electron will cross the plane exactly twice, first going in the positive y-direction and then returning to the cathode in the negative y-direction, if and only if

$$\sqrt{2\eta V_m} > v_{0y} > \sqrt{2\eta V}$$

since in this case the particle has sufficient energy to bypass the plane but insufficient energy to bypass the entire potential barrier, so it eventually gets repelled back to the cathode.

In region II, a particle passes a plane at y ($y > y_m$) once if and only if

$$v_{0y} \geq \sqrt{2\eta V_{\mathrm{m}}}$$

since, once a particle has bypassed the potential barrier, it will definitely reach the anode.

The minimum possible value of the y-component of the particle velocity $v_{\mathrm{m}y}$ at any location is therefore

$$v_{\mathrm{m}y} = \begin{cases} -\sqrt{-2\eta(V - V_{\mathrm{m}})} & y < y_{\mathrm{m}} \\ \sqrt{-2\eta(V - V_{\mathrm{m}})} & y > y_{\mathrm{m}} \end{cases} \tag{10}$$

This result will be used in subsequent integrations over velocity space.

Substituting Equation 3 for the space charge density into Equation 2 for the electric potential, taking into account the invariance of the electric potential in the transverse directions, and adjusting the lower limit of integration based on Equation 10 yields the following 1D Poisson equation for the electric potential V at any position y in the diode:

$$\frac{d^2V}{dy^2} = -\frac{e}{\varepsilon_0}\int_{-\infty}^{\infty}\int_{v_{my}}^{\infty}\int_{-\infty}^{\infty} n\,dv_x dv_y dv_z \tag{11}$$

This integro-differential equation is subject to the boundary conditions $V(0) = 0$ and $V(d) = V_{\mathrm{a}}$. The lower limit of integration on y is given by Equation 10.

This integro-differential equation can be solved to compute the location and magnitude of the minimum potential. It is convenient to replace the electric potential with the dimensionless variable Y,

$$Y = 2\eta F^2(V - V_{\mathrm{m}}) \tag{12}$$

Algebraic manipulation of Equation 11 (see for example Ref. 2) leads to

$$0 = \left(\frac{4\sqrt{\pi}}{\varepsilon_0}J_{\mathrm{th}}F^3\right)^{-\frac{1}{2}}\exp\left(\frac{Y_{\mathrm{c}}}{2}\right)\left(\int_0^{Y_c}\frac{1}{\sqrt{Q_{\mathrm{I}}(Y)}}dY + \int_0^{Y_a}\frac{1}{\sqrt{Q_{\mathrm{II}}(Y)}}dY\right) - d \tag{13}$$

where Y_{c} is the value of the nondimensionalized potential Y at the cathode,

$$Y_{\mathrm{c}} = -2\eta F^2 V_{\mathrm{m}}$$

Y_{a} is the value of Y at the anode,

$$Y_a = 2\eta F^2 (V_a - V_m)$$

or in terms of Y_c,

$$Y_a = 2\eta F^2 V_a + Y_c$$

and the dimensionless functions $Q_I(Y)$ and $Q_{II}(Y)$ have been defined as follows:

$$Q_I(Y) = (\exp(Y) - 1) + \mathrm{erf}(\sqrt{Y})\exp(Y) - \frac{2\sqrt{Y}}{\sqrt{\pi}}$$

$$Q_{II}(Y) = (\exp(Y) - 1) - \mathrm{erf}(\sqrt{Y})\exp(Y) + \frac{2\sqrt{Y}}{\sqrt{\pi}}$$

Thus $Q_I(Y)$ is used when integrating over values of the nondimensionalized potential in region I, and similarly $Q_{II}(Y)$ is used when integrating over values of the nondimensionalized potential in region II.

