No. 678

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April 1996

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April 1996

Abstract—The decomposition method (DM) is a nonnumerical method for solving strongly nonlinear differential equations. In this paper, the DM is used to solve the one-dimensional nonlinear Poisson's equations governing the linearly graded p-n junctions in semiconductor devices, and the error analysis for the approximate analytic solutions obtained by the DM is carried out. Also, the whole solution procedure has been realized by the mathematics-mechanization (MM) with microcomputers. The simulated results are accurate and reliable, and the quantitative analysis of the linearly graded p-n junctions has been realized. This work indicates that the DM has some quite significant advantages, and that it will open up a new way for the numerical analysis of semiconductor devices.

Keywords—Decomposition method, One-dimensional nonlinear Poisson's equation, Mathematics-mechanization with computers, Approximate analytic solutions, linearly graded p-n junctions.

1. Introduction

The numerical analysis for semiconductor devices consists of obtaining the solution of a set of differential equations under appropriate boundary and initial conditions. The equations are nonlinear, and the nonlinearity involved is of an exponential type, which deviates strongly from a linear relation [1]. For the linearly graded p-n junction, when

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considered under a nonsignificant current, we only need to solve nonlinear Poisson's equation of one-dimension [1]. Morgan and Smits [2] analyzed the linearly graded p-n junction by the explicit numerical-integration method. However, the numerical integration tends to diverge unless the electric-field magnitude at the junction point is given in an extraordinary accuracy, for example, to thirty digits. Even then, the solution obtained is restricted to a very small region around the junction point. Kurata [1] used the implicit method, where the matrix equation resulting from the difference approximation must be solved many times accoding to Newton's iteration principle. The method is complicated and time-consuming. It is obvious that both these methods are numerical methods. We must assume the extent of the depletion layer of the junction before the application of them, but the reasonable choice of this parameter in advance is very difficult.

Since the beginning of the 80's, G. Adomian [3-5] has developed an original method, named the decomposition method (DM), that has substantial advantages in solving nonlinear differential equations. It is based on the decomposition of unknown function into an infinite sum of functions defined by a recurrent relation. The nonlinearity is also expressed in terms of an infinite sum of special polynomials called Adomian's polynomials. The method is well-suited to physical problems since it needs neither the linearization and perturbation nor other restrictive assumptions which may change, sometimes seriously, the problem being solved. In this paper, the one-dimensional nonlinear Poisson's equation is solved by the DM, and the error analysis for the approximate solutions obtained by the DM is carried out. The whole solution procedure has been realized by the MM with microcomputers. Also, some simulated results are given, which are in good agreement with the qualitative conclusions in [1,2]. The error analysis results indicate that the approximate analytic solution determined by the DM is accurate and reliable and that it can be used to analyze quantitatively the linearly graded p-n junctions.

2. Basic Equations and the Boundary Conditions

According to the semiconductor device principle, the basic equation for every semiconductor device is a set of nonlinear differential equations with appropriate boundary and initial conditions. However, under the nonsignificant-current assumption, the basic equa-

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tion for the linearly graded p-n junction in the one-dimensional case can be expressed as nonlinear Poisson's equation, with appropriate boundary conditions. Poisson's equation in the one-dimensional case is written as [1]

$$\frac{d^2\psi}{dx^2} = -\frac{q}{\epsilon}[N(x) + p - n], \tag{1}$$

where ψ stands for the potential, x the distance, $N(x)$ the net impurity concentration, q the electronic charge, ϵ the dielectric constant, p the hole density, and n the electron density. For the linearly graded junction,

$$N(x) = mx. \tag{2}$$

The nonsignificant-current assumption allows the free carrier densities p and n to be written approximately as functions of a single-variable, namely ψ. The electron and hole densities in the depletion layer are written as [1]

$$n = n_i e^{\theta\psi}, p = n_i e^{\theta(v-\psi)}, \tag{3}$$

where $\theta = q/KT$, K stands for the Boltzmann constant, T the temperature, n_i the intrinsic free-electron density, v the applied voltage. The quotient θ is called the Boltzmann factor. Substituting (2)(3) into (1) yields

$$\frac{d^2\psi}{dx^2} = -\frac{q}{\epsilon}[mx + n_i e^{\theta(v-\psi)} - n_i e^{\theta\psi}]. \tag{4}$$

Boundary conditions for ψ can be expressed as [1]

$$\begin{cases} \psi(-a) = \frac{1}{\theta}\ln[\sqrt{(\frac{ma}{2n_i})^2 + 1} - \frac{ma}{2n_i}] + v, \\ \\ \psi(a) = \frac{1}{\theta}\ln[\sqrt{(\frac{ma}{2n_i})^2 + 1} + \frac{ma}{2n_i}], \end{cases} \tag{5}$$

where a is a parameter concerning the extent of the depletion layer. Outside the depletion layer, the space-charge neutrality holds. In view of the structural symmetry of the junction, the extent of the depletion layer of the junction is $2a$. Notice that the applied voltage v should not take the positive value, since in that case a significant current flows, making the solution physically meaningless. Therefore, v must be nonpositive.

