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半导体器件探测器计算流体力学的数值方法和分析

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摘要: 对三维光导型半导体探测器瞬态问题的计算流体力学数值模拟, 提出了一类修正迎风分数步差分格式 应用变分形式、能量方法、归纳法假定、微分方程的先验估计理论和技巧, 得到最佳阶误差估计 该文数值方法已成功地应用到光导型半导体探测器瞬态问题的数值模拟中

关 键 词: 光导型探测器; 流体力学模型; 迎风分数步方法; 理论分析; 实际应用

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引 言

半导体器件的迅速发展, 传统的近似方法已不适用, 需要研究通常称为扩散型的非线性偏微分方程组的初边值问题 建立在光电效应基础上的光导型光电探测器, 是利用光生载流子引起材料的电导率发生变化来对光进行探测的 其数学模型由 4 个方程组成的非线性偏微分方程组的初边值问题决定[1-5] 电子和空穴浓度方程是对流-扩散型的, 电场强度方程是一阶的, 温度方程是热传导型的

Gummel 于 1964 年提出用序列迭代法计算半导体问题[5], 开创了半导体数值模拟这一新领域 Douglas 和作者对一维、二维简单模型(不考虑温度影响, 常系数的情况) 提出了便于实用的差分方法, 并第一个得到理论分析成果[6-7] 本文研究现代强激光辐照半导体探测器时, 即产生光电效应又产生热效应, 应用流体力学方法, 提出了漂移-扩散模型, 建立相应的非线性耦合偏微分方程组的初、边值问题, 和一类新型的迎风差分格式, 它能克服经典方法可能出现的数值解的振荡和失真, 并可用大步长计算[8-10] 应用变分形式, 能量方法, 归纳法假定和先验估计理论, 得到最佳阶 l^2 模误差估计, 并应用到半导体光电探测器中载流子输运过程的数值模拟实践, 成功解决了这一著名问题[2,6], 对现代半导体器件数值模拟这一重要领域的模型

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分析、数值方法、机理研究和软件研制均有重要的理论和实用价值[10-12]

本文从载流子输运角度出发, 建立了光导型半导体光电探测器内载流子输运的模型及其流体动力学方程　HgCdTe 红外探测器以其诸多优势被广泛使用, 我们就以 HgCdTe 探测器为例, 通过对方程进行数值求解得到不同激光辐射功率密度下探测器内载流子及电场的分布规律

当激光辐照半导体探测器时, 由于半导体材料对光的吸收, 产生光生载流子　载流子在探测器内输运所遵循的连续性方程为[1-5]

$$\frac{p}{t} = G - R - \frac{1}{e} \quad J_p, \tag{1}$$

$$\frac{n}{t} = G - R + \frac{1}{e} \quad J_n, \tag{2}$$

式中 p, n 分别为空穴、电子的浓度, G, R 分别为空穴、电子对的产生函数和复合函数, J_p, J_n 分别为空穴、电子的电流密度, $\quad = (\ / \ x, \ / \ y, \ / \ z)^{\mathrm{T}}$

载流子的电流密度为其漂移电流密度和扩散电流密度之和, 即

$$J_p = e \ {}_p p\boldsymbol{E} - eD_p \quad p, \tag{3}$$

$$J_n = e \ {}_n n\boldsymbol{E} + eD_n \quad n, \tag{4}$$

其中 $\boldsymbol{E}$ 为载流子所在点的电场强度, ${}_p$, ${}_n$ 分别为空穴、电子的迁移率, D_p, D_n 分别为空穴、电子的扩散系数, $D_p(T) = {}_p kT/e$, $D_n(T) = {}_n kT/e$, k 为 Planck 常数, T 为温度　$G(\boldsymbol{X}, t)$ 为单位体积内光生载流子的产生函数　$R(p, n)$ 为载流子的复合函数

将电流密度表达式(3)、(4) 代入连续性方程(1)、(2), 并利用 Poission 方程　$\boldsymbol{E} = e(p - n)/$ 可以导出空穴、电子的动力学方程为

$$\frac{p}{t} = G - R - \ {}_p\boldsymbol{E} \quad p - \frac{e \ {}_p}{} p(p - n) + \quad (D_p(T) \quad p),$$

$$\boldsymbol{X} = (x, y, z)^{\mathrm{T}} \quad , \ t \quad J = (0, \bar{T}], \tag{5}$$

$$\frac{n}{t} = G - R + \ {}_n\boldsymbol{E} \quad n + \frac{e \ {}_n}{} n(p - n) + \quad (D_n(T) \quad n),$$

$$\boldsymbol{X} \quad , \ t \quad J \tag{6}$$

在载流子输运过程中, 探测器内电流密度为载流子电流密度与位移电流密度之和, 得到电场的动力学方程为

$$\frac{\boldsymbol{E}}{t} = \boldsymbol{J}_s - e[\ {}_p p + \ {}_n n]\boldsymbol{E} + eD_p(T) \quad p - eD_n(T) \quad n,$$

$$(\boldsymbol{X}, t) \qquad J, \tag{7}$$

此处 $\boldsymbol{J}_s$ 是探测器内总电流密度, 通常为常矢量函数, $\boldsymbol{E} = (E_1, E_2, E_3)^{\mathrm{T}}$

光照使得材料吸收热量而升温, 有热传导方程:

$$c \quad \frac{T}{t} = \quad (K(\boldsymbol{X}, t) \quad T) + g(\boldsymbol{X}, t), \qquad (\boldsymbol{X}, t) \qquad J, \tag{8}$$

式中 c, 　分别为与材料有关的常数, $K(\boldsymbol{X}, t)$, $g(\boldsymbol{X}, t)$ 为已知函数

方程(5)、(6)、(7) 和(8) 联立, 形成了完整地描述光导型半导体探测器内载流子输运现象的流体动力学方程, 这是一个耦合的非线性偏微分方程组

初始条件

$$\begin{cases} \boldsymbol{E}(\boldsymbol{X}, 0) = \boldsymbol{E}_0(\boldsymbol{X}), \ p(\boldsymbol{X}, 0) = p_0(\boldsymbol{X}), \\ n(\boldsymbol{X}, 0) = n_0(\boldsymbol{X}), \ T(\boldsymbol{X}, 0) = T_0(\boldsymbol{X}), \end{cases} \quad \boldsymbol{X} \tag{9}$$

在半导体器件数值模拟中, 应用最多的是第一类(Dirichlet) 和第二类(Neumann) 边界条件

问题 Dirichlet 边界条件

$$\boldsymbol{E} = \boldsymbol{E}(\boldsymbol{X}, t),\ p = p(\boldsymbol{X}, t),\ n = n(\boldsymbol{X}, t),\ T = T(\boldsymbol{X}, t),\quad (\boldsymbol{X}, t) \quad J, \tag{10}$$