The current density at the anode is

$$J_a = \int_{-\infty}^{\infty} \int_{v_{0my}}^{\infty} \int_{-\infty}^{\infty} e v_y n dv_x dv_y dv_z \tag{14}$$

where instead of being zero as in Equation 4, the lower limit of integration v_{0my} is the minimum velocity needed for the emitted particles to cross the potential barrier and thus reach the anode. Substituting the number density from Equation 6 yields

$$J_a = \int_{-\infty}^{\infty} \int_{v_{0my}}^{\infty} \int_{-\infty}^{\infty} \frac{2}{\pi} J_{th} F^4 v_y \exp[-F^2(v_x^2 + v_y^2 + v_z^2)] dv_x dv_y dv_z \tag{15}$$

This integral can be rearranged as follows:

$$J_a = \int_{-\infty}^{\infty} \frac{F}{\sqrt{\pi}} \exp(-F^2 v_x^2) dv_x \int_{v_{0my}}^{\infty} 2 J_{th} F^2 v_y \exp(-F^2 v_y^2) dv_y \int_{-\infty}^{\infty} \frac{F}{\sqrt{\pi}} \exp(-F^2 v_z^2) dv_z$$

Integrating the above expression, and noting that, by definition,

$$Y_c = F^2 v_{0my}^2$$

yields a simplified expression for the anode current in terms of the known thermionic current and the nondimensionalized potential at the cathode,

$$J_a = J_{th} \exp(-Y_c)$$

This leads to definitions of Y_c and Y_a in terms of the cathode and anode currents,

$$Y_c = \log\left(\frac{J_{th}}{J_a}\right) \tag{16}$$

$$Y_a = 2\eta F^2 V_a + \log\left(\frac{J_{th}}{J_a}\right) \tag{17}$$

Thus, given the electron properties, thermionic current, and potential difference between the cathode and the anode, it is possible to solve numerically for the anode current J_a by substituting Equation 16 and Equation 17 into Equation 13 and then evaluating the integrals over Y.

Any value of Y corresponds to a unique value of the electric potential greater than or equal to the minimum potential V_m. This value of the potential may correspond to a value of y on one or both sides of the potential minimum. The corresponding value of y in region I, denoted y_I, is

$$y_I = y_m - \left(\frac{4\sqrt{\pi}}{\varepsilon_0} J_{th} F^3\right)^{-\frac{1}{2}} \exp\left(\frac{Y_c}{2}\right) \left(\int_0^Y \frac{1}{\sqrt{Q_I(Y')}} dY' \right) \tag{18}$$

The corresponding value of y in region II, denoted y_{II}, is

$$y_{II} = y_m + \left(\frac{4\sqrt{\pi}}{\varepsilon_0} J_{th} F^3\right)^{-\frac{1}{2}} \exp\left(\frac{Y_c}{2}\right) \left(\int_0^Y \frac{1}{\sqrt{Q_{II}(Y')}} dY' \right) \tag{19}$$

Similarly it is possible to compute the potential at a specified y-coordinate. One viable approach is to integrate Equation 18 and Equation 19 for a list of Y-values, then generate a pair of interpolation functions giving y_I and y_{II} as approximate functions of Y. These interpolation functions can be inverted and combined to display the electric potential as a function of the y-coordinate in the diode.

Results and Discussion

Figure 2 shows the electric potential profile near the cathode for both the particle tracing simulation and the analytical solution. The **Reference** curve was created by defining an interpolation function containing numerical integrations of the results of the previous section.

