

多层不均匀材料中光吸收系数深度分布计算的理论处理*

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摘 要 提出了一种通过光热法测定与样品表面温度有关的光热信号, 重构反映多层不均匀材料中光吸收系数深度分布的理论处理和新的有效数值计算方法。数值模拟显示了较好的逼近效果。

关键词 深度, 分布, 光吸收, 多层材料。

1 引 言

Rosencwaig 和 Gersho^[1]对光热特性均匀的固体样品首次确定了与光热信号有关的样品表面温度、样品的光热特性和射到样品表面的入射光调制频率三者之间的定量关系。Afromowitz、Yeh 和 Yee^[2]研究了热特性均匀、光特性变化样品的表面温度与调制频率关系, 利用反拉氏变换, 将一组调制频率与表面温度的关系反演成样品中随深度变化的光吸收系数。但他们反演计算出的吸收系数分布与实际值之间的偏差随深度增加而增大, 且偏差超过允许值。

本文针对热特性不均匀、光吸收系数变化的三层固体样品, 推导了不同调制频率下表面温度与样品内部光热特性的解析表达式, 采用三种数值反演方法, 并用计算机模拟、比较, 得到一种最佳反演计算方法, 且与给定分布值对比, 其分布的绝对偏差和相对偏差都得到极大改善。

2 多层不均匀材料的表面温度与其内部光热特性之间的关系

图 1 所示 GaP·N 样品分别用 p 型、n 型外延层和衬底 b 三层组成, 每层边界分别为 $d_1 (= 0)$ 、 d_2 、 d_3 、 d_4 , 由于三层掺杂成份及浓度不同, 引起各层热参数不同, 而每层内部热均匀。样品受到调制频率为 ω 的单色光照射, 假定单色激励光为平面光波形式, 样品对激励

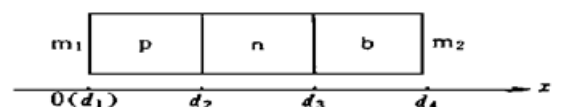


Fig. 1 GaP·N sample

* 国家自然科学基金资助项目。

光吸收沿 x 轴方向连续变化, 样品周围介质对激励光的吸收为零。

在平面波照射下横向尺寸无限大, 第 i 层热均匀样品的一维热扩散方程为

$$D_i \frac{\partial^2 \mathcal{F}_i(x, t)}{\partial x^2} + \frac{Q_i(x, t)}{\rho c} = \frac{\partial \mathcal{F}_i(x, t)}{\partial t} \quad (1)$$

式中 $\mathcal{F}_i(x, t)$ 为 t 时刻第 i 层离表面 x 处的温度, D_i 为第 i 层样品热扩散系数, ρ 、 c 分别为样品密度和热容; $Q_i(x, t)$ 为第 i 层 t 时刻 x 处单位体积样品内吸收光能后, 通过非辐射复合获得的热能; 脚标 i 取 0, 1, 2, 3, 4 分别表示介质 m_1 、 p 型外延层、 n 型外延层、衬底 b 及介质 m_2 。

设激励光的调制频率为 ω , 则样品表面光强表示为: $I(t) = I_0[1 + \exp(j\omega t)]/2$; 由于样品吸收系数 α 是空间坐标 x 的函数, 在样品内部的光强的衰减形式为 $\exp[-\int_0^x \alpha(y) dy]$, 所以 $Q_i(x, t)$ 写为以下形式:

$$Q_i(x, t) = \frac{1}{2}(1 - R_i)I_0\eta_i(x)\alpha(x) \exp[-\int_0^x \alpha(y) dy][1 + \exp(j\omega t)] \quad (2)$$

式中 $\eta_i(x)$ 、 R_i 分别为样品第 i 层光能转化为热能的效率及光反射系数, $\alpha(x)$ 是随空间坐标 x 变化的吸收系数。由于光热偏转法检测的是周期性变化温度场, 仅考虑交流项, 舍去 $Q_i(x, t)$ 中与时间无关的直流项后, 代入(1)式, 令 $\mathcal{F}_i(x, t) = T_i(x, \omega) \exp(j\omega t)$, (1)式可化为:

$$[\partial^2 T_i(x, \omega)/\partial x^2] - S_i^2 T_i(x, \omega) = -H(x), \quad (d_i \leq x \leq d_{i+1}) \quad (3)$$

式中 $H(x) = \frac{(1 - R_i)}{2k_i} I_i \eta_i \alpha(x) \exp[-\int_{d_i}^x \alpha(y) dy]$, $(d_i \leq x \leq d_{i+1})$,

$S_i^2 = j\omega/D_i$, $D_i = k_i/\rho c$, k_i 为样品第 i 层热导率, $I_i = I_0 \exp[-\int_{d_i}^x \alpha(y) dy]$ 为入射到第 i 层的光强, η_i 为第 i 层光转移为热的效率且是一个给定的常数。方程(3)最终解的表达式为

$$T_i(x, \omega) = C_{i1} \exp(S_i x) + C_{i2} \exp(-S_i x) + T_{E_i}(x, \omega)$$