此处 $\boldsymbol{E}, p, n$ 和 T 为给定的已知的矢量函数和数量函数

问题 Neumann 边界条件

$$\boldsymbol{E} = 0,\quad p = 0,\quad n = 0,\quad T = 0,\quad (\boldsymbol{X}, t) \quad J, \tag{11}$$

此处 为边界面 的外法线方向

通常问题是正定的, 即满足

(C) $0 < D_* \quad D_s(T) \quad D^*,\ s = p, n,\ 0 < K_* \quad K(\boldsymbol{X}, t) \quad K^*,$

此处 D_*, D^*, K_*, K^* 均为正常数

假定问题的精确解具有一定的光滑性, 即满足

(R) $p, n, \boldsymbol{E}, T \quad L\ (W^{4,}\ ),\ \frac{^2 p}{t^2}, \frac{^2 n}{t^2}, \frac{^2 \boldsymbol{E}}{t^2}, \frac{^2 T}{t^2} \quad L\ (L\ ),$

且 $R(p, n)$ 在解的 $_0$ 领域关于二个变量均是Lipschitz 连续的, 即存在常数 M, 当$|\ _i|\quad _0(1\quad i\quad 4)$ 时有

$$|R(p(\boldsymbol{X}, t) + \ _1, n(\boldsymbol{X}, t) + \ _2) - R(p(\boldsymbol{X}, t) + \ _3, n(\boldsymbol{X}, t) + \ _4)|$$
$$M\left\{|\ _1 - \ _3| + |\ _2 - \ _4|\right\},\quad (\boldsymbol{X}, t) \quad J \tag{12}$$

这样的假定在物理上是合理的[2-4] 最后指出, 在本文中记号 M 和 $_i$ 分别表示普通正常数和小的正数, 在不同之处可有不同的含义

1 二阶迎风差分格式

为了用差分方法求解, 用网格区域 $_h$ 代替 在三维空间 $\boldsymbol{X} = (x, y, z)^{\mathrm{T}}$ 上 x 方向步长为 h_1, y 方向步长为 h_2, z 方向步长为 h_3, $x_i = ih_1$, $y_j = jh_2$, $z_k = kh_3$, 如图 1 所示

$$_h = \left\{ (x_i, y_j, z_k) \left| \begin{array}{l} i_1(j, k) < i < i_2(j, k) \\ j_1(i, k) < j < j_2(i, k) \\ k_1(i, j) < k < k_2(i, j) \end{array} \right. \right\},$$

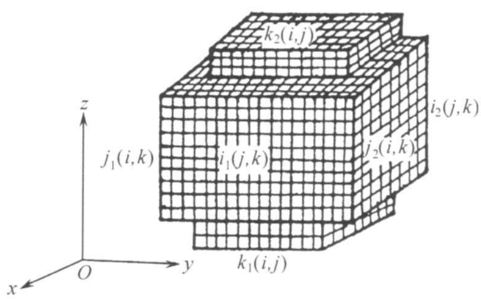

图 1 网域 $_h$ 示意图

用 $_h$ 代替 , 用 $_h$ 表示 的边界

记 $\boldsymbol{E}^m_{h,ijk}, p^m_{h,ijk}, n^m_{h,ijk}$ 和 $T^m_{h,ijk}$ 为对应于 $\boldsymbol{E}(X_{ijk}, t^m), p(X_{ijk}, t^m), n(X_{ijk}, t^m)$ 和 $T(X_{ijk}, t^m)$ 的差分解 设 t^m 时刻的 $\boldsymbol{E}^m_h, p^m_h, n^m_h$ 和 T^m_h 已知, 寻求下一时刻的差分解 $\boldsymbol{E}^{m+1}_h, p^{m+1}_h, n^{m+1}_h$ 和 T^{m+1}_h 为叙述简便, 这里仅讨论第一边值问题

由于热传导方程(8) 是独立的, 首先提出其分数步差分格式:

$$(c - \ t\ _z(K^{m+1}\ _z))T^{m+1/3}_{h,ijk} = c\,T^m_{h,ijk} + \ t g^{m+1}_{ijk},\quad k_1(i,j) < k < k_2(i,j), \tag{13a}$$

$$T^{m+1/3}_{h,ijk} = T(X_{ijk}, t^{m+1}),\quad X_{ijk} \quad _h; \tag{13b}$$

$$(c - \ t\ _y(K^{m+1}\ _y))T^{m+2/3}_{h,ijk} = c\,T^{m+1/3}_{h,ijk},\quad j_1(i,k) < j < j_2(i,k), \tag{14a}$$

$$T^{m+2/3}_{h,ijk} = T(X_{ijk}, t^{m+1}),\quad X_{ijk} \quad _h; \tag{14b}$$

$$(c - \quad t_{\ x}(K^{m+1}\ \ _x))T^{m+1}_{h,ijk} = \ c\,T^{m+2/3}_{h,ijk}, \qquad i_1(j,k) < \ i < \ i_2(j,k), \tag{15a}$$

$$T^{m+1}_{h,ijk} = \ T(X_{ijk},\ t^{m+1}), \qquad X_{ijk} \qquad _h \tag{15b}$$

其次,提出电场强度方程的中心差分格式:

$$(\boldsymbol{E}^{m+1}_{h,ijk} - \ \boldsymbol{E}^{m}_{h,ijk})/\ \ t = \ \boldsymbol{J}_s - \ e[\ \ _p\,p^{m}_{h,ijk} + \quad _n n^{m}_{h,ijk}]\,\boldsymbol{E}^{m+1}_{h,ijk} +$$
$$eD_p(\,T^{m+1}_{h,ijk}) \quad _h\,p^{m}_{h,ijk} - \ eD_n(T^{m+1}_{h,ijk}) \quad _h n^{m}_{h,ijk},$$
$$k_1(i,j) < \ k < \ k_2(i,j),\ \ j_1(i,k) < \ j < \ j_2(i,k), \tag{16a}$$

$$\boldsymbol{E}^{m+1}_{h,ijk} = \ \boldsymbol{E}(X_{ijk},\ t^{m+1}), \qquad X_{ijk} \qquad _h, \tag{16b}$$