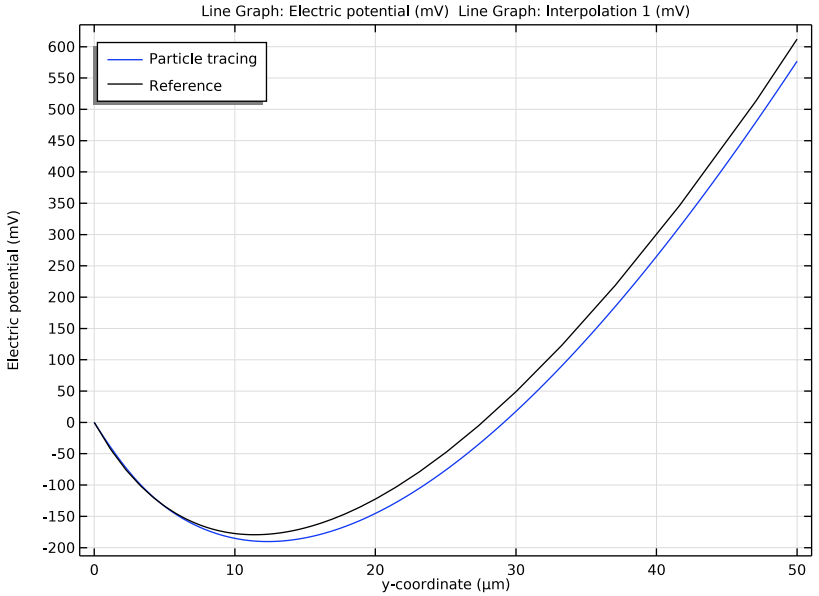

Figure 2: Electric potential next to the cathode. The black solid curve represents the electric potential calculated using the numerical integration. The solid blue curve shows the electric potential obtained from the thermionic emission feature.

Table 1 shows a comparison of the anode current density J_a, minimum potential V_m and minimum potential location y_m obtained from the model and from the analytical solution.

The values in the **Model** column may change slightly when the model is run on different architectures because the initial velocity of each electron is generated pseudorandomly.

TABLE 1: COMPARISON BETWEEN THE MODEL AND THE ANALYTICAL SOLUTION.

PARAMETER	MODEL	REFERENCE	RELATIVE ERROR (%)
J_a (A/cm^2)	-0.26932	-0.25356	6.2150
V_m (mV)	-179.97	-179.37	0.33268
y_m (µm)	11.788	11.412	3.2946

References

1. T.C. Fry, "The thermionic current between parallel plane electrodes; velocities of emission distributed according to Maxwell's law," *Physical Review*, vol. 17, no. 4, p. 441, 1921.

2. I. Langmuir, "The effect of space charge and initial velocities on the potential distribution and thermionic current between parallel plane electrodes," *Physical Review*, vol. 21, no. 4, 419, 1923.

3. P. T. Kirstein, G. S. Kino, and W. E. Waters, "Space charge flow," in *Physical and Quantum Electronics Series*, McGraw-Hill, pp. 265–275, 1967.

Application Library path: `Particle_Tracing_Module/Charged_Particle_Tracing/planar_diode`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 In the **Select Physics** tree, select **AC/DC>Particle Tracing>Particle Field Interaction, Non-Relativistic**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Charged Particle Tracing>Bidirectionally Coupled Particle Tracing**.

6 Click **Done**.

GEOMETRY 1

Load the parameters for the geometry and physics setup from a file. This file also includes the expected values of the anode current, minimum electric potential, and location of the minimum potential, which are also given in the **Reference** column in Table 1.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `planar_diode_parameters.txt`.

GEOMETRY 1

Block 1 (blk1)

1 In the **Geometry** toolbar, click **Block**.

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type `rc`.

4 In the **Depth** text field, type `d`.

5 In the **Height** text field, type `rc`.

6 Locate the **Position** section. In the **x** text field, type `-rc/2`.

7 In the **z** text field, type `-rc/2`.

Add a thin layer adjacent to the cathode. This will be used to plot the electric potential in a small region surrounding the potential barrier, making the results easier to visualize.

8 Click to expand the **Layers** section. Find the **Layer position** subsection. Clear the **Bottom** check box.

9 Select the **Front** check box.

10 In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	d/20

The section The Langmuir-Fry Model includes a derivation of the electric potential in the planar diode that can be integrated numerically. Load this numeric data from the reference file and use it to define an interpolation function.

DEFINITIONS

Interpolation 1 (int1)

1 In the **Home** toolbar, click **Functions** and choose **Global>Interpolation**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `planar_diode_reference.txt`.