其中 C_{i1} 和 C_{i2} 为待定常数, 特解 $T_{E_i}(x, \omega)$ 为

$$T_{E_i}(x, \omega) = \frac{1}{2S_i} [\exp(-S_i x) \int_{d_i}^x \exp(S_i y) H(y) dy - \exp(S_i x) \int_{d_i}^x \exp(-S_i y) H(y) dy], \quad (d_i \leq x \leq d_{i+1}),$$

可以证明在第 i 层中 $H(x)$ 和 $\alpha(x)$ 之间的关系如下:

$$\alpha(x) = H(x) \left[\frac{(1 - R_i)}{2k_i} I_i \eta_i - \int_{d_i}^x H(y) dy \right]^{-1}, \quad (d_i \leq x \leq d_{i+1}) \quad (4)$$

其中 $I_i = \frac{H(d_i)}{\alpha(d_i)} \times \frac{2k_i}{(1 - R_i)\eta_i}$, 且在 $[d_i, d_{i+1}]$ ($i = 1, 2, 3$) 上 $\alpha(x)$ 可表示成 $H(x)$ 的函数。

对于如图 1 所示的三层样品, 同时考虑在样品周围的介质吸收系数为零, 介质厚度远大于介质中的热波长度, 可以认为是半无界的, 根据自然边界条件得到介质及样品各层中的温度为:

$$\begin{aligned} T_0(x, \omega) &= C_{m1} \exp(S_{m1} x) & x \leq d_1; \\ T_1(x, \omega) &= C_{p1} \exp(S_p x) + C_{p2} \exp(-S_p x) + T_{E_1}(x, \omega) & d_1 \leq x \leq d_2; \end{aligned}$$

$$\begin{aligned}
T_2(x, \omega) &= C_{n1} \exp(S_n x) + C_{n2} \exp(-S_n x) + T_{E_2}(x, \omega) & d_2 \leq x \leq d_3; \\
T_3(x, \omega) &= C_{b1} \exp(S_b x) + C_{b2} \exp(-S_b x) + T_{E_3}(x, \omega) & d_3 \leq x \leq d_4; \\
T_4(x, \omega) &= C_{m_2} \exp(-S_{m_2} x) & x \geq d_4;
\end{aligned}$$

式中 S_{m_1} 、 S_p 、 S_n 、 S_b 、 S_{m_2} 分别为介质 m_1 、 p 型外延层、 n 型外延层、衬底及介质 m_2 的热扩散; C_{m_1} 、 C_{m_2} 、 C_{p1} 、 C_{p2} 、 C_{n1} 、 C_{n2} 、 C_{b1} 、 C_{b2} 为待定系数, 可以利用图 1 所示的各层边界上温度连续、热流连续条件确定。同时为了表达简便起见, 将式中各变数在边界上的取值分别用下列系数表示。令

$$\begin{aligned}
A &= \exp(S_p d_2) & B &= \exp(-S_p d_2) & C &= \exp(S_n d_2) & D &= \exp(-S_n d_2) \\
G &= \exp(S_n d_3) & E &= \exp(-S_n d_3) & J &= \exp(S_b d_3) & K &= \exp(-S_b d_3) \\
M &= \exp(S_b d_4) & N &= \exp(-S_b d_4)
\end{aligned}$$

$$\begin{aligned}
c_1 &= \exp(-S_p d_2) \int_{d_1}^{d_2} \exp(S_b y) H(y) dy & c_2 &= \exp(S_p d_2) \int_{d_1}^{d_2} \exp(-S_b y) H(y) dy \\
f_1 &= \exp(-S_n d_2) \int_{d_2}^{d_3} \exp(S_n y) H(y) dy = 0 & f_2 &= \exp(S_n d_2) \int_{d_2}^{d_3} \exp(-S_n y) H(y) dy = 0 \\
i_1 &= \exp(-S_n d_3) \int_{d_2}^{d_3} \exp(S_n y) H(y) dy & i_2 &= \exp(S_n d_3) \int_{d_2}^{d_3} \exp(-S_n y) H(y) dy \\
l_1 &= \exp(-S_b d_3) \int_{d_3}^{d_4} \exp(S_b y) H(y) dy = 0 & l_2 &= \exp(S_b d_3) \int_{d_3}^{d_4} \exp(-S_b y) H(y) dy = 0 \\
o_1 &= \exp(-S_b d_4) \int_{d_3}^{d_4} \exp(S_b y) H(y) dy & o_2 &= \exp(S_p d_4) \int_{d_3}^{d_4} \exp(-S_b y) H(y) dy \\
P &= \exp(-S_{m_2} d_4).
\end{aligned}$$

由边界条件:

$$\left. \begin{aligned}
T_i(d_{i+1}, \omega) &= T_{i+1}(d_{i+1}, \omega) \\
k_i \frac{dT_i(x, \omega)}{dx} \Big|_{x=d_{i+1}} &= k_{i+1} \frac{dT_{i+1}(x, \omega)}{dx} \Big|_{x=d_{i+1}} \quad (i = 0, 1, 2, 3),
\end{aligned} \right\} \quad (5)$$