此处

$$\boldsymbol{E}_h = \ (E_{1h},\ E_{2h},\ E_{3h})^{\mathrm{T}},$$

$$_h\,p^{m}_{h,ijk} = \ \left(\frac{p^{m}_{h,i+1,jk} - \ p^{m}_{h,i-1,jk}}{2h_1},\ \frac{p^{m}_{h,i,j+1,k} - \ p^{m}_{h,i,j-1,k}}{2h_2},\ \frac{p^{m}_{h,ij,k+1} - \ p^{m}_{h,ij,k-1}}{2h_3}\right)^{\mathrm{T}},$$

$$_h n^{m}_{h,ijk} =$$

最后提出空穴、电子浓度的二阶迎风分数步差分格式:

$$(1 - \quad t(1 + \ (h_3/2) \ \ _p\,|\ E^{m}_{3h}\ |\ D^{-1}_p(T^{m+1}_h))^{-1}_{ijk}\ \ _z(D_p(T^{m+1}_h) \ \ _z) + \quad t\ \ _{E^{m}_{3h}})p^{m+1/3}_{h,ijk} =$$
$$p^{m}_{h,ijk} + \quad t\left\{- \ (e\ \ _p/\ \ )p^{m}_{h,ijk}(p^{m}_{h,ijk} - \ n^{m}_{h,ijk}) + \ (G^{m+1}_{ijk} - \ R(p^{m}_{h,ijk},\ n^{m}_{h,ijk}))\right\},$$
$$k_1(i,j) < \ k < \ k_2(i,j), \tag{17a}$$

$$p^{m+1/3}_{h,ijk} = \ p(X_{ijk},\ t^{m+1}), \qquad X_{ijk} \qquad _h; \tag{17b}$$

$$(1 - \quad t(1 + \ (h_2/2) \ \ _p\,|\ E^{m}_{2h}\ |\ D^{-1}_p(T^{m+1}_h))^{-1}_{ijk}\ \ _y(D_p(T^{m+1}_h) \ \ _y) + \quad t\ \ _{E^{m}_{2h}})p^{m+2/3}_{h,ijk} =$$
$$p^{m+1/3}_{h,ijk}, \qquad j_1(i,k) < \ j < \ j_2(i,k), \tag{18a}$$

$$p^{m+2/3}_{h,ijk} = \ p(X_{ijk},\ t^{m+1}), \qquad X_{ijk} \qquad _h; \tag{18b}$$

$$(1 + \quad t(1 + \ (h_1/2) \ \ _p\,|\ E^{m}_{1h}\ |\ D^{-1}_p(T^{m+1}_h))^{-1}_{ijk}\ \ _x(D_p(T^{m+1}_h) \ \ _x) + \quad t\ \ _{E^{m}_{1h}})p^{m+1}_{h,ijk} =$$
$$p^{m+2/3}_{h,ijk}, \qquad i_1(j,k) < \ i < \ i_2(j,k), \tag{19a}$$

$$p^{m+1}_{h,ijk} = \ p(X_{ijk},\ t^{m+1}), \qquad X_{ijk} \qquad _h; \tag{19b}$$

此处

$$\begin{cases} _{E^{m}_{1h}}\,p_{h,ijk} = \quad _p E^{m}_{1h,ijk}\Big\{H(E^{m}_{1h,ijk})\,D^{-1}_p(T^{m+1}_{h,ijk})\,D_p(T^{m+1}_{h,i-1/2,jk}) \ \ _x + \\ \qquad (1 - \ H(E^{m}_{1h,ijk}))\,D^{-1}_p(T^{m+1}_{h,ijk})\,D_p(T^{m+1}_{h,i+1/2,jk}) \ \ _x\Big\}p_{h,ijk}, \\ _{E^{m}_{2h}}\,p_{h,ijk} = \qquad , \qquad _{E^{m}_{3h}}\,p_{h,ijk} = \qquad , \\ H(z) = \ 1, \qquad z \quad 0,\ \ H(z) = \ 0, \qquad z < \ 0 \end{cases} \tag{20}$$

$$(1 - \quad t(1 + \ (h_3/2) \ \ _n\,|\ E^{m}_{3h}\ |\ D^{-1}_n(T^{m+1}_h))^{-1}_{ijk}\ \ _z(D_n(T^{m+1}_h) \ \ _z) - \quad t\ \ _{E^{m}_{3h}})\,n^{m+1/3}_{h,ijk} =$$
$$n^{m}_{h,ijk} + \quad t\left\{(e\ \ _p/\ \ )\,n^{m}_{h,ijk}(p^{m}_{h,ijk} - \ n^{m}_{h,ijk}) + \ (G^{m+1}_{ijk} - \ R(p^{m}_{h,ijk},\ n^{m}_{h,ijk}))\right\},$$
$$k_1(i,j) < \ k < \ k_2(i,j), \tag{21a}$$

$$n^{m+1/3}_{h,ijk} = \ n(X_{ijk},\ t^{m+1}), \qquad X_{ijk} \qquad _h; \tag{21b}$$

$$(1 - \quad t(1 + \ (h_2/2) \ \ _n\,|\ E^{m}_{2h}\ |\ D^{-1}_n(T^{m+1}_h))^{-1}_{ijk}\ \ _y(D_n(T^{m+1}_h) \ \ _y) -$$
$$t\ \ _{E^{m}_{2h}})\,n^{m+2/3}_{h,ijk} = \ n^{m+1/3}_{h,ijk}, \qquad j_1(i,k) < \ j < \ j_2(i,k), \tag{22a}$$

$$n^{m+2/3}_{h,ijk} = \ n(X_{ijk},\ t^{m+1}), \qquad X_{ijk} \qquad _h; \tag{22b}$$

$$(1 - \quad t(1 + \ (h_1/2) \ \ _n\,|\ E^{m}_{1h}\ |\ D^{-1}_p(T^{m+1}_h))^{-1}_{ijk}\ \ _x(D_n(T^{m+1}_h) \ \ _x) - \quad t\ \ _{E^{m}_{1h}})\,n^{m+1}_{h,ijk} =$$

$$n_{h,ijk}^{m+2/3},\qquad i_1(j,k) < i < i_2(j,k), \tag{23a}$$

$$n_{h,ijk}^{m+1} = n(X_{ijk}, t^{m+1}),\qquad X_{ijk}\ \ {}_h; \tag{23b}$$

此处 $E_{1h}^{m} n_{h,ijk}$ 的定义是类似的

格式(13) ~ (23)的计算程序: 首先由式(13) ~ (15)用追赶法计算出 $\{T_{h,ijk}^{m+1}\}$, 再由式(16)分别在3个方向用追赶法计算出 $\boldsymbol{E}_{h,ijk}^{m+1}$, 最后由式(17) ~ (20)用追赶法计算出 $\{p_{h,ijk}^{m+1}\}$, 同时并行的由式(21) ~ (23)计算出 $\{n_{h,ijk}^{m+1}\}$ 由于问题满足正定性条件(C), 故格式(13) ~ (23)的解存在且唯一

2 收敛性分析

为理论分析简便, 设

$$= \{(x,y,z)^{\mathrm{T}} \mid 0 < x < 1, 0 < y < 1, 0 < z < 1\},$$

$$h = 1/N,\quad t = T/L,\quad t^m = m\ t$$

设 $\quad R = \boldsymbol{E} - \boldsymbol{E}_h,\ F = p - p_n,\ N = n - n_h,\ V = T - T_h,$