In the two-point boundary-value problem (4)(5), ϵ, q, θ and n_i are all physical constants, m and v are parameters given in advance, while a is an unknown quantity. The

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condition for determining a value is that the electric-field values in positions $\pm a$ are 0, which can be written as

$$\frac{d\psi}{dx}\Big|_{x=\pm a} = 0. \tag{6}$$

Until now, we have established the analysis model (4)-(6). In the next section, we first solve problem (4)(5) by the DM to obtain the analytic approximate solution with a as a parameter, then we solve equation (6) to find a value. The accurate determination of the extent of the depletion layer by this technique is one of the great advantages of our method, which other numerical methods are difficult to accomplish.

3. The Computational Procedure

The DM is a general method for solving nonlinear problems. For its general principle, refer to [3-5]. Here, we take the boundary-value problem (4)(5) as an example to illustrate the solution procedure of the DM and our improvement on the iteration scheme of the method.

Let $L = \frac{d^2}{dx^2}$, $f(\psi) = \frac{qn_i}{\epsilon}[e^{\theta(v-\psi)} - e^{\theta\psi}]$, then the equation (4) can be written

$$L\psi = -\frac{qm}{\epsilon}x - f(\psi). \tag{7}$$

Solving for $L\psi$ and operating with L^{-1}, the two-fold indefinite integral operator, we have

$$\psi = \Phi - L^{-1}(\frac{qm}{\epsilon}x) - L^{-1}f(\psi), \tag{8}$$

where Φ satisfies $L\Phi = 0$. $\Phi = c_0 + c_1 x$, c_0 and c_1 are integration constants. By using the double decomposition strategy [6], we now decompose the solution ψ as well as the integration constant term Φ. Let $\psi = \sum\limits_{m=0}^{\infty} \psi_m, \Phi = \sum\limits_{m=0}^{\infty}(c_{0,m} + c_{1,m}x)$. The nonlinear term $f(\psi)$ will be equated to $\sum\limits_{m=0}^{\infty} A_m$, where A_m are polynomials of $\psi_0, \psi_1, \ldots, \psi_m$ called Adomian's polynomials and are calculated by the formulae

$$A_m = \frac{1}{m!}\frac{d^m}{d\lambda^m}f[\overline{\psi}(\lambda)]|_{\lambda=0}, m = 0, 1, 2, \ldots \tag{9}$$

where $\overline{\psi}(\lambda) = \sum\limits_{m=0}^{\infty}\psi_m\lambda^m$. Putting these relations into (8) gives

$$\sum_{m=0}^{\infty}\psi_m = \sum_{m=0}^{\infty}(c_{0,m} + c_{1,m}x) - \frac{qm}{6\epsilon}x^3 - L^{-1}\sum_{m=0}^{\infty}A_m. \tag{10}$$

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The basic iteration scheme of the DM can be expressed as

$$\begin{cases} \psi_0 = c_{0,0} + c_{1,0}x - \frac{qm}{6\epsilon}x^3, \\ \\ \psi_m = c_{0,m} + c_{1,m}x - L^{-1}A_{m-1}, m \geq 1. \end{cases} \tag{11}$$

In order to avoid the difficult integrations and to express the integration results with elementary functions, we improve the iteration scheme of the method. From (10), the ψ_m's can be determined by the recurrent relation

$$\begin{cases} \psi_0 = c_{0,0} + c_{1,0}x, \\ \\ \psi_1 = c_{0,1} + c_{1,1}x - \frac{qm}{6\epsilon}x^3 - L^{-1}A_0, \\ \\ \psi_m = c_{0,m} + c_{1,m}x - L^{-1}A_{m-1}, m \geq 2. \end{cases} \tag{12}$$

Let

$$r_m = \psi_0 + \psi_1 + \cdots + \psi_{m-1}, \tag{13}$$

then $c_{0,m}$ and $c_{1,m}$ are determined by satisfying the boundary conditions (5) with r_{m+1}. Denote

$$\begin{cases} \beta_1(a) = \frac{1}{\theta}\ln[\sqrt{(\frac{ma}{2n_i})^2 + 1} - \frac{ma}{2n_i}] + v, \\ \\ \beta_2(a) = \frac{1}{\theta}\ln[\sqrt{(\frac{ma}{2n_i})^2 + 1} + \frac{ma}{2n_i}], \end{cases} \tag{14}$$

then the boundary conditions (5) become

$$\psi(-a) = \beta_1(a), \psi(a) = \beta_2(a). \tag{15}$$

Matching $r_1 = \psi_0$ to the boundary conditions (15), $c_{0,0}$ and $c_{1,0}$ are determined by two linear equations, and

$$\begin{cases} c_{0,0} = \frac{\beta_1(a)+\beta_2(a)}{2}, \\ \\ c_{1,0} = \frac{\beta_2(a)-\beta_1(a)}{2a}. \end{cases} \tag{16}$$

So we get $r_1 = \psi_0$. From (9), we have $A_0 = f(\psi_0)$. Then

$$\psi_1 = c_{0,1} + c_{1,1}x - \frac{qm}{6\epsilon}x^3 - L^{-1}A_0. \tag{17}$$

Matching $r_2 = \psi_0 + \psi_1$ to the boundary conditions (15), we require $\psi_1(-a) = \psi_1(a) = 0$. By solving two linear equations, we have

$$\begin{cases} c_{0,1} = \frac{L^{-1}A_0(-a)+L^{-1}A_0(a)}{2}, \\ \\ c_{1,1} = \frac{qm}{6\epsilon}a^2 + \frac{L^{-1}A_0(a)-L^{-1}A_0(-a)}{2a}. \end{cases} \tag{18}$$