得到以下线性方程组:

$$\begin{pmatrix}
1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\
\zeta & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & A & B & -C & -D & 0 & 0 & 0 \\
0 & \beta A & -\beta B & -C & D & 0 & 0 & 0 \\
0 & 0 & 0 & G & E & -J & -K & 0 \\
0 & 0 & 0 & \gamma G & -\gamma E & -J & K & 0 \\
0 & 0 & 0 & 0 & 0 & M & N & -P \\
0 & 0 & 0 & 0 & 0 & \theta M & -\theta M & P
\end{pmatrix}
\begin{pmatrix}
C_{m_1} \\
C_{p1} \\
C_{p2} \\
C_{n1} \\
C_{n2} \\
C_{b1} \\
C_{b2} \\
C_{m_2}
\end{pmatrix}
=
\begin{pmatrix}
0 \\
0 \\
-(c_1 - c_2)/(2S_p) \\
\beta(c_1 + c_2)/(2S_p) \\
-(i_1 - i_2)/(2S_n) \\
\gamma(i_1 + i_2)/(2S_n) \\
-(o_1 - o_2)/(2S_b) \\
\theta(o_1 + o_2)/(2S_b)
\end{pmatrix} \quad (6)$$

$$\zeta = \frac{k_{m_1}}{k_p} \frac{\sqrt{D_p}}{\sqrt{D_{m_1}}}, \quad \beta = \frac{k_p}{k_n} \frac{\sqrt{D_n}}{\sqrt{D_p}}, \quad \gamma = \frac{k_n}{k_b} \frac{\sqrt{D_b}}{\sqrt{D_n}}, \quad \theta = \frac{k_b}{k_{m_2}} \frac{\sqrt{D_{m_2}}}{\sqrt{D_b}}$$

由于光热信号反映样品表面的周期温度 $T_s(0, \omega)$, 所以仅考虑线性方程组 8 个未知数中的系数 C_{m_1} , 即

$$T_s(0, \omega) = T_0(0, \omega) = C_{m_1} = u/v \quad (7)$$

$$\text{其中} \quad u = - \left[\frac{(c_1 - c_2)}{2S_p} M_{31} + \frac{\beta}{2S_p} (c_1 + c_2) M_{41} + \frac{i_1 - i_2}{2S_n} M_{51} + \frac{\gamma}{2S_n} (i_1 + i_2) M_{61} + \frac{o_1 - o_2}{2S_b} M_{71} + \frac{\theta}{2S_b} (o_1 + o_2) M_{81} \right]$$

上式结果是按第 1 列拉普拉斯展开得到的, 这里 M_{i1} 是(6) 式系数矩阵的第 i 行第 1 列所对应的子式($i = 3, 4, \dots, 8$) 且与 $H(x)$ 无关, v 是(6) 式系数矩阵的行列式(可以证明: 当选取的 ω 大于某一正值或 ω 小于某一正值时, 则相应的 v 不等于零)。

由(7) 式看出, 对于非均匀样品, 其表面温度受样品内部各层热参数及吸收系数变化的影响。当 p 型外延层、n 型外延层和衬底的热参数相等 ($\equiv k$), 令 $d_2 = d_3 = d_4 \equiv d$, $S_p = S_n = S_b \equiv S$ (即 $D_1 = D_2 = D_3 \equiv D$), m_1 代表空气介质, m_2 代表透明介质, 得到

$$\begin{aligned} \beta = 1, \quad \gamma = 1, \quad A = C = G = J = M = \exp(Sd), \\ B = E = K = N = \exp(-Sd), \quad P = \exp(-Sd), \\ c_1 = \exp(-Sd) \int_0^d \exp(Sy) H(y) dy, \quad c_2 = \exp(Sd) \int_0^d \exp(-Sy) H(y) dy, \\ f_1 = f_2 = i_1 = i_2 = l_1 = l_2 = o_1 = o_2 = 0, \end{aligned}$$

代入(7) 式, 得到

$$C_{m_1} = \frac{1}{S} \frac{(1 + \tilde{b}) \Phi(S) A + (1 - \tilde{b}) \Phi(-S) B}{(1 + \tilde{b})(g + 1) A - (1 - \tilde{b})(1 - g) B} \quad (8)$$

$$\text{其中 } g = \zeta = \frac{k_g}{k} \frac{\sqrt{D}}{\sqrt{D_g}}, \quad \tilde{b} = \frac{1}{\theta}, \quad \Phi(S) = \int_0^{\infty} \exp(-Sy) H(y) dy = \int_0^d \exp(-Sy) H(y) dy =$$

$\frac{c_2}{A}$, $\Phi(-S) = c_1/B$ 。(8) 式与 Afromowitz 在热参数相等时所得的单层材料表面温度表达式相同^[2]。