此处 $\boldsymbol{E}, p, n, T$ 为问题的精确解, $\boldsymbol{E}_h, p_h, n_h, T_h$ 为相应的差分解, 为了进行误差分析, 引入离散空间 $l^2(\Omega)$ 和 $h^1(\Omega)$ 的内积与范数[8-9],

$$\langle v, w\rangle = \sum_{i,j,k=1}^{N} v_{ijk} w_{ijk} h^3,\quad \|v\|_0 = \|v\| = \langle v, v\rangle^{1/2};$$

$$[v, w)_1 = \sum_{i=0}^{N-1}\sum_{j,k=1}^{N} v_{ijk} w_{ijk} h^3,\ [v, w)_2 = \sum_{j=0}^{N-1}\sum_{i,k=1}^{N} v_{ijk} w_{ijk} h^3,$$

$$[v, w)_3 = \sum_{k=0}^{N-1}\sum_{i,j=1}^{N} v_{ijk} w_{ijk} h^3,$$

$$|[D_x v\|_0 = [D_x v, D_x v)_1^{1/2},\ |[D_y v\|_0 = [D_y v, D_y v)_2^{1/2},\ |[D_z v\|_0 = [D_z v, D_z v)_3^{1/2},$$

$$\|v\|_1^2 = \|v\|_0^2 + |[D_x v\|_0^2 + |[D_y v\|_0^2 + |[D_z v\|_0^2.$$

首先讨论热传导方程, 由式(13) ~ (15)消去 $T_h^{m+1/3}, T_h^{m+2/3}$, 并整理可得下述等价方程:

$$\begin{aligned}
&c\rho(T_{h,ijk}^{m+1} - T_{h,ijk}^{m})/\Delta t - \{D_x(K^{m+1}D_x) + D_y(K^{m+1}D_y) + \\
&\quad D_z(K^{m+1}D_z)\}T_{h,ijk}^{m+1} + (\Delta t/(c\rho))\{D_z(K^{m+1}D_z(D_y(K^{m+1}D_y))) + \\
&\quad D_z(K^{m+1}D_z(D_x(K^{m+1}D_x))) + D_y(K^{m+1}D_y(D_x(K^{m+1}D_x)))\}T_{h,ijk}^{m+1} - \\
&\quad (\Delta t/(c\rho))^2 D_z(K^{m+1}D_z(D_y(K^{m+1}D_y(D_x(K^{m+1}D_x T_h^{m+1})))))_{ijk} = \\
&\quad g(X_{ijk}, t^{m+1}),\qquad 1 \le i,j,k \le N-1,
\end{aligned} \tag{24a}$$

$$T_{h,ijk}^{m+1} = T(X_{ijk}, t^{m+1}),\qquad X_{ijk} \in \partial\Omega_h. \tag{24b}$$

由方程(8) $(t = t^{m+1})$ 和式(24)相减可得下述误差方程:

$$\begin{aligned}
&c\rho(V_{ijk}^{m+1} - V_{ijk}^{m})/\Delta t - \{D_x(K^{m+1}D_x V^{m+1})_{ijk} + D_y(K^{m+1}D_y V^{m+1})_{ijk} + \\
&\quad D_z(K^{m+1}D_z V^{m+1})_{ijk}\} + (\Delta t/(c\rho))\{D_z(K^{m+1}D_z(D_y(K^{m+1}D_y V^{m+1})))_{ijk} + \\
&\quad D_z(K^{m+1}D_z(D_x(K^{m+1}D_x V^{m+1})))_{ijk} + D_y(K^{m+1}D_y(D_x(K^{m+1}D_x V^{m+1})))_{ijk}\} - \\
&\quad (\Delta t/(c\rho))^2 D_z(K^{m+1}D_z(D_y(K^{m+1}D_y(D_x(K^{m+1}D_x V^{m+1})))))_{ijk} = \\
&\quad E_1(X_{ijk}, t^{m+1}),\qquad 1 \le i,j,k \le N-1,
\end{aligned} \tag{25a}$$

$$V_{ijk}^{m+1} = 0\qquad X_{ijk} \in \partial\Omega_h, \tag{25b}$$

此处 $|E_1(X_{ijk}, t^{m+1})| \le M\{\Delta t + h^2\}$.

对式(25)乘以 $V_{ijk}^{m+1}\Delta t$，作内积并应用分部求和公式和 Gronwall 引理可得

$$\| V \|_{L^{\infty}((0,T];l^2)} \leq M\{\Delta t + h^2\}. \tag{26}$$

其次讨论电场强度方程组(7)，由方程组(7) $(t = t^{m+1})$ 和式(16)相减可得下述误差方程组:

$$\varepsilon(R_{ijk}^{m+1} - R_{ijk}^{m})/\Delta t = -e\{[L_p p^{m+1} + L_n n^{m+1}]_{ijk}\boldsymbol{E}_{ijk}^{m+1} - [L_p p_n^m + L_n n_n^m]_{ijk}\boldsymbol{E}_{h,ijk}^{m+1}\} +$$
$$e\{[D_p(T^{m+1})\nabla p^{m+1} - D_p(T_h^{m+1})\nabla_h p_h^m]_{ijk} -$$
$$[D_n(T^{m+1})\nabla n^{m+1} - D_n(T_h^{m+1})\nabla_h n_h^m]_{ijk}\} +$$
$$E_2(X_{ijk}, t^{m+1}), \quad 1 \leq i,j,k \leq N-1, \tag{27a}$$

$$R_{h,ijk}^{m+1} = 0, \quad X_{ijk} \in \partial\Omega_h, \tag{27b}$$

此处 $0 = (0,0,0)^{\mathrm{T}}$，$|E_2(X_{ijk}, t^{m+1})| \leq M\{\Delta t + h^2\}.$

对式(27)乘以 $R_{ijk}^{m+1}\Delta t$，作内积可得

$$\varepsilon\langle R^{m+1} - R^m, R^{m+1}\rangle =$$
$$-e\langle [L_p p^{m+1} + L_n n^{m+1}]\boldsymbol{E}^{m+1} - [L_p p_h^m + L_n n_h^m]\boldsymbol{E}_h^{m+1}, R^{m+1}\rangle\Delta t +$$
$$e\langle D_p(T^{m+1})\nabla p^{m+1} - D_p(T_h^{m+1})\nabla_h p_h^m, R^{m+1}\rangle - e\langle D_n(T^{m+1})\nabla n^{m+1} -$$
$$D_n(T_h^{m+1})\nabla_h n_h^m, R^{m+1}\rangle\Delta t + \langle E_2^{m+1}, R^{m+1}\rangle\Delta t. \tag{28}$$

我们引入归纳法假定

$$\max_{0\leq m\leq L}\{\| R^m \|_{0,\infty}, \| F^m \|_{0,\infty}, \| N^m \|_{0,\infty}\} \to 0, \quad (\Delta t, h) \to 0. \tag{29}$$

对估计式(28)，应用归纳法假定式(29)可得

$$\| R^{m+1} \|^2 - \| R^m \|^2 \leq \varepsilon\{\| \nabla_h F^m \|^2 + \| \nabla_h N^m \|^2\}\Delta t +$$
$$M\{\| F^m \|^2 + \| N^m \|^2 + \| R^{m+1} \|^2 + (\Delta t)^2 + h^4\}\Delta t. \tag{30}$$

