

《激光烧蚀固体碳氢材料的离子组分分离研究》附加材料*

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A.1 线性化离子碰撞项

异类粒子碰撞算符为

$$C_{ab}^{\Phi} \equiv C_{ab}(f_a^M \Phi_a, f_b^M) + C_{ab}(f_a^M, f_b^M \Phi_b) = T_{ab}(\Phi_a) + M_{ab}(\Phi_b), \quad (\text{A.1})$$

其中 $T_{ab}(\Phi_a)$ 是分布发生扰动的电荷与背景为麦克斯韦分布的电荷之间的碰撞项,

$$T_{ab}(\Phi_a) = \frac{3\sqrt{\pi}f_a^M v_a^3}{4\tau_{ab} v_b^3} \left[-\frac{e^{w_a^2}}{2w_b^2} \frac{\partial}{\partial w_b} \left(e^{-w_a^2} w_b \frac{\partial H_b^M}{\partial w_b} \frac{\partial \Phi_a}{\partial w_b} \right) + \frac{\partial G_b^M}{2w_b^3 \partial w_b} \hat{L}^2(\Phi_a) \right], \quad (\text{A.2})$$

$M_{ab}(\Phi_b)$ 是麦克斯韦分布的电荷与扰动背景电荷之间的碰撞,

$$M_{ab}(\Phi_b) = \frac{3\sqrt{\pi}f_a^M v_a^3}{4\tau_{ab} v_b^3} \left\{ \frac{4}{\sqrt{\pi}} \frac{m_a}{m_b} e^{-w_b^2} \Phi_b - 2 \frac{m_b - m_a}{m_b} \frac{v_b^2}{v_a^2} w_b \frac{\partial H_b^{\Phi}}{\partial w_b} - \frac{2v_b^2}{v_a^2} \left(H_b^{\Phi} - \frac{v_b^2}{v_a^2} w_b^2 \frac{\partial^2 G_b^{\Phi}}{\partial w_b^2} \right) \right\}. \quad (\text{A.3})$$

为此再引入两个无量纲的算子 T_{ab} 和 M_{ab} , 其定义为

$$T_{ab}(\Phi_a) = \frac{3\sqrt{\pi}f_a^M v_a^3}{4\tau_{ab} v_b^3} T_{ab}(\Phi_a), \quad M_{ab}(\Phi_b) = \frac{3\sqrt{\pi}f_a^M v_a^3}{4\tau_{ab} v_b^3} M_{ab}(\Phi_b). \quad (\text{A.4})$$

异类粒子的碰撞时间定义为

$$\tau_{ab} = \frac{3m_a^{1/2} T_a^{3/2}}{4\sqrt{2\pi} Z_a^2 Z_b^2 n_b e^4 \ln \Lambda_{ab}}, \quad (\text{A.5})$$

v 为粒子热速度, $w_a = w/v_a$ 和 $w_b = w/v_b$ 为无量纲速度, H_b^M 和 G_b^M 为无量纲化的扰动 Rosenbluth 势, 其表达式为

$$H_b^{\Phi}(w) = \frac{1}{\pi^{3/2}} \int e^{-w^2} \frac{\Phi_b(w')}{|w - w'|} d^3 w', \quad (\text{A.6})$$

$$G_b^{\Phi}(w) = \frac{1}{\pi^{3/2}} \int e^{-w^2} \Phi_b(w') |w - w'| d^3 w'. \quad (\text{A.7})$$

角动量算符平方 \hat{L}^2 为

$$\hat{L}^2 \equiv \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}. \quad (\text{A.8})$$

对于同类粒子而言:

$$T_a(\Phi_a) = \frac{3\sqrt{\pi}f_a^M}{2\sqrt{2}\tau_{aa}} \left[-\frac{e^{w^2}}{2w^2} \frac{\partial}{\partial w} \left(e^{-w^2} w \frac{\partial H^M}{\partial w} \frac{\partial \Phi_a}{\partial w} \right) + \frac{1}{2w^3} \frac{\partial G^M}{\partial w} \hat{L}^2(\Phi) \right], \quad (\text{A.9})$$

$$M_a(\Phi_a) = \frac{3\sqrt{\pi}f_a^M}{2\sqrt{2}\tau_{aa}} \left\{ \frac{4}{\sqrt{\pi}} e^{-w^2} \Phi_a - 2 \left(H_a^\Phi - w^2 \frac{\partial^2 G_a^\Phi}{\partial w^2} \right) \right\}, \quad (\text{A.10})$$

定义

$$I_{aa}(\Phi_a) = C_{aa}(f_a^M \Phi_a, f_a^M) + C_{aa}(f_a^M, f_a^M \Phi_a) = T_a(\Phi_a) + M_a(\Phi_a). \quad (\text{A.11})$$