(7) 式可用于预示多层热参数不同, 而在同一层中热参数均匀、吸收系数连续变化的层状样品在不同调制频率下, 表面温度的变化。因为光热信号直接与样品表面温度 $T_s(0, \omega)$ 有关, 因此, 若能从(7) 式中的 $T_s(0, \omega)$ 反演计算出 $H(x)$, 根据(4) 式, 则可计算出光吸收系数 $\alpha(x)$ 。即当 $\alpha(x)$ 是未知的空间函数时, 测量出一组调制频率下的光热信号, 通过反演运算, 可求出样品纵向吸收系数的变化。

3 数值反演计算方法及其结果比较

3.1 数值反演计算方法

由(4) 式可知, 欲反演 $\alpha(x)$, 只要能反演出 $H(x)$ 即可。为了检验数值反演的可行性, 可以分二步进行。

第一步: 需要精确的 $T_s(0, \omega)$, 故设(3) 式中的 $H(x)$ 为假定函数, 令

$$F(x, y) = \int \exp(xy)H(y)dy,$$

由微积分牛顿-莱布尼兹公式, 得到(7) 式中系数的精确计算为:

$$\begin{cases} c_1 = B[F(S_p, d_2) - F(S_p, d_1)] & \begin{cases} i_1 = E[F(S_n, d_3) - F(S_n, d_2)] \\ i_2 = G[F(-S_n, d_3) - F(-S_n, d_2)] \end{cases} & \begin{cases} f_1 = 0 \\ f_2 = 0 \end{cases} \\ c_2 = A[F(-S_p, d_2) - F(-S_p, d_1)] & \begin{cases} o_1 = N[F(S_b, d_4) - F(S_b, d_3)] \\ o_2 = M[F(-S_b, d_4) - F(-S_b, d_3)] \end{cases} & \begin{cases} l_1 = 0 \\ l_2 = 0 \end{cases} \end{cases}$$

将上述精确计算值代入(7) 式, 得到 $T_s(0, \omega)$ 的精确计算值。

第二步, 由上面计算出的表面信号 $T_s(0, \omega)$ 数值反演 $H(x)$ 。这里构造具有代数精度为 2 的数值积分公式近似计算(7) 式, 即

$$\int_a^b \exp(Sx)f(x)dx \approx A_0f(a) + A_1f\left(\frac{a+b}{2}\right) + A_2f(b) \tag{9}$$

其中

$$\begin{aligned} A_0 &= A_0(S, a, b) = \frac{2}{(b-a)^2} \frac{1}{S} \left[\left(\frac{2}{S^2} - \frac{b-a}{2S} \right) \exp(Sb) - \left(\frac{1}{2}(b-a)^2 + \frac{3}{2S}(b-a) + \frac{2}{S^2} \right) \exp(Sa) \right], \\ A_1 &= A_1(S, a, b) = \frac{4}{(b-a)^2 S^2} \left[(b-a - \frac{2}{S}) \exp(Sb) + (b-a + \frac{2}{S}) \exp(Sa) \right], \\ A_2 &= A_2(S, a, b) = \frac{2}{(b-a)^2 S} \left\{ \left[\frac{1}{2}(b-a)^2 - \frac{3(b-a)}{2S} + \frac{2}{S^2} \right] \exp(Sb) - \left(\frac{b-a}{2S} + \frac{2}{S^2} \right) \exp(Sa) \right\}; \end{aligned}$$

从而得到: $T_s(0, \omega) \approx \sum_{j=1}^{13} H_j \tilde{A}_j(\omega)$, 其中 $\tilde{A}_j(\omega)$ 是与频率、样品的热参数有关。为了获得 $H(x)$ 的分布, 可采用下面几种模型, 寻求 $H_j(j = 1, 2, \dots, 13)$ 的近似值[H_j 表示第 j 个取样点所对应 $H(x)$ 的值]:

1) 逼近模型 1: 求 $H_j(j = 1, 2, \dots, 13)$, 满足

$$\min_{H_j \in R} \sum_{k=1}^{\hat{m}} |T_s(0, \omega_k) - \sum_{j=1}^{13} \tilde{A}_j(\omega_k) H_j|^2 = \sum_{k=1}^{\hat{m}} |T_s(0, \omega_k) - \sum_{j=1}^{13} \tilde{A}_j(\omega_k) H_j^*|^2$$

其中 \hat{m} 代表所取调制频率的个数;

2) 逼近模型 2: 求 $H_j^*(j = 1, 2, \dots, 13)$, 满足

$$\max_{1 \leq k \leq 13} \left| \sum_{j=1}^{13} \tilde{A}_j(\omega_k) H_j^* - T_s(0, \omega_k) \right| = \min_{H_j \geq 0} \max_{01 \leq k \leq 13} \left| \sum_{j=1}^{13} \tilde{A}_j(\omega_k) H_j - T_s(0, \omega_k) \right|;$$

3) 逼近模型 3: 一般, $T_s(0, \omega) \approx \sum_{j=1}^m H_j \tilde{A}_j(\omega)$, 求 $\tilde{H}_j(j = 1, 2, \dots, m)$ 满足

$$\sum_{j=1}^m \operatorname{Re}[\tilde{A}_j(\omega_k)] \tilde{H}_j = \operatorname{Re}[T_s(0, \omega_k)], \quad (k = 1, 2, \dots, m)$$