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So we get ψ_1 and $r_2 = \psi_0 + \psi_1$. From (9), A_1 can be determined by ψ_0 and ψ_1. Generally, if $\psi_0, \psi_1, \ldots, \psi_{m-1}$ have been found for $m \geq 2$, A_{m-1} can be determined by $\psi_0, \psi_1, \ldots, \psi_{m-1}$ and (9). Matching $r_{m+1} = \psi_0 + \cdots + \psi_{m-1} + \psi_m$ to the boundary conditions (15), we require $\psi_m(-a) = \psi_m(a) = 0$. By solving two linear equations, we have

$$
\begin{cases}
c_{0,m} = \dfrac{L^{-1}A_{m-1}(-a) + L^{-1}A_{m-1}(a)}{2}, \\[3mm]
c_{1,m} = \dfrac{L^{-1}A_{m-1}(a) - L^{-1}A_{m-1}(-a)}{2a}.
\end{cases}
\tag{19}
$$

So we get ψ_m and $r_{m+1} = \psi_0 + \psi_1 + \cdots + \psi_m$.

From the above-mentioned procedure, we will arrive at an approximate analytic solution $r(x,a)$ for the boundary-value problem (4)(5). By solving equation

$$
\frac{dr(x,a)}{dx}\Big|_{x=\pm a} = 0,
\tag{20}
$$

we can obtain the value a and the extent of the depletion layer $2a$.

4. The MM with Computers and the Error Analysis

Although the DM is a general method that is well-suited to solving many nonlinear problems, the artificial derivation of its computational procedure for the solution of complex nonlinear equations is cumbersome as well as time-consuming, and the complex approximate solutions with high accuracy are hard to calculate. Computers and new softwares can be of a great help for the computations. It is necessary to realize the DM for the solution of complex nonlinear equations by the MM with computers and the symbolic software such as Maple and Mathematica. Now we state the concrete steps of the MM briefly.

- Compute $c_{0,0}$ and $c_{1,0}$ with boundary conditions, then obtain ψ_0.

- According to the recurrent scheme, derive $A_{m-1}, c_{0,m}, c_{1,m}$, and $\psi_m (m = 1, 2, \ldots)$ successively.

- Adding these ψ_m's, obtain the approximate analytic solution $r(x,a)$. By solving equation (20), find the parameter a. Simplify the approximant $r(x,a)$.

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- Carry out the error analysis for the approximate solution obtained by the DM, by using the technique described below.

- Quantitatively analyze the potential r and the electric field $-\frac{dr}{dx}$, and reveal the objective laws governing the linearly graded p-n junctions.

With the computational procedure and the MM method, we have studied the boundary-value problem (4)(5) carefully. Considering the concise expression of the approximate solution and the limited microcomputer memory, the two-term approximation to the solution is given by

$$r_2(x, a) = \psi_0 + \psi_1 = \frac{\beta_1(a) + \beta_2(a)}{2}$$

$$- \frac{2qa^2 n_i}{[\beta_2(a) - \beta_1(a)]^2 \epsilon \theta^2} \{e^{\beta_1(a)\theta} + e^{\beta_2(a)\theta} - e^{\theta[v - \beta_1(a)]} - e^{\theta[v - \beta_2(a)]}\}$$

$$+ \frac{2qa n_i}{[\beta_2(a) - \beta_1(a)]^2 \epsilon \theta^2} \{e^{\beta_1(a)\theta} - e^{\beta_2(a)\theta} - e^{\theta[v - \beta_1(a)]} + e^{\theta[v - \beta_2(a)]}\}x$$

$$+ \frac{\beta_2(a) - \beta_1(a)}{2a}x + \frac{qma^2}{6\epsilon}x - \frac{qm}{6\epsilon}x^3 + \frac{4qa^2 n_i}{[\beta_2(a) - \beta_1(a)]^2 \epsilon \theta^2}$$

$$\{e^{\frac{\theta[\beta_1(a) + \beta_2(a)]}{2} + \frac{\theta[\beta_2(a) - \beta_1(a)]}{2a}x} - e^{-\frac{\theta[\beta_1(a) + \beta_2(a)]}{2} + v\theta - \frac{\theta[\beta_2(a) - \beta_1(a)]}{2a}x}\}.$$

The parameter a can be determined easily by solving equation $\frac{dr_2}{dx}|_{x = \pm a} = 0$ with a symbolic program such as Mathematica.

The method's convergence has been studied by Y. Cherruault [7,8] by using the fixed point theorems [7] and the properties of the substituted series [8], but problems still remain with differential equations. P. Nelson [9] proposed a counterexample to the convergence assertion of the DM. Because there is no theoretical proof that is entirely satisfactory, we must verify the validity of the approximate solution obtained with a symbolic program such as Mathematica.

It is obvious that r_2 satisfies the boundary conditions (5). We need to verify that r_2 satisfies the equation (4). For this purpose, we define the following absolute error and

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relative error functions

$$AE(x) = \frac{d^2 r_2}{dx^2} + \frac{q}{\epsilon}[mx + f(r_2)],$$ (21)

$$RE(x) = 2 \times AE(x)/\{\frac{d^2 r_2}{dx^2} - \frac{q}{\epsilon}[mx + f(r_2)]\},$$ (22)

and the criterion whether these two functions are close to 0 in $[-a, a]$ can be used to test the degree of accuracy of the approximate solution r_2.