下面讨论空穴和浓度方程(5)和(6)的误差估计. 对于空穴浓度方程的迎风分数步格式(17)~(20)，消去 $p_h^{m+1/3}, p_h^{m+2/3}$ 可得下述等价方程:

$$(p_{h,ijk}^{m+1} - p_{h,ijk}^m)/\Delta t - \{(1 + (h/2)L_p|E_{1h}^m|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_x(D_p(T_h^{m+1})\delta_{\bar{x}}) +$$
$$(1 + (h/2)L_p|E_{2h}^m|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_y(D_p(T_h^{m+1})\delta_{\bar{y}}) +$$
$$(1 + (h/2)L_p|E_{3h}^m|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_{\bar{z}})\}p_{h,ijk}^{m+1} +$$
$$\{\delta_{E_{1h}^m} + \delta_{E_{2h}^m} + \delta_{E_{3h}^m}\}p_{h,ijk}^{m+1} +$$
$$\Delta t\{(1 + (h/2)L_p|E_{3h}^m|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_{\bar{z}}((1 +$$
$$(h/2)L_p|E_{2h}^m|D_p^{-1}(T_h^{m+1}))^{-1}\delta_y(D_p(T_h^{m+1})\delta_{\bar{y}}))) +$$
$$(1 + (h/2)L_p|E_{3h}^m|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_{\bar{z}}((1 +$$
$$(h/2)L_p|E_{1h}^m|D_p^{-1}(T_h^{m+1}))^{-1}\delta_x(D_p(T_h^{m+1})\delta_{\bar{x}}))) + \cdots\}p_{h,ijk}^{m+1} -$$
$$(\Delta t)^2(1 + (h/2)L_p|E_{3h}^m|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_{\bar{z}}((1 +$$
$$(h/2)L_p|E_{2h}^m|D_p^{-1}(T_h^{m+1}))^{-1}\delta_y(D_p(T_h^{m+1})\delta_{\bar{y}}((1 +$$
$$(h/2)L_p|E_{1h}^m|D_p^{-1}(T_h^{m+1}))^{-1}\delta_x(D_p(T_h^{m+1})\delta_{\bar{x}}p_h^{m+1})))))_{ijk} +$$
$$\Delta t\{\delta_{E_{3h}^m}(\delta_{E_{2h}^m}) + \delta_{E_{3h}^m}(\delta_{E_{1h}^m}) + \delta_{E_{2h}^m}(\delta_{E_{1h}^m})\}p_{h,ijk}^{m+1} +$$
$$(\Delta t)^2\delta_{E_{3h}^m}(\delta_{E_{2h}^m}(\delta_{E_{1h}^m}p_h^{m+1})))_{ijk} -$$
$$\Delta t\{(1 + (h/2)L_p|E_{3h}^m|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_{\bar{z}}(\delta_{E_{2h}^m})) +$$

$$E_{3h}^{m}((1+(h/2)L_p|E_{2h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\delta_y(D_p(T_h^{m+1})\delta_y))+\cdots\}p_{h,ijk}^{m+1}+$$
$$(\Delta t)^2\{(1+(h/2)L_p|E_{3h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_z((1+$$
$$(h/2)L_p|E_{2h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\delta_y(D_p(T_h^{m+1})\delta_y(\delta_{E_{1h}^{m}}p_h^{m+1}))))_{ijk}+\cdots\}=$$
$$-(eL_p/\mu)p_{h,ijk}^{m}(p_{h,ijk}^{m}-n_{h,ijk}^{m})+(G_{h,ijk}^{m}-R(p_{h,ijk}^{m},n_{h,ijk}^{m})),$$
$$1\le i,j,k\le N-1, \tag{31a}$$
$$p_{h,ijk}^{m+1}=p(X_{ijk},t^{m+1}),\qquad X_{ijk}\in\partial\Omega_h. \tag{31b}$$

由方程(5) $(t=t^{m+1})$ 和式(31),可得下述空穴浓度误差方程:

$$(\xi_{ijk}^{m+1}-\xi_{ijk}^{m})/\Delta t-\{(1+(h/2)|E_{1h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_x(D_p(T_h^{m+1})\delta_x\xi^{m+1})_{ijk}+$$
$$(1+(h/2)|E_{2h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_y(D_p(T_h^{m+1})\delta_y\xi^{m+1})_{ijk}+$$
$$(1+(h/2)|E_{3h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_z\xi^{m+1})_{ijk}\}=$$
$$-\{\delta_{E_{1h}^{m}}\xi_{ijk}^{m+1}+\delta_{E_{2h}^{m}}\xi_{ijk}^{m+1}+\delta_{E_{3h}^{m}}\xi_{ijk}^{m+1}\}-$$
$$\Delta t\{(1+(h/2)L_p|E_{3h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_z((1+$$
$$(h/2)L_p|E_{2h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\delta_y(D_p(T_h^{m+1})\delta_y\xi^{m+1})))_{ijk}+\cdots\}+$$
$$(\Delta t)^2(1+(h/2)|E_{3h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_z((1+$$
$$(h/2)|E_{2h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\delta_y(D_p(T_h^{m+1})\delta_y((1+$$
$$(h/2)|E_{1h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\delta_x(D_p(T_h^{m+1})\delta_x\xi^{m+1})))))_{ijk}+$$
$$\{[(1+(h/2)L_p|E_3^{m+1}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_x(D_p(T_h^{m+1})\delta_x p^{m+1})_{ijk}-$$
$$(1+(h/2)L_p|E_{1h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_x(D_p(T_h^{m+1})\delta_x p^{m+1})_{ijk}]+\cdots\}-$$
$$\{[\delta_{E_1^{m+1}}p_{ijk}^{m+1}-\delta_{E_{1h}^{m}}p_{ijk}^{m+1}]+\cdots\}-$$
$$\Delta t\{[(1+(h/2)L_p|E_3^{m+1}|D_p^{-1}(T^{m+1}))_{ijk}^{-1}\delta_z(D_p(T^{m+1})\delta_z((1+$$
$$(h/2)L_p|E_2^{m+1}|D_p^{-1}(T^{m+1}))^{-1}\delta_y(D_p(T^{m+1})\delta_y p^{m+1})))_{ijk}-$$
$$(1+(h/2)L_p|E_{3h}^{m}|D_p^{-1}(T_h^{m+1}))_{ijk}^{-1}\delta_z(D_p(T_h^{m+1})\delta_z((1+$$
$$(h/2)L_p|E_{2h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\delta_y(D_p(T_h^{m+1})\delta_y p^{m+1})))_{ijk}]+\cdots\}+$$
$$(\Delta t)^2\{(1+(h/2)L_p|E_3^{m+1}|D_p^{-1}(T^{m+1}))_{ijk}^{-1}\delta_z(D_p(T^{m+1})\delta_z((1+$$
$$(h/2)L_p|E_2^{m+1}|D_p^{-1}(T^{m+1}))^{-1}\delta_y((1+$$
$$(h/2)L_p|E_1^{m+1}|D_p^{-1}(T^{m+1}))^{-1}\delta_x(D_p(T^{m+1})\delta_x p_h^{m+1}))))_{ijk}-\cdots\}+\cdots+$$
$$\varepsilon_3(X_{ijk},t^{m+1}),\qquad 1\le i,j,k\le N-1, \tag{32a}$$
$$\xi_{ijk}^{m+1}=0,\qquad X_{ijk}\in\partial\Omega_h, \tag{32b}$$

此处 $|\varepsilon_3(X_{ijk},t^{m+1})|\le M\{\Delta t+h^2\}$.