其中记号 Re 表示取复数的实部, m 代表剖分点的个数。

3.2 数值结果及其比较

为了比较这些反演模型的数值逼近程度, 给定样品各层厚度及热参数, 并令介质 m_1 和介质 m_2 为同一介质, 记作 \bar{m} 。

取 $d_1 = 0.0 \text{ cm}$, $d_2 = 40.0 \times 10^{-4} \text{ cm}$, $d_3 = 100.0 \times 10^{-4} \text{ cm}$, $d_4 = 180.0 \times 10^{-4} \text{ cm}$, $D_{\bar{m}} = 0.00762 (\text{W} \cdot \text{cm}^2 \cdot \text{s}^{-1})$, $D_p = 0.019 (\text{W} \cdot \text{cm}^2 \cdot \text{s}^{-1})$, $D_n = 0.0175 (\text{W} \cdot \text{cm}^2 \cdot \text{s}^{-1})$, $D_b = 0.0420 (\text{W} \cdot \text{cm}^2 \cdot \text{s}^{-1})$, $\zeta = 20.0$, $\beta = 1.07387$, $\gamma = 0.9$ 和 $\theta = 0.06$ 。记

$$\overline{D_1} = \{d_1, d_1 + \frac{1}{4}(d_2 - d_1), d_1 + \frac{2}{4}(d_2 - d_1), \dots, d_2, d_2 + \frac{1}{4}(d_3 - d_2), \dots, d_3, d_3 + \frac{1}{4}(d_4 - d_3), \dots, d_4\};$$

$$\overline{D_2} = \{d_1, d_1 + \frac{1}{8}(d_2 - d_1), d_1 + \frac{2}{8}(d_2 - d_1), \dots, d_2, d_2 + \frac{1}{8}(d_3 - d_2), \dots, d_3, d_3 + \frac{1}{8}(d_4 - d_3), \dots, d_4\};$$

$$\overline{D_3} = \{d_1, d_1 + \frac{1}{6}(d_2 - d_1), d_1 + \frac{2}{6}(d_2 - d_1), \dots, d_2, d_2 + \frac{1}{6}(d_3 - d_2), \dots, d_3, d_3 + \frac{1}{6}(d_4 - d_3), \dots, d_4\};$$

$\hat{H}(x)$ 是用高斯列主元消去法求解模型 3 中的线性方程组获得的近似曲线, 而 $H^*(x)$ 是以 $\hat{H}(x)$ 为初始迭代值用迭代改善方法得到。

图 2 用模型 1 求解, 取 $\omega_k = 100\pi k$, ($k = 1, 2, \dots, \hat{m}$); “ \square ”表示取 $\hat{m} = 13$, “ \circ ”表示取 $\hat{m} = 20$ 反演计算所得到的近似曲线 $H^*(x)$, $x \in \overline{D_1}$; “ \bullet ”表示精确曲线 $H(x) = x$, $x \in \overline{D_1}$; 图像表明: “ \circ ”代表的近似曲线与 “ \square ”代表的近似曲线两者都远偏离精确曲线 $H(x)$, 且 “ \circ ”比 “ \square ”的偏差大得多。图 3 用模型 2 求解, 取 $\omega_k = 100\pi k$, ($k = 1, 2, \dots, 13$); “ \circ ”表示反演

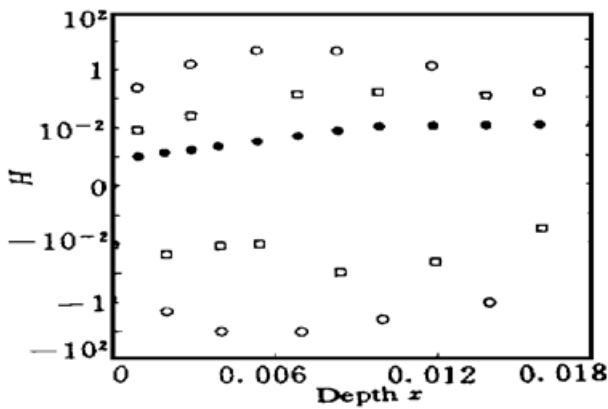


Fig. 2 Finding solution by model 1 where $\omega_k = 100\pi k$ ($k = 1, 2, \dots, \hat{m}$). The centers of “ \square ” and the centers of “ \circ ” are represented as approximate curves $H^*(x)$, $x \in \overline{D_1}$ when $\hat{m} = 13$ and $\hat{m} = 20$, respectively; and the centers of “ \bullet ” are represented as accurate curve $H(x) = x$, $x \in \overline{D_1}$