5. Simulated Results

Let us now discuss some examples. At this stage, the following numerical data are given for physical constants: $q = 1.6 \times 10^{-19}$ Coul, $\epsilon = 1.064 \times 10^{-16}$ F/μm, $\theta = 38.5$ V^{-1}, $n_i = 1.4 \times 10^{-2}$ (μm)$^{-3}$. By using the MM method, four cases with $v = 0$ V, $m = 10^4$ (μm)$^{-4}$; $v = -5$ V, $m = 10^4$ (μm)$^{-4}$; $v = -10$ V, $m = 10^4$ (μm)$^{-4}$ and $v = -100$ V, $m = 10^3$ (μm)$^{-4}$ are simulated, and the corresponding a values are 0.4377 μm, 0.8355 μm, 1.026 μm and 4.65 μm, respectively. The potential, electric field, absolute error and relative error distributions in the depletion layers for these four cases are shown in Figure 1 to Figure 16. The computational results are in good agreement with the qualitative conclusions given in [1,2]. The error analysis results show that the approximate analytic solutions obtained are accurate and reliable, especially when the absolute values of v's are large. Also, our technique can be used to find the accurate extent of the depletion layer for the linearly graded p-n junctions and to analyze quantitatively their various electric performance indices, such as the potential distribution and the electric field distribution.

6. Conclusions

The application of the DM to the solution of the one-dimensional Poisson's equation has been studied, and the approximate analytic solution for this strongly nonlinear equation has been found, depending on the MM method with microcomputer. Also, the technique for determining the extent of the depletion layer has been presented, and the error analysis for the obtained approximate solutions has been carried out. Our research work indicates that the approximate analytic solution determined by the DM is accurate and reliable, and that it can be used to analyze quantitatively the linearly graded p-n junctions.

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The DM is an efficient method that can solve many nonlinear equations. For the first time, its efficiency has been proved with the quantitative analysis of the linearly graded p-n junctions. The method has some quite significant advantages over numerical methods such as finite element method and finite difference method, and it gives much more information. Although the linearly graded p-n junction just has been analyzed quantitatively, maybe the DM will open up a new way for the numerical analysis of semiconductor devices. The approximate solution determined by the DM can be viewed as usual functions. It can be used to solve very interesting problems such as quantitative analysis and optimization design.

Acknowledgments

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Figure 1 plot:

0.4

a=0.4377 (μm)
m=10⁴ (μm⁻⁴)
v=0 (V)

0.2

Potential (V)

0

-0.2

-0.4
-0.4377   -0.21885   0   0.21885   0.4377

Distance x (μm)
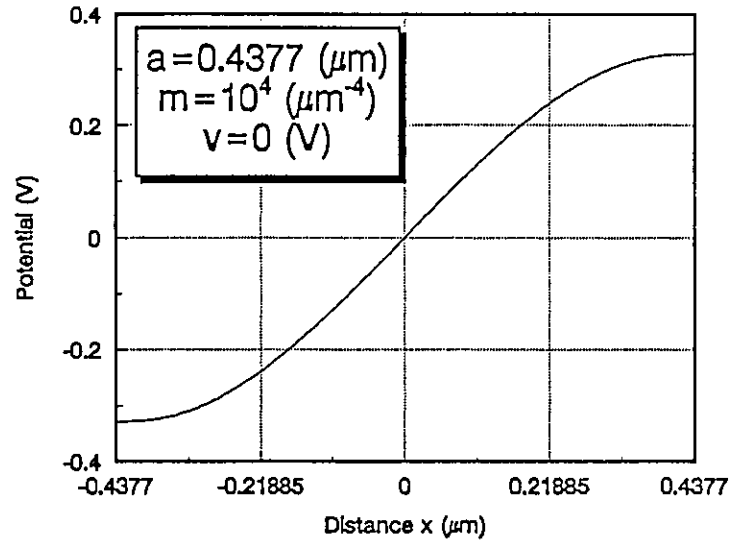
Figure 1: Potential distribution with $v = 0$ V and $m = 10^4$ $(\mu m)^{-4}$

Figure 2 plot:

0

a=0.4377 (μm)
m=10⁴ (μm⁻⁴)
v=0 (V)

-0.325

E (V/μm)

