《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

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

其中$T_{ab}\left(\Phi_a\right)$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，

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

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

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

为此再引入两个无量纲的算子$\mathcal{T}_{ab}$和$\mathcal{M}_{ab}$，其定义为

$$T_{ab}\left(\Phi_a\right) = \frac{3\sqrt{\pi} f_a^{\mathrm{M}}}{4\tau_{ab}}\frac{v_a^3}{v_b^3}\mathcal{T}_{ab}\left(\Phi_a\right),\ M_{ab}\left(\Phi_b\right) = \frac{3\sqrt{\pi} f_a^{\mathrm{M}}}{4\tau_{ab}}\frac{v_a^3}{v_b^3}\mathcal{M}_{ab}\left(\Phi_b\right)。 \tag{A.4}$$

异类粒子的碰撞时间定义为

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

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

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

$$G_b^{\Phi}(w) = \frac{1}{\pi^{3/2}}\int \mathrm{e}^{-w'^2}\Phi_b\left(\boldsymbol{w}'\right)\left|\boldsymbol{w} - \boldsymbol{w}'\right|\mathrm{d}^3 w'。 \tag{A.7}$$

角动量算符平方 $\hat{L}^2$ 为

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

对于同类粒子而言：

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

$$M_a(\varPhi_a)=\frac{3\sqrt{\pi}f_a^{\rm M}}{2\sqrt{2}\tau_{aa}}\left\{\frac{4}{\sqrt{\pi}}{\rm e}^{-w^2}\varPhi_a-2\left(H_a^{\varPhi}-w^2\frac{\partial^2 G_a^{\varPhi}}{\partial w^2}\right)\right\}, \tag{A.10}$$

定义

$$I_{aa}(\varPhi_a)=C_{aa}\left(f_a^{\rm M}\varPhi_a, f_a^{\rm M}\right)+C_{aa}\left(f_a^{\rm M}, f_a^{\rm M}\varPhi_a\right)=T_a(\varPhi_a)+M_a(\varPhi_a)\text{。} \tag{A.11}$$

同类粒子的碰撞时间 τ_{aa} 为

$$\tau_{aa}=\frac{3\sqrt{m_a}T_a^{3/2}}{4\sqrt{\pi}Z_a^4e^4n_a\ln\varLambda_{aa}}, \tag{A.12}$$

引入无量纲的算子 $\hat{I}_{aa}$，

$$I_{aa}(\varPhi_a)=\frac{3\sqrt{\pi}f_a^{\rm M}}{2\sqrt{2}\tau_{aa}}\hat{I}_{aa}\text{。}$$

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 $\eta_{\alpha\beta}W_{\alpha\beta}$，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：

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

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

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

(A.15)

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

(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：

$$\left\langle n\left|\hat{I}_{aa}\right|m\right\rangle\equiv\int_0^{\infty}\mathrm{e}^{-w_a^2}w_aS_{3/2}^n\left(w_a^2\right)\hat{I}_{aa}\left[w_aS_{3/2}^m(w_a^2)\right]w_a^2\mathrm{d}w_a\text{，}\tag{A.17}$$

$$\left\langle n\left|\hat{I}_{bb}\right|m\right\rangle\equiv\int_0^{\infty}\mathrm{e}^{-w_b^2}w_bS_{3/2}^n\left(w_b^2\right)\hat{I}_{bb}\left[w_bS_{3/2}^m(w_b^2)\right]w_b^2\mathrm{d}w_b\text{，}\tag{A.18}$$

$$\left\langle n\left|T_{ab}\right|m\right\rangle\equiv\int_0^{\infty}\mathrm{e}^{-w_a^2}w_aS_{3/2}^n\left(w_a^2\right)T_{ab}\left[w_aS_{3/2}^m(w_a^2)\right]w_a^2\mathrm{d}w_a\text{，}\tag{A.19}$$

$$\left\langle n\left|T_{ba}\right|m\right\rangle\equiv\int_0^{\infty}\mathrm{e}^{-w_b^2}w_bS_{3/2}^n\left(w_b^2\right)T_{ba}\left[w_bS_{3/2}^m(w_b^2)\right]w_b^2\mathrm{d}w_b\text{，}\tag{A.20}$$

$$\left\langle n\left|M_{ab}\right|m\right\rangle\equiv\int_0^{\infty}\mathrm{e}^{-w_a^2}w_aS_{3/2}^n\left(w_a^2\right)M_{ab}\left(w_bS_{3/2}^m(w_b^2)\right)w_a^2\mathrm{d}w_a\text{，}\tag{A.21}$$

$$\left\langle n\left|M_{ba}\right|m\right\rangle\equiv\int_0^{\infty}\mathrm{e}^{-w_b^2}w_bS_{3/2}^n\left(w_b^2\right)M_{ba}\left[w_aS_{3/2}^m(w_a^2)\right]w_b^2\mathrm{d}w_b\text{。}\tag{A.22}$$

利用索宁多项式生成函数的性质：

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

那么

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

(A.24)

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

(A.25)

对(A.24)式和(A.25)式的右边积分，有

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

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

通过对 $\sum_{n,m=0}^{\infty}t^n s^m\left\langle n\left|T_{ab}\right|m\right\rangle$ 和 $\sum_{n,m=0}^{\infty}t^n s^m\left\langle n\left|M_{ab}\right|m\right\rangle$ 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