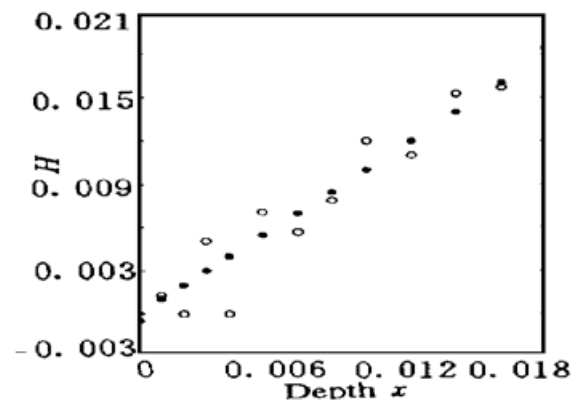


Fig. 3 Finding solution by model 2 where $\omega_k = 100\pi k$ ($k = 1, 2, \dots, 13$). The centers of “ \circ ” are represented as approximate curves $H^*(x)$, $x \in \overline{D_1}$; and the centers of “ \bullet ” are represented as accurate curve $H(x) = x$, $x \in \overline{D_1}$

计算所得到的近似曲线 $H^*(x)$, $x \in \overline{D_1}$; “ \bullet ”表示精确曲线 $H(x) = x$, $x \in \overline{D_1}$; 绝对误差及相对误差:

$$\max_{x \in \overline{D_1}} |H^*(x) - H(x)| = 4.0 \times 10^{-3}, \quad \frac{\max_{x \in \overline{D_1}} |H^*(x) - H(x)|}{\max_{x \in \overline{D_1}} |H(x)|} = 22.22\%;$$

图 4 用模型 3 求解, $m = 13$, 取 $\omega_k = 100\pi k$, ($k = 1, 2, \dots, 13$); “ \square ”表示反演计算所得

到的近似曲线 $\hat{H}(x)$, $x \in \overline{D_1}$; “ ⊖ ”表示改善 $\hat{H}(x)$ 后的曲线 $\hat{H}^*(x)$, $x \in \overline{D_1}$; “ ⊕ ”表示精确曲线 $H(x) = x$, $x \in \overline{D_1}$;

$$\max_{x \in \overline{D_1}} |\hat{H}^*(x) - H(x)| = 3.57755 \times 10^{-7},$$

$$\frac{\max_{x \in \overline{D_1}} |\hat{H}^*(x) - H(x)|}{\max_{x \in \overline{D_1}} |H(x)|} = 0.001988\%.$$

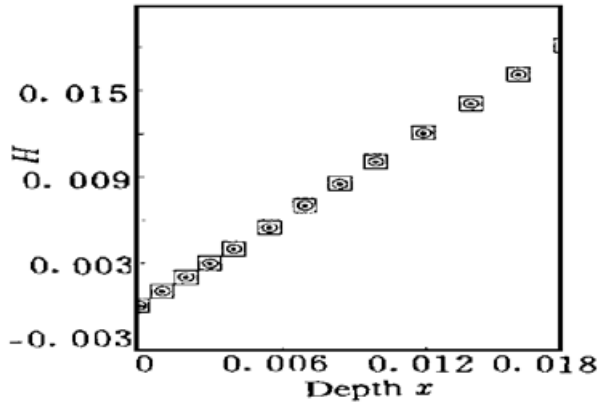


Fig. 4 Finding solution by model 3 where $\omega_k = 100\pi k$ ($k = 1, 2, \dots, 13$) and $m = 13$. The centers of “ ⊖ ” are represented as approximate curves $\hat{H}(x)$, $x \in \overline{D_1}$; the centers of “ ⊕ ” are represented as approximate curve $\hat{H}^*(x)$ obtained by improving $\hat{H}(x)$, $x \in \overline{D_1}$; and the centers of “ • ” are represented as accurate curve $H(x) = x$, $x \in \overline{D_1}$

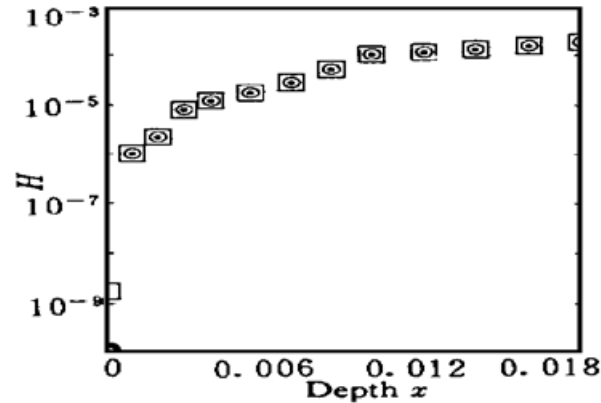


Fig. 5 Finding solution by model 3 where $\omega_k = 100\pi k$ ($k = 1, 2, \dots, 13$) and $m = 13$. The centers of “ ⊖ ” are represented as approximate curves $\hat{H}(x)$, $x \in \overline{D_1}$; the centers of “ ⊕ ” are represented as approximate curve $\hat{H}^*(x)$ obtained by improving $\hat{H}(x)$, $x \in \overline{D_1}$; and the centers of “ • ” are represented as accurate curve $H(x) = x^2$, $x \in \overline{D_1}$