-0.65

-0.975

-1.3
-0.4377   -0.21885   0   0.21885   0.4377

Distance x (μm)
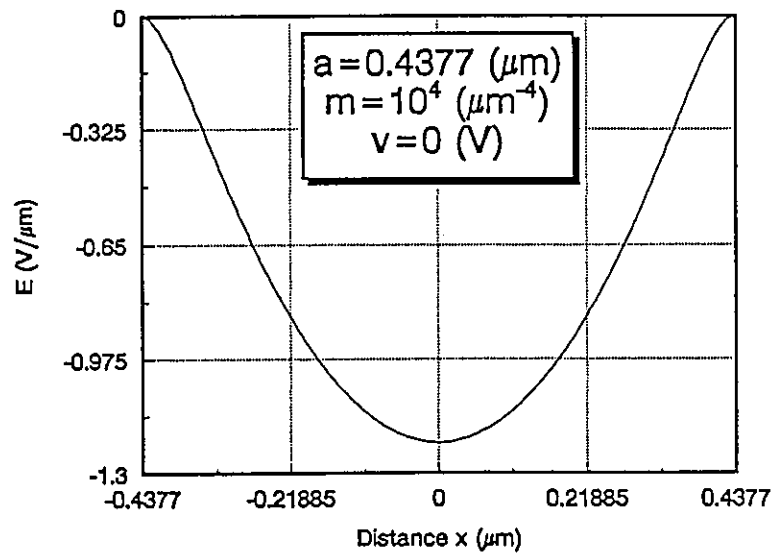
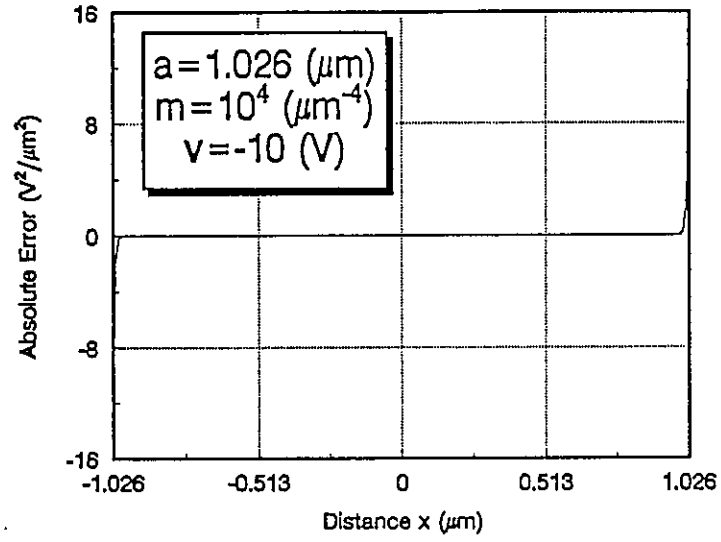Figure 2: Electric field distribution with $v = 0$ V and $m = 10^4$ $(\mu m)^{-4}$
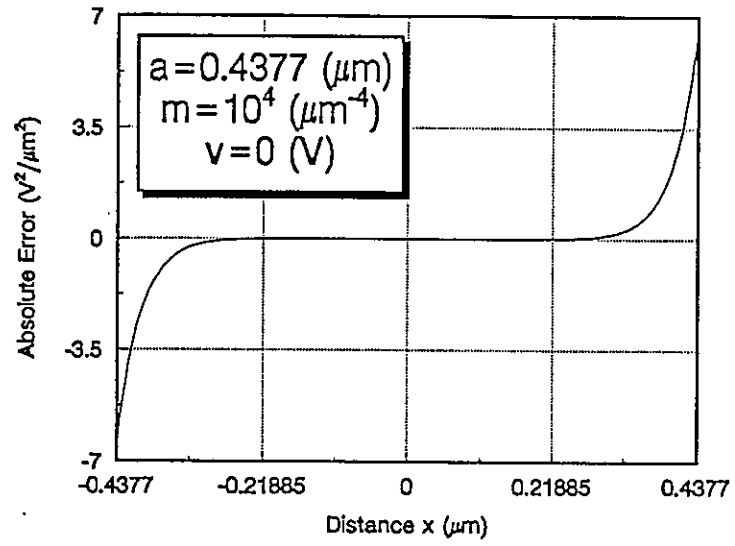
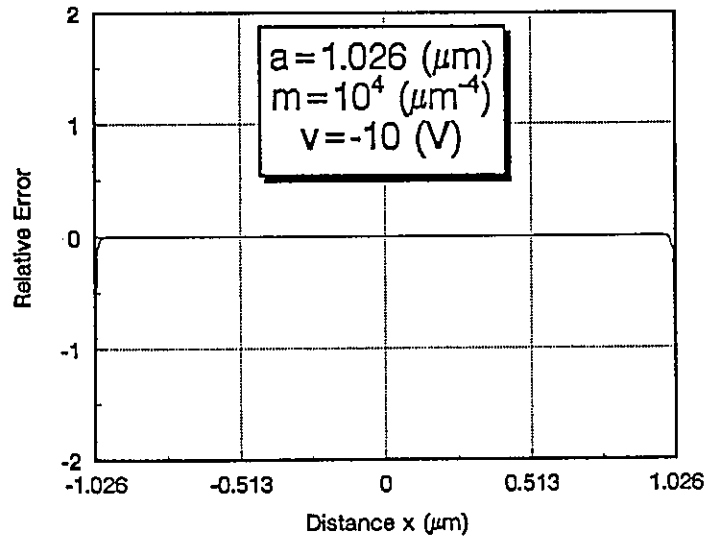Figure 3: Absolute error distribution with $v = 0$ V and $m = 10^4$ $(\mu m)^{-4}$
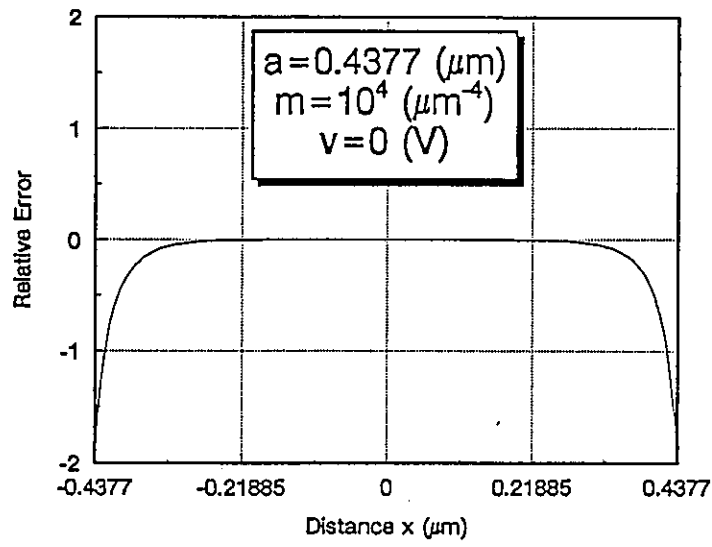
Figure 4: Relative error distribution with $v = 0$ V and $m = 10^4$ $(\mu m)^{-4}$