假定时间和空间剖分参数满足限制性条件:

$$\Delta t=O(h^2). \tag{33}$$

对式(32)乘以 $\xi_{ijk}^{m+1}\Delta t$,作内积并分部求和可得

$$\langle\xi^{m+1}-\xi^{m},\xi^{m+1}\rangle+\Delta t\{\langle D_p(T_h^{m+1})\delta_x\xi^{m+1},$$
$$\delta_x[(1+(h/2)|E_{1h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\xi^{m+1}]\rangle+$$
$$\langle D_p(T_h^{m+1})\delta_y\xi^{m+1},\delta_y[(1+(h/2)|E_{2h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\xi^{m+1}]\rangle+$$
$$\langle D_p(T_h^{m+1})\delta_z\xi^{m+1},\delta_z[(1+(h/2)|E_{3h}^{m}|D_p^{-1}(T_h^{m+1}))^{-1}\xi^{m+1}]\rangle\}=$$

$$
\begin{aligned}
&-\Delta t\langle D_{E^m_{1h}}F^{m+1}+D_{E^m_{2h}}F^{m+1}+D_{E^m_{3h}}F^{m+1},F^{m+1}\rangle-\\
&(\Delta t)^2\langle(1+(h/2)L_p|E^m_{3h}|D_p^{-1}(T_h^{m+1}))^{-1}D_z(D_p(T_h^{m+1})D_z((1+\\
&(h/2)L_p|E^m_{2h}|D_p^{-1}(T_h^{m+1}))^{-1}D_y(D_p(T_h^{m+1})D_yF^{m+1})))+\cdots,F^{m+1}\rangle+\\
&(\Delta t)^3\langle(1+(h/2)|E^m_{3h}|D_p^{-1}(T_h^{m+1}))^{-1}D_z(D_p(T_h^{m+1})D_z((1+\\
&(h/2)L_p|E^m_{2h}|D_p^{-1}(T_h^{m+1}))^{-1}D_y(D_p(T_h^{m+1})D_y((1+\\
&(h/2)L_p|E^m_{1h}|D_p^{-1}(T_h^{m+1}))^{-1}D_x(D_p(T_h^{m+1})D_xF^{m+1}))))),F^{m+1}\rangle+\\
&\Delta t\langle[(1+(h/2)L_p|E_1^{m+1}|D_p^{-1}(T_h^{m+1}))^{-1}D_x(D_p(T^{m+1})D_xp^{m+1})-\\
&(1+(h/2)L_p|E^m_{1h}|D_p^{-1}(T_h^{m+1}))^{-1}D_x(D_p(T_h^{m+1})D_xp^{m+1})]+\cdots,F^{m+1}\rangle-\\
&\Delta t\langle[D_{E_1^{m+1}}p^{m+1}-D_{E^m_{1h}}p^{m+1}]+\cdots,F^{m+1}\rangle-\\
&(\Delta t)^2\langle[(1+(h/2)L_p|E_3^{m+1}|D_p^{-1}(T^{m+1}))_{ijk}^{-1}D_z(D_p(T^{m+1})D_z((1+\\
&(h/2)L_p|E_2^{m+1}|D_p^{-1}(T^{m+1}))^{-1}D_y(D_p(T^{m+1})D_yp^{m+1})))-\\
&(1+(h/2)L_p|E^m_{3h}|D_p^{-1}(T_h^{m+1}))^{-1}D_z(D_p(T_h^{m+1})D_z((1+\\
&(h/2)L_p|E^m_{2h}|D_p^{-1}(T_h^{m+1}))^{-1}D_y(D_p(T_h^{m+1})D_yp^{m+1})))]+\cdots,F^{m+1}\rangle+\\
&(\Delta t)^3\langle(1+(h/2)L_p|E_1^{m+1}|D_p^{-1}(T^{m+1}))^{-1}D_z(D_p(T^{m+1})D_z((1+\\
&(h/2)L_p|E_2^{m+1}|D_p^{-1}(T^{m+1}))^{-1}D_z((1+\\
&(h/2)L_p|E_1^{m+1}|D_p^{-1}(T^{m+1}))^{-1}D_x(D_p(T_h^{m+1})D_xp^{m+1}))))-\\
&\cdots,F^{m+1}\rangle+\cdots+\Delta t\langle E_3^{m+1},F^{m+1}\rangle.
\end{aligned}\tag{34}
$$

首先对误差方程(34)的左端进行估计可得

$$
\begin{aligned}
&\langle F^{m+1}-F^m,F^{m+1}\rangle+\Delta t\Big\{\langle D_p(T_h^{m+1})D_xF^{m+1},\\
&D_x[(1+(h/2)L_p|E^m_{1h}|D_p^{-1}(T_h^{m+1}))^{-1}F^{m+1}]\rangle+\\
&\langle D_p(T_h^{m+1})D_yF^{m+1},D_y[(1+(h/2)L_p|E^m_{2h}|D_p^{-1}(T_h^{m+1}))^{-1}F^{m+1}]\rangle+\\
&\langle D_p(T_h^{m+1})D_zF^{m+1},D_z[(1+(h/2)L_p|E^m_{3h}|D_p^{-1}(T_h^{m+1}))^{-1}F^{m+1}]\rangle\Big\}\geq\\
&(1/2)\Big\{\|F^{m+1}\|^2-\|F^m\|^2\Big\}+\\
&\Delta t\Big\{\langle D_p(T_h^{m+1})D_xF^{m+1},(1+(h/2)L_p|E^m_{1h}|D_p^{-1}(T_h^{m+1}))^{-1}D_xF^{m+1}\rangle+\\
&\langle D_p(T_h^{m+1})D_yF^{m+1},(1+(h/2)L_p|E^m_{2h}|D_p^{-1}(T_h^{m+1}))^{-1}D_yF^{m+1}\rangle+\\
&\langle D_p(T_h^{m+1})D_zF^{m+1},(1+(h/2)L_p|E^m_{3h}|D_p^{-1}(T_h^{m+1}))^{-1}D_zF^{m+1}\rangle\Big\}+\\
&\Delta t\Big\{\langle D_p(T_h^{m+1})D_xF^{m+1},D_x(1+(h/2)L_p|E^m_{1h}|D_p^{-1}(T_h^{m+1}))^{-1}F^{m+1}\rangle+\\
&\langle D_p(T_h^{m+1})D_yF^{m+1},D_y(1+(h/2)L_p|E^m_{2h}|D_p^{-1}(T_h^{m+1}))^{-1}F^{m+1}\rangle+\\
&\langle D_p(T_h^{m+1})D_zF^{m+1},D_z(1+(h/2)L_p|E^m_{3h}|D_p^{-1}(T_h^{m+1}))^{-1}F^{m+1}\rangle\Big\}\geq\\
&(1/2)\Big\{\|F^{m+1}\|^2-\|F^m\|^2\Big\}+D_0\Delta t\,|\nabla_hF^{m+1}|^2-\\
&E|\nabla_hF^{m+1}|^2\Delta t-M\|F^{m+1}\|^2\Delta t,
\end{aligned}\tag{35a}
$$