图 5 用模型 3 求解, $m = 13$, 取 $\omega_k = 100\pi k$, ($k = 1, 2, \dots, 13$); “ ⊖ ”表示反演计算所得到的近似曲线 $\hat{H}(x)$, $x \in \overline{D_1}$; “ ⊕ ”表示改善 $\hat{H}(x)$ 后的曲线 $\hat{H}^*(x)$, $x \in \overline{D_1}$; “ ⊕ ”表示精确曲线 $H(x) = x^2$, $x \in \overline{D_1}$;

$$\max_{x \in \overline{D_1}} |\hat{H}^*(x) - H(x)| = 7.9247 \times 10^{-10},$$

$$\frac{\max_{x \in \overline{D_1}} |\hat{H}^*(x) - H(x)|}{\max_{x \in \overline{D_1}} |H(x)|} = 0.0002446\%.$$

图 6 用模型 3 求解, $m = 13$, 取 $\omega_k = 100\pi k$, ($k = 1, 2, \dots, 13$); “ ⊖ ”表示反演计算所得到的近似曲线 $\hat{H}(x)$, $x \in \overline{D_1}$; “ ⊕ ”表示改善 $\hat{H}(x)$ 后的曲线 $\hat{H}^*(x)$, $x \in \overline{D_1}$; “ ⊕ ”表示精确曲线 $H(x) = x^3$, $x \in \overline{D_1}$;

$$\max_{x \in \overline{D_1}} |\hat{H}^*(x) - H(x)| = 8.7486884 \times 10^{-8},$$

$$\frac{\max_{x \in \overline{D_1}} |\hat{H}^*(x) - H(x)|}{\max_{x \in \overline{D_1}} |H(x)|} = 1.500\%.$$

图 7 用模型 3 求解, 仅增加剖分数, $m = 25$, 求积公式的代数精度仍为 2, 取 $\omega_k = 100\pi k$, ($k = 1, 2, \dots, 25$); “ ⊖ ”表示反演计算所得到的近似曲线 $\hat{H}(x)$, $x \in \overline{D_2}$; “ ⊕ ”表示改善 $\hat{H}(x)$ 后的曲线 $\hat{H}^*(x)$, $x \in \overline{D_2}$; “ ⊕ ”表示精确曲线 $H(x) = x^3$, $x \in \overline{D_2}$ 。

由图 7 看出, 为了获得 $H(x)$ 的更多信息, 假如仅增加剖分数(如两倍), 只能得到图 7 所示的糟糕结果, 而不能得到真实的 $H(x)$ 。然而, 可以构造一个具有较高代数精度为 3 的数值

求积公式, 得到较好的结果如图 8 所示。

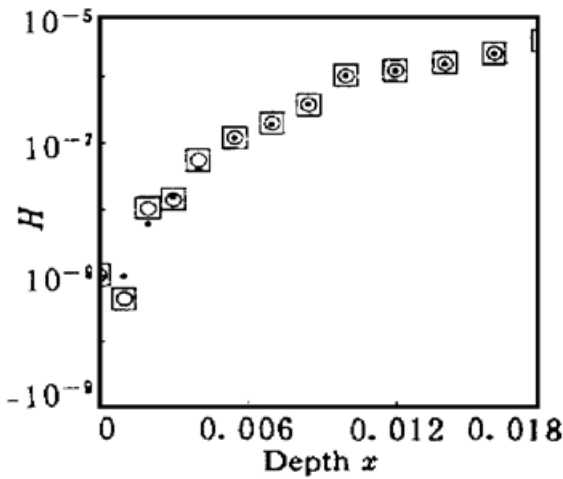


Fig. 6 Finding solution by model 3 where $\omega_k = 100\pi k$ ($k = 1, 2, \dots, 13$) and $m = 13$. The centers of “□” are represented as approximate curves $\tilde{H}(x)$, $x \in \overline{D_1}$; the centers of “○” are represented as approximate curve $\tilde{H}^*(x)$ obtained by improving $\tilde{H}(x)$, $x \in \overline{D_1}$; and the centers of “•” are represented as accurate curve $H(x) = x^3$, $x \in \overline{D_1}$

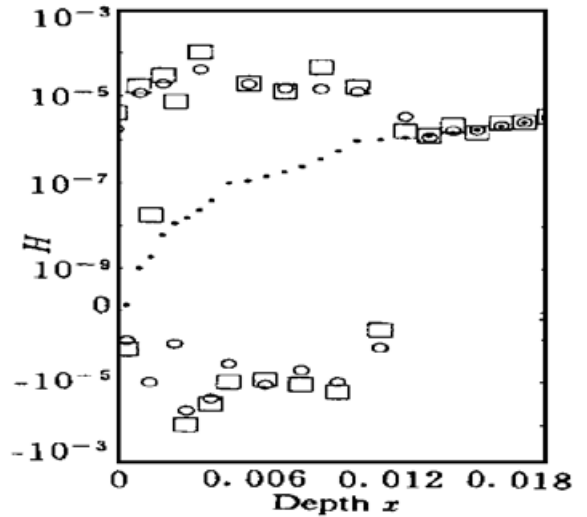


Fig. 7 Finding solution by model 3 only increasing dividing number where $\omega_k = 100\pi k$ ($k = 1, 2, \dots, 25$) and $m = 25$. The centers of “□” are represented as approximate curves $\tilde{H}(x)$, $x \in \overline{D_2}$ with algebraic precision 2; the centers of “○” are represented as approximate curve $\tilde{H}^*(x)$ obtained by improving $\tilde{H}(x)$, $x \in \overline{D_2}$; and the centers of “•” are represented as accurate curve $H(x) = x^3$, $x \in \overline{D_2}$