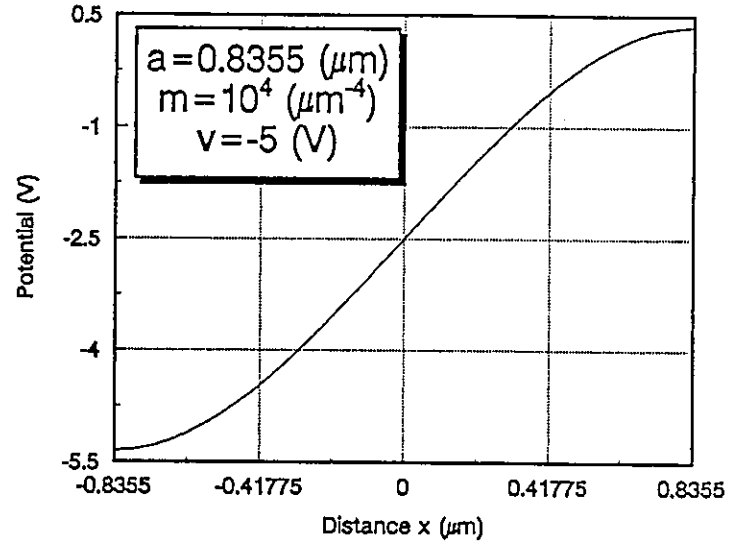
Figure 5: Potential distribution with $v = -5$ V and $m = 10^4$ $(\mu\text{m})^{-4}$
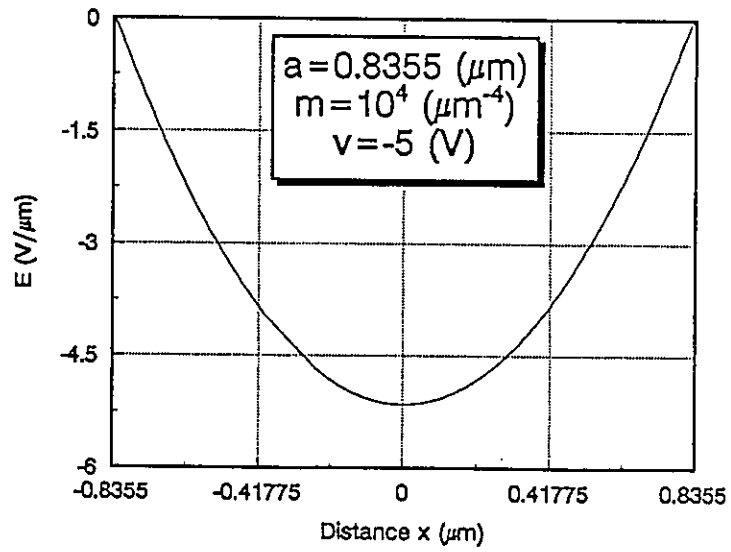
Figure 6: Electric field distribution with $v = -5$ V and $m = 10^4$ $(\mu\text{m})^{-4}$
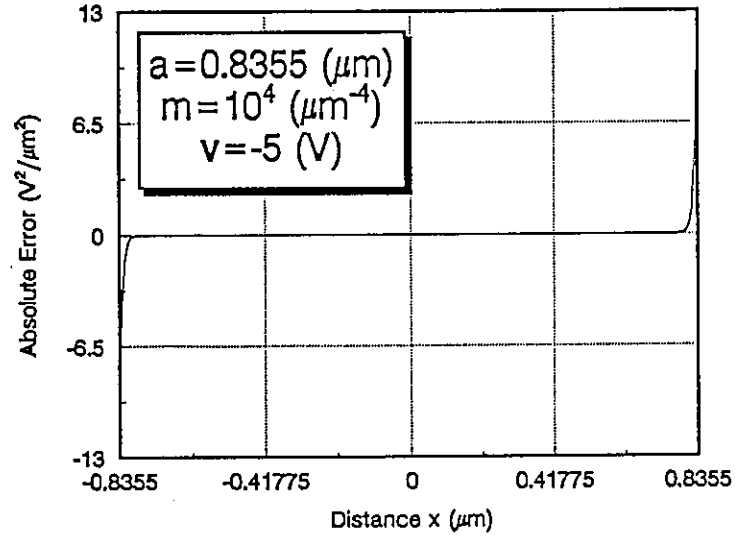
Figure 7: Absolute error distribution with $v = -5$ V and $m = 10^4$ $(\mu m)^{-4}$
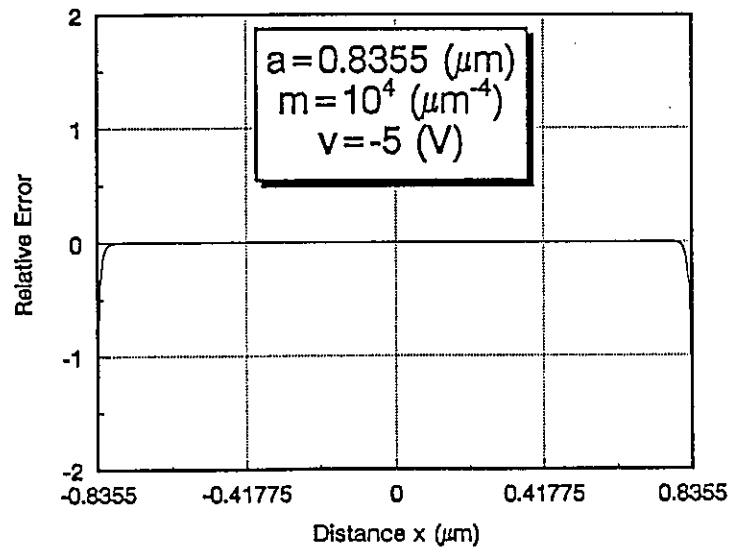
Figure 8: Relative error distribution with $v = -5$ V and $m = 10^4$ $(\mu m)^{-4}$