此处 D_0 为某一确定的正常数.

对于式(34)的右端逐项依次估计,对第1项由归纳假定式(30)得知 $\|E_h^m\|_{0,\infty}$ 是有界的,则可推出

$$
\begin{aligned}
&-\Delta t\langle D_{E^n_{1h}}F^{m+1}+D_{E^n_{2h}}F^{m+1}+D_{E^n_{3h}}F^{m+1},F^{m+1}\rangle\leq\\
&E|\nabla_hF^{m+1}|^2\Delta t+M\|F^{m+1}\|^2\Delta t.
\end{aligned}\tag{35b}
$$

对于式(34)右端的其他诸项,虽然 $-D_x(D_pD_x)$, $-D_y(D_pD_y)$, $-D_z(D_pD_z)$ 是自共轭的、正定

有界算子, 区域为正立方体, 但它们的乘积是不可交换的, 利用 $\mathrm{D}_y D_z = D_z D_y$, $D_y D_z = D_z D_y$ 对右端第 2 项的第 1 部分进行详细分析, 其余部分是类似的1

$$
\begin{aligned}
- & (\$t)^2 3(1+ (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_z(D_p(T_h^{m+1}) D_z((1+ \\
& (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y(D_p(T_h^{m+1}) D_y F^{m+1}))), F^{m+1} 4 = \\
& (\$t)^2 3\, D_p(T_h^{m+1}) D_z((1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y(D_p(T_h^{m+1}) D_y F^{m+1})), \\
& D_z[(1+ (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{F}^{m+1}] 4 = \\
& (\$t)^2 3\, D_p(T_h^{m+1})(1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y D_z(D_p(T_h^{m+1}) D_y F^{m+1}) + \\
& D_p(T_h^{m+1}) D_z(1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y(D_p(T_h^{m+1}) D_y F^{m+1}), \\
& (1+ (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_z F^{m+1} + \\
& D_z(1+ (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{F}^{m+1} 4 = \\
- & (\$t)^2 \Big\{ 3\, D_p(T_h^{m+1}) D_y D_z F^{m+1}, (1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1}(1+ \\
& (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y D_z F^{m+1} 4 + \\
& 3\, D_z D_p(T_h^{m+1}) D_y F^{m+1}, (1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1}(1+ \\
& (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y D_z F^{m+1} 4 + \\
& 3 D_p(T_h^{m+1}) D_y D_z F^{m+1}, D_y[(1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1}(1+ \\
& (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1}] D_z F^{m+1} + \ , 4 + \\
& 3\, D_z D_p(T_h^{m+1}) D_y F^{m+1}, D_y[(1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1}(1+ \\
& (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1}] D_z F^{m+1} + \ , 4 + \\
& 3 D_p(T_h^{m+1}) D_y F^{m+1}, D_p(T_h^{m+1}) D_z(1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1} @ \\
& (1+ (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y D_z F^{m+1} 4 + \\
& 3 D_p(T_h^{m+1}) D_y F^{m}, D_y[D_p(T_h^{m+1}) D_z(1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1} @ \\
& (1+ (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1}] D_z F^{m+1} + \ , 4 \Big\} 1
\end{aligned}
\tag{35c}
$$

对于上述估计式(35c) 的第 1 项, 利用正定性条件(C) 和归纳法假定式(29), 可得

$$
\begin{aligned}
- & (\$t)^2 3\, D_p(T_h^{m+1}) D_y D_z F^{m+1}, (1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1}(1+ \\
& (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y D_z F^{m+1} 4 \ [\\
& - (\$t)^2 D_1 + \mathrm{D}_y D_z F^{m+1} +^2 1
\end{aligned}
\tag{35d}
$$

此处 D_1 为某一确定的正常数1 对式(35c) 中某余诸项有

$$
\begin{aligned}
- & (\$t)^2 \Big\{ 3\, \mathrm{D}_z D_p(T_h^{m+1}) D_y F^{m+1}, (1+ (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1}(1+ \\
& (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y D_z F^{m+1} 4 + \ , \Big\} [\\
& (\$t)^2 (D_1/2) + D_y D_z F^{m+1} +^2 + M + F^{m+1} +^2 \$ t 1
\end{aligned}
\tag{35e}
$$

于是对式(34) 右端的第 2 项有下述估计式:

$$
\begin{aligned}
- & (\$t)^2 3(1+ (h/2) L_p \mid E^m_{3h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_z(D_p(T_h^{m+1}) D_z((1+ \\
& (h/2) L_p \mid E^m_{2h} \mid D_p^{-1}(T_h^{m+1}))^{-1} \mathrm{D}_y(D_p(T_h^{m+1}) D_y F^{m+1}))) + \ , \ , F^{m+1} 4 \ [\\
& - (\$t)^2 (D_1/2) \Big\{ + D_y D_z F^{m+1} +^2 + \ + D_x D_z F^{m+1} +^2 + \ + D_x D_y F^{m+1} +^2 \Big\} + \\
& M + F^{m+1} +^2 \$ t 1
\end{aligned}
\tag{35f}
$$

对式(34) 右项其余诸项可以进行类似的分析, 并综合式(35a) ~ (35f) 经整理可得估计式:

$$
+ \mathrm{F}^{m+1} +^2 - + F^m +^2 + \ + \ \ {}_h F^{m+1} +^2 \$ t \ [
$$

$$M\left\{\|F^{m+1}\|^2+\|N^m\|^2+\|F^m\|^2+(\Delta t)^2+h^4\right\}\Delta t. \tag{36}$$

对上式关于时间 t 求和$(0\leq m\leq L)$ 可得

$$\|F^{L+1}\|^2+\sum_{m=0}^{L}\|{}_hF^{m+1}\|^2\Delta t\leq$$
$$M\left\{\sum_{m=0}^{L}\left[\|F^{m+1}\|^2+\|N^{m+1}\|^2\right]\Delta t+(\Delta t)^2+h^4\right\}. \tag{37}$$