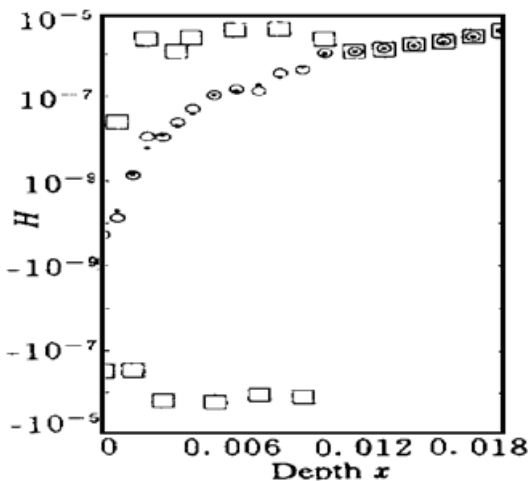


Fig. 8 Finding solution by model 3 where $\omega_k = 100\pi k$ ($k = 1, 2, \dots, 19$) and $m = 19$. The centers of “□” are represented as approximate curves $\tilde{H}(x)$, with algebraic precision 3, $x \in \overline{D_3}$; the centers of “○” are represented as approximate curve $\tilde{H}^*(x)$ obtained by improving $\tilde{H}(x)$, $x \in \overline{D_3}$; and the centers of “•” are represented as accurate curve $H(x) = x^3$, $x \in \overline{D_3}$

图 8 用模型 3 求解, 在增加剖分数的同时, 提高求积公式的代数精度至 3, $m = 19$, 取 $\omega_k = 100\pi k$, ($k = 1, 2, \dots, 19$); “□”表示反演计算所得到的近似曲线 $\tilde{H}(x)$, $x \in \overline{D_3}$; “○”表示改善 $\tilde{H}(x)$ 后的曲线 $\tilde{H}^*(x)$, $x \in \overline{D_3}$; “•”表示精确曲线 $H(x) = x^3$, $x \in \overline{D_3}$;

$$\max_{x \in D_3} |\tilde{H}^*(x) - H(x)| = 1.408618281 \times 10^{-7},$$

$$\frac{\max_{x \in D_3} |\tilde{H}^*(x) - H(x)|}{\max_{x \in D_3} |H(x)|} = 2.4\%;$$

这里构造的求积公式为

$$\int_a^b \exp(Sx)f(x) dx \approx A_0 f(a) + A_1 f\left(a + \frac{b-a}{3}\right) + A_2 f\left[a + \frac{2(b-a)}{3}\right] + A_3 f(b)$$

其中

$$\begin{aligned}
 A_0 &= -\frac{\exp(-Sa)}{6S(Sh)^3} \{6(Sh)^3 + 11(Sh)^2 + 12(Sh) + 6 + \\
 &\quad [\exp(3Sh)][-2(Sh)^2 + 6(Sh) - 6]\}, \\
 A_1 &= -\frac{\exp(-Sa)}{2S(Sh)^3} \{[\exp(3Sh)][3(Sh)^2 - 8(Sh) + 6] - 6(Sh)^2 - 10Sh - 6\}, \\
 A_2 &= \frac{\exp(-Sa)}{2S(Sh)^3} \{[\exp(3Sh)][6(Sh)^2 - 10Sh + 6] - 3(Sh)^2 - 8(Sh) - 6\}, \\
 A_3 &= \frac{\exp(-Sa)}{6S(Sh)^3} \{[\exp(3Sh)][6(Sh)^3 - 11(Sh)^2 + 12(Sh) - 6] + \\
 &\quad 2(Sh)^2 + 6(Sh) + 6\}, \\
 h &= (b - a)/3.
 \end{aligned}$$

比较图 2~ 图 4, 得到模型 3 是最佳的。图 4~ 图 8 表明: 采用同一模型 3, 在取定剖分数的情况下, 要选择恰当的求积公式, 才能更准确地反演计算 $H(x)$ 的分布。

结 论 综上所述, 利用计算机模拟数据, 也就是模拟光热信号和入射光调制频率 ω 之间的关系, 应用模型 3 能较好地得到吸收系数 $\alpha(x)$ 。用光热实验数据反演材料中吸收系数分布的进一步研究正在进行之中。

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A Theoretical Treatment for Computation on Depth Distribution of Optical Absorption Coefficient in Multilayer Inhomogeneous Material

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(Received 17 June 1997; revised 2 October 1997)

Abstract A theoretical treatment and a new effective numerical method are proposed to reconstruct the depth distribution of optical absorption coefficient in multilayer inhomogeneous material by the optical and thermal signals, which are related to the surface temperature of the sample measured with the optical and thermal method. Numerical simulations demonstrate the performance of the approach is better.

Key words depth, distribution, optical absorption, multilayer material.