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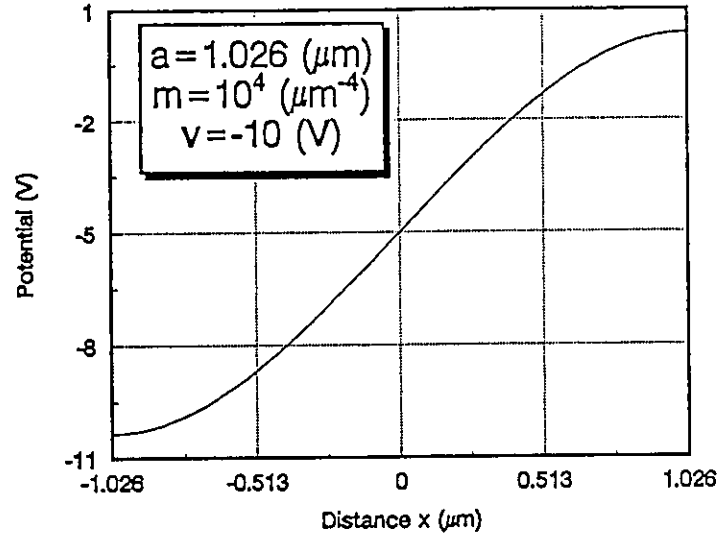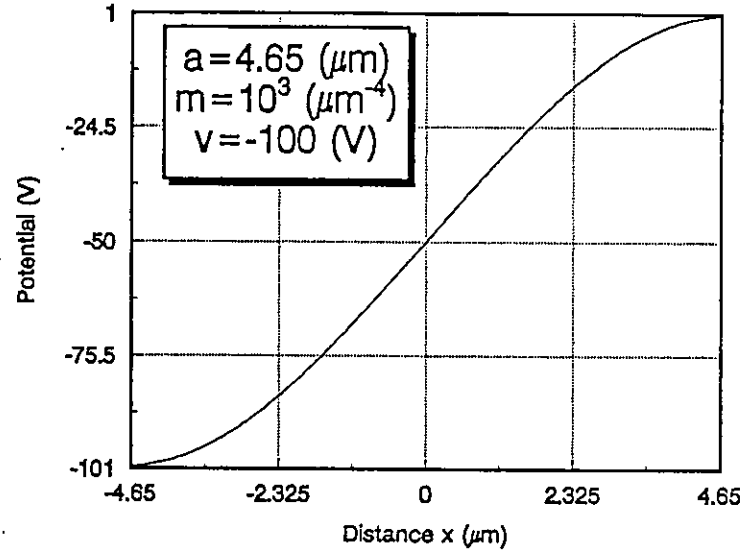
Figure 9: Potential distribution with $v = -10$ V and $m = 10^4$ $(\mu m)^{-4}$
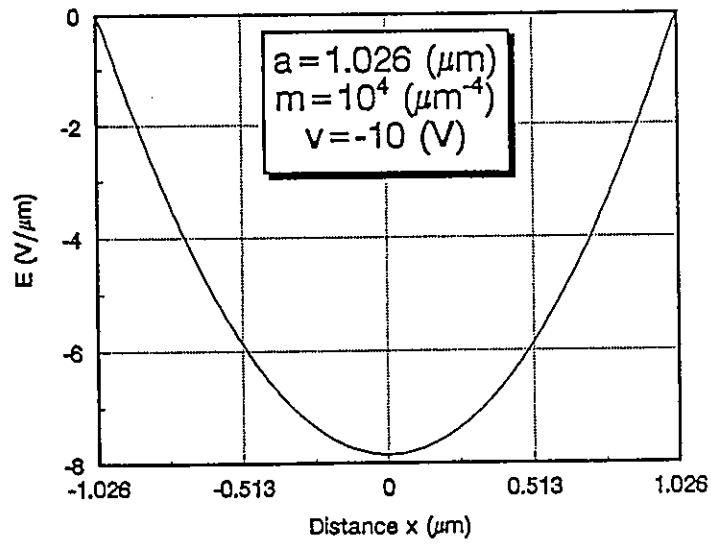
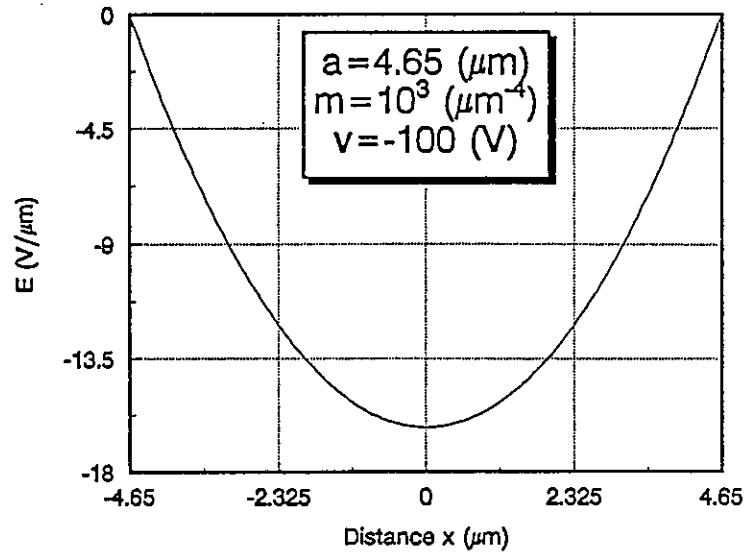Figure 10: Electric field distribution with $v = -10$ V and $m = 10^4$ $(\mu m)^{-4}$
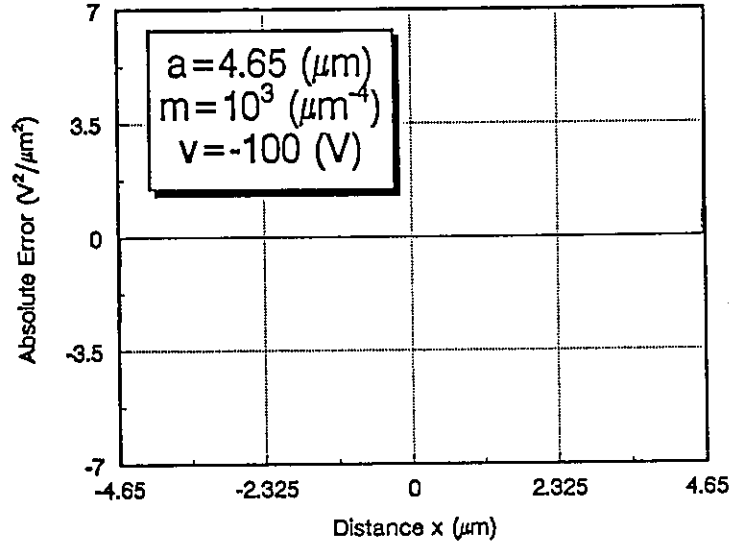
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Figure 11: Absolute error distribution with $v = -10$ V and $m = 10^4$ $(\mu\mathrm{m})^{-4}$