对电子浓度方程(23),经同样的估计过程和复杂的计算,可得下述误差估计式:

$$\|N^{L+1}\|^2+\sum_{m=0}^{L}\|{}_hN^{m+1}\|^2\Delta t\leq$$
$$M\left\{\sum_{m=0}^{L}\left[\|N^{m+1}\|^2+\|F^{m+1}\|^2\right]\Delta t+(\Delta t)^2+h^4\right\}. \tag{38}$$

对式(30)关于时间 t 求和$(0\leq m\leq L)$,并组合式(37)和(38)可得

$$\|F^{L+1}\|^2+\|N^{L+1}\|^2+\|R^{L+1}\|^2+$$
$$\sum_{m=0}^{L}\left[\|{}_hF^{m+1}\|^2+\|{}_hN^{m+1}\|^2\right]\Delta t\leq$$
$$M\left\{\sum_{m=0}^{L}\left[\|F^{m+1}\|^2+\|N^{m+1}\|^2+\|R^{m+1}\|^2\right]\Delta t+(\Delta t)^2+h^4\right\}. \tag{39}$$

应用 Gronwall 引理可得

$$\|F^{L+1}\|^2+\|N^{L+1}\|^2+\|R^{L+1}\|^2+$$
$$\sum_{m=0}^{L}\left[\|{}_hF^{m+1}\|^2+\|{}_hN^{m+1}\|^2\right]\Delta t\leq$$
$$M\left\{(\Delta t)^2+h^4\right\}. \tag{40}$$

归纳法假定式(29)满足是显然的1

定理 假定问题(5)~(11)的精确解满足正则性条件(R),采用修正迎风分数步格式(13)~(23)逐层并行计算,若剖分参数满足条件(33),则下述最佳阶 l^2 误差估计式成立:

$$\|p-p_h\|_{L^\infty(J,l^2)}+\|n-n_h\|_{L^\infty(J,l^2)}+\|\boldsymbol{E}-\boldsymbol{E}_h\|_{L^\infty(J,l^2)}+$$
$$\|T-T_h\|_{L^\infty(J,l^2)}+\|p-p_h\|_{L^2(J,h^1)}+\|n-n_h\|_{L^2(J,h^1)}\leq$$
$$M^*\left\{\Delta t+h^2\right\}, \tag{41}$$

此处常数 M^* 依赖于 $p, n, T, \boldsymbol{E}$ 及其导函数1

3 数值模拟结果

经计算得到,不同激光辐照功率密度下,光生电子密度随光照时间的变化情况如图 2 所示,从中可看出在稳定功率的激光辐照下,电子密度很快达到稳定分布,其大小与辐照光的功率密度成正比1 载流子寿命对载流子密度的影响情况如图 3 所示,可看出达到稳定分布所需的时间与载流子寿命成正比1 光生空穴密度有着同样的变化规律1

图 4 表示激光辐照时载流子密度的空间分布,图 5 表示不同掺杂密度下探测器内电子密度随光照时间的变化1 从对探测器温度的计算得知,在激光辐照密度较小或辐照时间较短的情况下,探测器的温度并不升高1 引起温度升高的时间为毫秒量级,所以当计算时间小于温升时间时,计算出的载流子密度的变化是指光生电子(光生空穴)密度的变化1

从上述计算结果指明

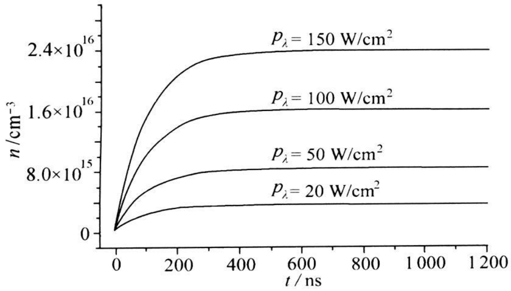

图 2 不同激光功率密度下探测器内 x = 0.1 Lm 处光生电子密度随光照时间的变化 (pK= (20, 50, 100, 150) W/cm^2)

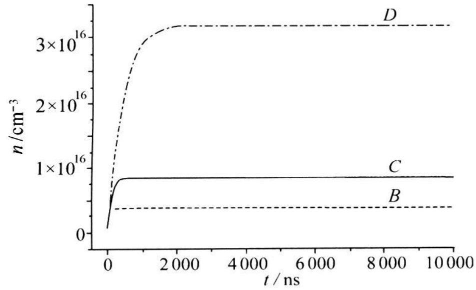

图 3 载流子寿命对载流子密度的影响 (pK= 50 W/cm^2, B, C, D 分别对应 S = (4 @10^{-8}, 10^{-7}, 4 @ 10^{-7}) s)

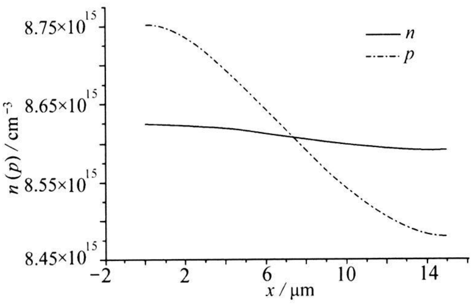

图 4 光照时间 t = 1 Ls 时探测器内载流子密度的分布 (pK= 50 W/cm^2)

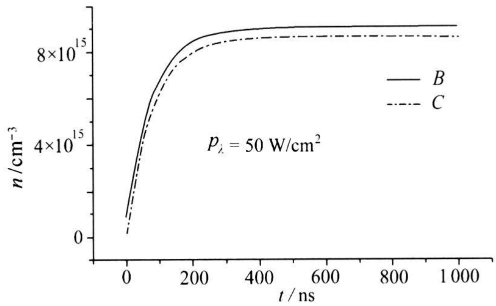

图 5 不同掺杂密度下探测器内 x = 0.1 Lm 处电子密度随光照时间的变化 (C, B 分别对应 N_D = 0, 8 @10^{14} cm^{-3})

1) 在稳定功率的激光辐照下, 探测器内光生载流子密度经过一段时间后达到稳定分布, 达到稳定分布所需的时间与载流子寿命成正比1

2) 光照时光生载流子产生的数量与激光辐照功率密度成正比, 与载流子寿命也成正比1

3) 材料掺杂质密度的大小只影响探测器内载流子的数量, 不影响其分布规律1

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Numerical Method and Analysis of Computational Fluid Mechanics for Photoelectric Semiconducting Detector

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Abstract: For computational fluid mechanics simulations of a three-dimensional photoelectric semiconducting detector, a modified upwind finite difference fractional step scheme was proposed. The optimal error estimated by using techniques including calculus of variations, energy method, induction hypothesis, and a prior estimates were obtained. The proposed scheme has been applied to simulate the photoelectric semiconducting detector.

Key words: photoelectric detector; fluid mechanics model; upwind fractional step; theoretical analysis; actual application