6 Click **Import**.

7 In the **Function name** text field, type `reference`.

8 Locate the **Units** section. In the **Arguments** text field, type `um`.

9 In the **Function** text field, type `mV`.

Define a nonlocal minimum coupling at one of the edges in the thin layer adjacent to the cathode. This coupling will be used to compute the value and location of the minimum electric potential.

Minimum 1 (minop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Minimum**.

2 In the **Settings** window for **Minimum**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Edge**.

4 Select Edge 4 only.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	1	1	Basic

ELECTROSTATICS (ES)

Set up the boundary conditions for the calculation of the electric potential.

Ground 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electrostatics (es)** and choose **Ground**.

2 Select Boundary 2 only.

Electric Potential 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Potential**.

2 Select Boundary 9 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the V_0 text field, type `Va`.

CHARGED PARTICLE TRACING (CPT)

In the **Model Builder** window, under **Component 1 (comp1)** click **Charged Particle Tracing (cpt)**.

Thermionic Emission 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Thermionic Emission**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Thermionic Emission**, locate the **Surface Properties** section.

4 In the T text field, type `Tc`.

5 In the Φ text field, type `Phim`.

6 In the A^* text field, type `A0`.

7 In the N text field, type `N`.

8 Locate the **Initial Velocity** section. In the N_{vel} text field, type `Nvel`.

9 From the **Weighting of macroparticles** list, choose **Uniform speed intervals**. Sampling at uniform speed intervals causes a disproportionately large number of model particles to have above-average speed. However, since the faster particles are more likely to cross the barrier and thus have more significant contributions to the charge density near the anode, it is reasonable to devote more degrees of freedom to them. This disproportionate sampling from the probability distribution function is offset by reducing the contributions of these energetic particles to the space charge density in the domain.

10 In the n text field, type `20`.

Particle Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Charged Particle Tracing (cpt)** click **Particle Properties 1**.

2 In the **Settings** window for **Particle Properties**, locate the **Particle Species** section.

3 From the **Particle species** list, choose **Electron**.

Apply the **Symmetry** boundary condition to the sides of the modeling domain. The **Symmetry** condition acts like a specularly reflecting boundary. The physical interpretation of this is that, on average, for every electron that leaves through the sides of the modeling domain, another electron enters the domain at the same time. This is consistent with the interpretation of the domain as a finite region of a semi-infinite diode.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.

2 Select Boundaries 1, 3–5, 7, 8, 10, and 11 only.

Use the **Particle Counter** feature to create a global variable for the total current at the anode.

Particle Counter 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Particle Counter**.

2 Select Boundary 9 only.

Electric Force 1

1 In the **Model Builder** window, click **Electric Force 1**.

2 In the **Settings** window for **Electric Force**, locate the **Electric Force** section.

3 From the **E** list, choose **Electric field (es/ccn1)**.

4 Locate the **Advanced Settings** section. Select the **Use piecewise polynomial recovery on field** check box.

To make the solution more robust and reproducible, modify the **Particle Field Interaction** node so that the space charge density used to compute the electric potential is the cumulative average over successive iterations of the solver sequence.

MULTIPHYSICS

Electric Particle Field Interaction 1 (epfi1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Electric Particle Field Interaction 1 (epfi1)**.

2 In the **Settings** window for **Electric Particle Field Interaction**, locate the **Continuation Settings** section.

3 Select the **Use cumulative space charge density** check box.

4 In the β text field, type 0. A value of zero means that the space charge is not ramped up for the purpose of computing the electric potential. Instead the full space charge contribution will be used even in the first iteration.

5 From the **Weights for subsequent iterations** list, choose **Arithmetic sequence**. Weighting the iterations in an arithmetic sequence minimizes the impact of the earlier iterations, which generally use only crude initial guesses for the potential distribution and will have larger relative error compared to later iterations.

The planar diode is essentially a one-dimensional model. Mesh the transverse directions of the geometry with only one mesh element to reduce the number of degrees of freedom. An additional benefit is that no spurious transverse electric forces can arise due to the discretization of the particle distribution in velocity space.