同类粒子的碰撞时间 τ_{aa} 为

$$\tau_{aa} = \frac{3\sqrt{m_a} T_a^{3/2}}{4\sqrt{\pi} Z_a^4 e^4 n_a \ln \Lambda_{aa}}, \quad (\text{A.12})$$

引入无量纲的算子 \hat{I}_{aa} ,

$$I_{aa}(\Phi_a) = \frac{3\sqrt{\pi}f_a^M}{2\sqrt{2}\tau_{aa}} \hat{I}_{aa}.$$

A.2 输运方程的求解

将扰动分布函数错误!未找到引用源。式代入离子输运方程错误!未找到引用源。，忽略黏滞项 $n_{\alpha\beta} W_{\alpha\beta}$ ，比较温度梯度 $\nabla \log T$ 项以及扩散驱动力项 D_a 的系数，并经过处理可以得到如下方程组:

$$\sum_{m=0}^{\infty} \left[\frac{n_a Z_a^2}{n_b Z_b^2} \langle n | \hat{I}_{aa} | m \rangle + \mu^3 \langle n | T_{ab} | m \rangle \right] g_m^{(a)} + \mu^3 \frac{n_b}{n_a} \sum_{m=0}^{\infty} \langle n | M_{ab} | m \rangle g_m^{(b)} = -\frac{5}{4} \delta_{n,1}, \quad (\text{A.13})$$

$$\frac{n_a}{n_b \mu^3} \sum_{m=0}^{\infty} \langle n | M_{ba} | m \rangle g_m^{(a)} + \sum_{m=0}^{\infty} \left[\frac{n_b Z_b^2}{n_a Z_a^2} \langle n | \hat{I}_{bb} | m \rangle + \frac{1}{\mu^3} \langle n | T_{ba} | m \rangle \right] g_m^{(b)} = -\frac{5}{4} \delta_{n,1}, \quad (\text{A.14})$$

$$\sum_{m=0}^{\infty} \left[\frac{n_a Z_a^2}{n_b Z_b^2} \langle n | \hat{I}_{aa} | m \rangle + \mu^3 \langle n | T_{ab} | m \rangle \right] h_m^{(a)} - \mu^3 \frac{n_b}{n_a} \sum_{m=0}^{\infty} \langle n | M_{ab} | m \rangle h_m^{(b)} = \frac{1}{2\zeta_a} \delta_{n,0},$$

(A.15)

$$-\frac{n_a}{n_b \mu^3} \sum_{m=0}^{\infty} \langle n | M_{ba} | m \rangle h_m^{(a)} + \sum_{m=0}^{\infty} \left[\frac{n_b Z_b^2}{n_a Z_a^2} \langle n | \hat{I}_{bb} | m \rangle + \frac{1}{\mu^3} \langle n | T_{ba} | m \rangle \right] h_m^{(b)} = \frac{1}{2\zeta_b} \delta_{n,0} \quad (\text{A.16})$$

这里, n 为粒子数密度, ζ 为粒子数丰度, 如 a 离子粒子数丰度为 $\zeta_a = n_a / n$,

$\mu = \sqrt{m_b} / \sqrt{m_a}$, Z 为电荷数。

各碰撞矩阵元的定义如下:

$$\langle n | \hat{I}_{aa} | m \rangle \equiv \int_0^{\infty} e^{-w_a^2} w_a S_{3/2}^n(w_a^2) \hat{I}_{aa} [w_a S_{3/2}^m(w_a^2)] w_a^2 dw_a, \quad (\text{A.17})$$

$$\langle n | \hat{I}_{bb} | m \rangle \equiv \int_0^{\infty} e^{-w_b^2} w_b S_{3/2}^n(w_b^2) \hat{I}_{bb} [w_b S_{3/2}^m(w_b^2)] w_b^2 dw_b, \quad (\text{A.18})$$

$$\langle n | T_{ab} | m \rangle \equiv \int_0^{\infty} e^{-w_a^2} w_a S_{3/2}^n(w_a^2) T_{ab} [w_a S_{3/2}^m(w_a^2)] w_a^2 dw_a, \quad (\text{A.19})$$

$$\langle n | T_{ba} | m \rangle \equiv \int_0^{\infty} e^{-w_b^2} w_b S_{3/2}^n(w_b^2) T_{ba} [w_b S_{3/2}^m(w_b^2)] w_b^2 dw_b, \quad (\text{A.20})$$

$$\langle n | M_{ab} | m \rangle \equiv \int_0^{\infty} e^{-w_a^2} w_a S_{3/2}^n(w_a^2) M_{ab} (w_b S_{3/2}^m(w_b^2)) w_a^2 dw_a, \quad (\text{A.21})$$

$$\langle n | M_{ba} | m \rangle \equiv \int_0^{\infty} e^{-w_b^2} w_b S_{3/2}^n(w_b^2) M_{ba} [w_a S_{3/2}^m(w_a^2)] w_b^2 dw_b. \quad (\text{A.22})$$