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

即：

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

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

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)式即可求得离子的输运系数。

A.3 离子输运系数

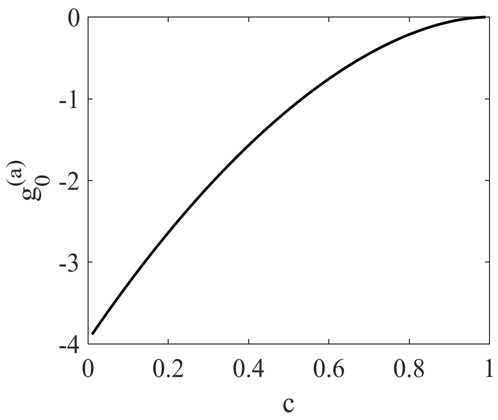

图 A1 离子输运系数 $g_0^{(a)}$ 作为 c 的函数

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

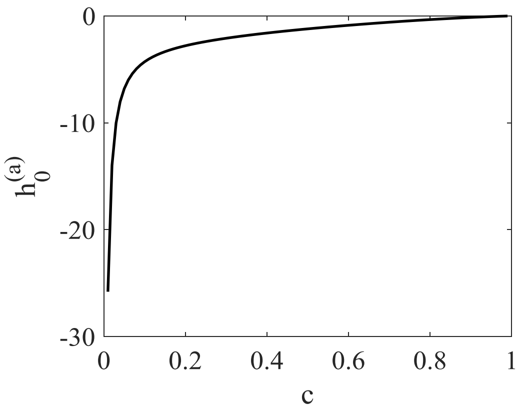

图 A2 离子输运系数 $h_0^{(a)}$ 作为 c 的函数

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

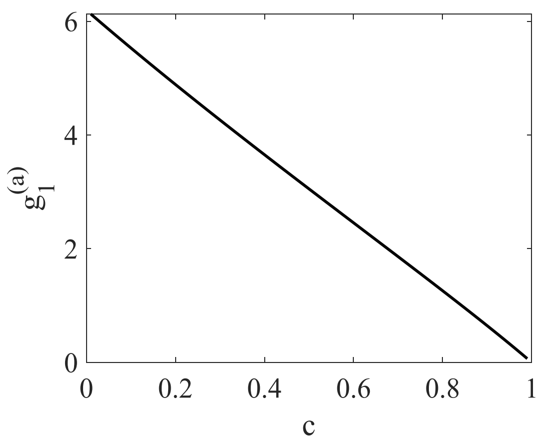

图 A3 离子输运系数 $g_1^{(a)}$ 作为 c 的函数

Fig. A3. Variation of ion transport coefficient $g_1^{(a)}$ with mass concentration c.

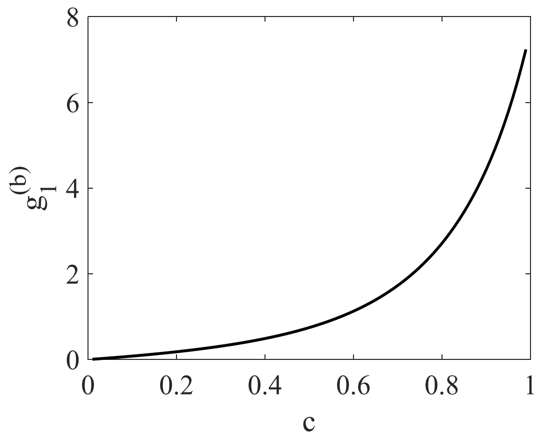

图 A4 离子输运系数 $g_1^{(b)}$ 作为 c 的函数

Fig. A4. Variation of ion transport coefficient $g_1^{(b)}$ versus mass concentration c.

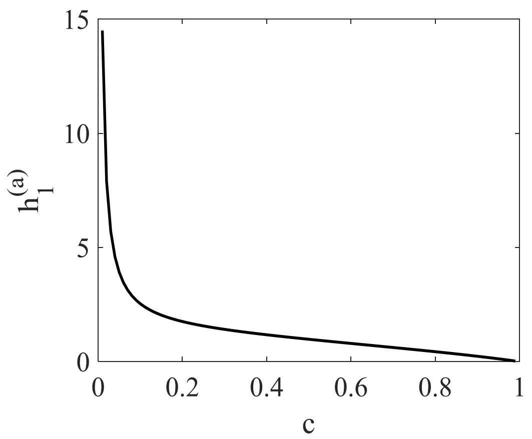

图 A5 离子输运系数 $h_1^{(a)}$ 作为 c 的函数

Fig. A5. Variation of ion transport coefficient $h_1^{(a)}$ versus mass concentration c.

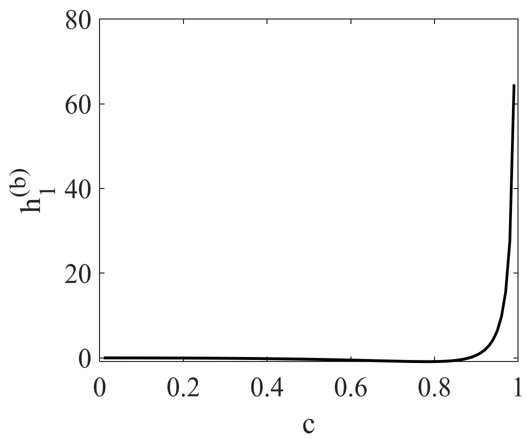

图 A6 离子输运系数 $h_1^{(b)}$ 作为 c 的函数

Fig. A6. Variation of ion transport coefficient $h_1^{(b)}$ versus massconcentration c.