MESH 1

Mapped 1

1 In the **Mesh** toolbar, click  **Boundary** and choose **Mapped**.

2 Select Boundary 2 only.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 In the **Number of elements** text field, type 1.

4 Select Edges 1, 3, 5, and 14 only.

Swept 1

In the **Mesh** toolbar, click  **Swept**.

Distribution 1

1 Right-click **Swept 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

3 Click  **Clear Selection**.

4 Select Domain 1 only.

5 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.

6 In the **Number of elements** text field, type 80.

7 In the **Element ratio** text field, type 10.

8 Select the **Reverse direction** check box.

Distribution 2

1 In the **Model Builder** window, right-click **Swept 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

3 Click **Clear Selection**.

4 Select Domain 2 only.

5 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.

6 In the **Number of elements** text field, type `100`.

7 In the **Element ratio** text field, type `10`.

8 Click **Build All**. The resulting swept mesh should be extremely fine near the cathode and coarser at greater distances from the cathode.

Increase the number of iterations in the solver sequence. As more iterations are taken, it becomes easier to obtain a more self-consistent solution.

STUDY 1

Step 1: Bidirectionally Coupled Particle Tracing

1 In the **Model Builder** window, under **Study 1** click **Step 1: Bidirectionally Coupled Particle Tracing**.

2 In the **Settings** window for **Bidirectionally Coupled Particle Tracing**, locate the **Study Settings** section.

3 From the **Time unit** list, choose **µs**.

4 In the **Output times** text field, type `0 0.1`.

5 Locate the **Iterations** section. In the **Number of iterations** text field, type `50`.

6 In the **Home** toolbar, click **Compute**.

RESULTS

Use the **Edge 3D** dataset to plot the electric potential in a narrow region adjacent to the cathode.

Edge 3D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Edge 3D**.

2 Select Edge 4 only.

Electric Potential Minimum

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Electric Potential Minimum` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Edge 3D 1**.

4 From the **Time selection** list, choose **Last**.

5 Locate the **Plot Settings** section. Select the **y-axis label** check box.

6 In the associated text field, type `Electric potential (mV)`.

7 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Line Graph 1

1 Right-click **Electric Potential Minimum** and choose **Line Graph**.

2 Use the default expression, which is V, the electric potential.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 From the **Unit** list, choose **mV**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `y`.

7 From the **Unit** list, choose **µm**.

8 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

9 Select the **Show legends** check box. In the table, enter `Particle tracing`.

Line Graph 2

1 In the **Model Builder** window, right-click **Electric Potential Minimum** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `reference(y)`.

4 From the **Unit** list, choose **mV**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `y`.

7 From the **Unit** list, choose **µm**.

8 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Black**.

9 Locate the **Legends** section. Select the **Show legends** check box.

10 From the **Legends** list, choose **Manual**. In the table, enter `Reference`.

11 In the **Electric Potential Minimum** toolbar, click **Plot**. Compare the resulting plot to Figure 2.

Global Evaluation 1

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Particle 1**.

4 From the **Time selection** list, choose **Last**.

5 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`cpt.pcnt1.It`	`A`	`Transmitted current, Particle Counter 1`
`minop1(V,y)`	`um`	`Location of the potential minimum`
`minop1(V)`	`mV`	`Potential minimum`

Compare the resulting values to the **References** column in Table 1. The values may differ slightly due to the random nature of the particle release feature.

6 Click **Evaluate**.

Global Evaluation 2

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Particle 1**.

4 From the **Time selection** list, choose **Last**.

5 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`abs((Iref-cpt.pcnt1.It)/Iref)*100`	`1`	`Relative error (%) for the transmitted current`
`abs((yref-minop1(V,y))/yref)*100`	`1`	`Relative error (%) for the location of the potential minimum`
`abs((Vref-minop1(V))/Vref)*100`	`1`	`Relative error (%) for the potential minimum`

The relative errors should be comparable in magnitude to the **Relative Error (%)** column in Table 1.

6 Click **Evaluate**.