利用索宁多项式生成函数的性质:

$$\frac{1}{(1-t)^{i+1}} e^{-\frac{t}{1-t}x} = \sum_{n=0}^{\infty} S_i^n(x) t^n, \quad (\text{A.23})$$

那么

$$\sum_{n,m=0}^{\infty} t^n s^m \langle n | T_{ab} | m \rangle = \frac{1}{[(1-t)(1-s)]^{5/2}} \int_0^{\infty} e^{-w_a^2} w_a e^{-\frac{t}{1-t}w_a^2} T_{ab} \left(w_a e^{-\frac{s}{1-s}w_a^2} \right) w_a^2 dw_a, \quad (\text{A.24})$$

$$\sum_{n,m=0}^{\infty} t^n s^m \langle n | M_{ab} | m \rangle = \frac{1}{[(1-t)(1-s)]^{5/2}} \int_0^{\infty} e^{-w_a^2} w_a e^{-\frac{t}{1-t}w_a^2} M_{ab} \left(w_b e^{-\frac{s}{1-s}w_b^2} \right) w_a^2 dw_a. \quad (\text{A.25})$$

对(A.24)式和(A.25)式的右边积分, 有

$$\begin{aligned} & \left[\mu^2(1-t)(1-s) + (1-ts) \right]^{3/2} \sum_{n,m=0}^{\infty} t^n s^m \langle n | T_{ab} | m \rangle \\ &= -\frac{1}{2\mu^2(1-ts)} \left\{ \frac{\mu^2 + 1 - (\mu^2 - 1)ts}{(1-ts)} + \frac{3ts}{\left[\mu^2(1-t)(1-s) + (1-ts) \right]} \right\}, \end{aligned} \quad (\text{A.26})$$

$$\begin{aligned} & \left[\mu^2(1-t) + (1-s) \right]^{5/2} \sum_{n,m=0}^{\infty} t^n s^m \langle n | M_{ab} | m \rangle \\ &= \frac{1}{2\mu} \left\{ 3 - \left[\mu^2(1-t) + (1-s) \right] + 3(1-t)(1-s) \right\} + \frac{1}{2\mu^3} \left\{ (\mu^2 - 1) \left[2\mu^2(1-t) - (1-s) \right] \right\}. \end{aligned} \quad (\text{A.27})$$

通过对 $\sum_{n,m=0}^{\infty} t^n s^m \langle n | T_{ab} | m \rangle$ 和 $\sum_{n,m=0}^{\infty} t^n s^m \langle n | M_{ab} | m \rangle$ 作展开即可得到各个碰撞矩阵元,

方程(A.13)、方程(A.14)、方程(A.15)以及方程(A.16)的可解条件(Enskog 条件)为

$$\sum_s \rho_s u_s = 0, \quad (\text{A.28})$$

即:

$$\tau_{ab} n_a b_a^{(0)} + \tau_{ba} n_b b_b^{(0)} = 0, \quad (\text{A.29})$$

$$\tau_{ab} n_a c_a^{(0)} - \tau_{ba} n_b c_b^{(0)} = 0. \quad (\text{A.30})$$

方程(A.13)和方程(A.14)结合可解条件(A.29)式, 方程(A.15)和方程(A.16)结合可解条件(A.30)式即可求得离子的运输系数。

A.3 离子运输系数

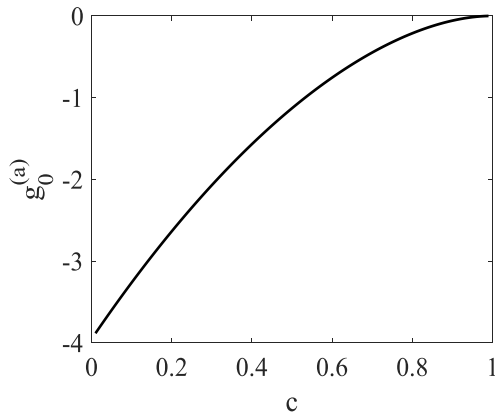


图 A1 离子运输系数 $g_0^{(a)}$ 作为 c 的函数

Fig. A1. Variation of ion transport coefficient $g_0^{(a)}$ with mass concentration c .