Figure 12: Relative error distribution with $v = -10$ V and $m = 10^4$ $(\mu\mathrm{m})^{-4}$

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Figure 13: Potential distribution with $v = -100$ V and $m = 10^3$ $(\mu m)^{-4}$

Figure 14: Electric field distribution with $v = -100$ V and $m = 10^3$ $(\mu m)^{-4}$

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Figure 15: Absolute error distribution with $v = -100$ V and $m = 10^3$ $(\mu\mathrm{m})^{-4}$
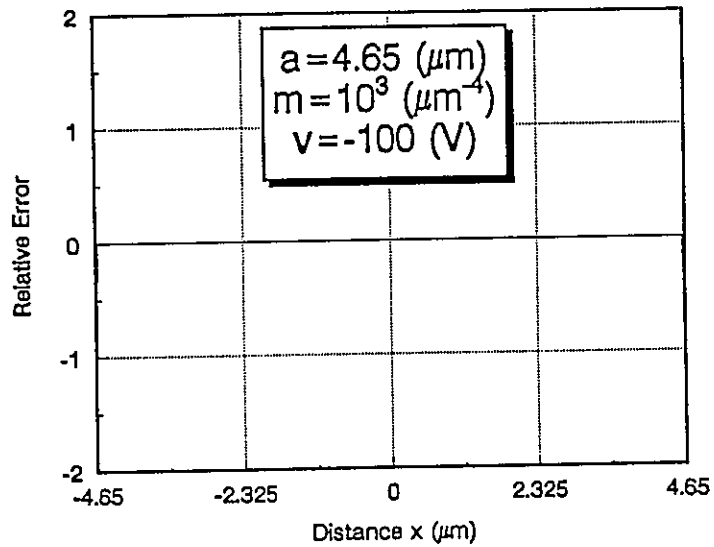

Figure 16: Relative error distribution with $v = -100$ V and $m = 10^3$ $(\mu\mathrm{m})^{-4}$

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