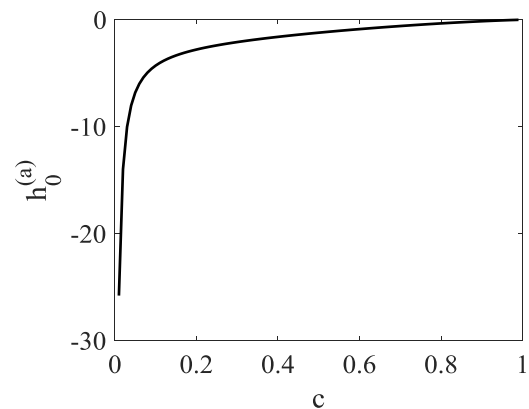


图 A2 离子运输系数 $h_0^{(a)}$ 作为 c 的函数

Fig. A2. Variation of ion transport coefficient $h_0^{(a)}$ with mass concentration c .

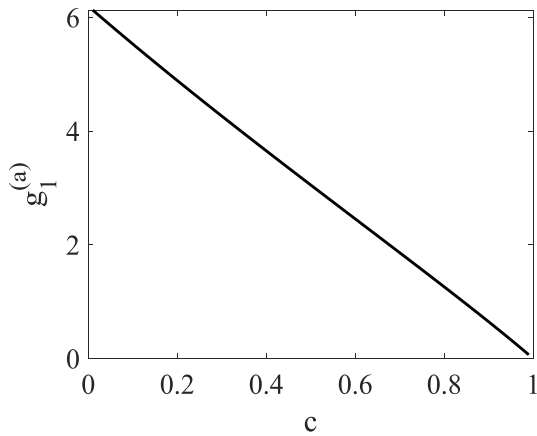


图 A3 离子运输系数 $g_1^{(a)}$ 作为 c 的函数

Fig. A3. Variation of ion transport coefficient

$g_1^{(a)}$ with mass concentration c .

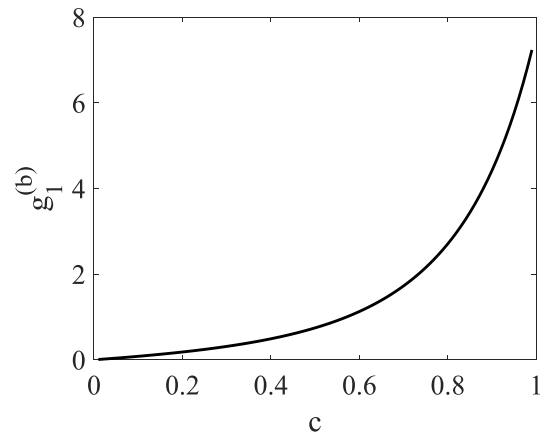


图 A4 离子运输系数 $g_1^{(b)}$ 作为 c 的函数

Fig. A4. Variation of ion transport

coefficient $g_1^{(b)}$ versus mass concentration c .

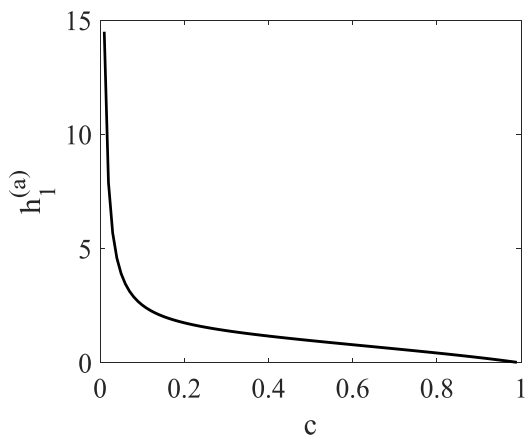


图 A5 离子运输系数 $h_1^{(a)}$ 作为 c 的函数

Fig. A5. Variation of ion transport

coefficient $h_1^{(a)}$ versus mass concentration c .

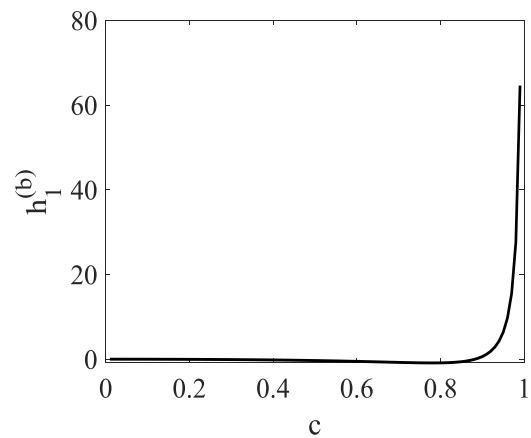


图 A6 离子运输系数 $h_1^{(b)}$ 作为 c 的函数

Fig. A6. Variation of ion transport coefficient

$h_1^{(b)}$ versus mass concentration c .