

《中子辐照诱导钨再结晶的模拟研究》*的补充材料

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1. 团簇动力学主方程^[1]

$$\begin{aligned} \frac{dC_1}{dt} = & G_1 + 2\alpha_2^- C_{I_2} + \sum_{n=3}^{N_1} \alpha_n^- C_{I_n} + \beta_3^- C_{I_3} + (k_{I_2+v}^+ + k_{V_1+I_2}^+) C_V C_{I_2} + k_{I+v}^+ C_V^{\text{eq}} C_1^{\text{eq}} \\ & - 2\alpha_1^+ C_1^2 - (\alpha_2^+ + \beta_1^+) C_1 C_{I_2} - \sum_{n=3}^{N_1-1} \alpha_n^+ C_1 C_{I_n} - k_{I+v}^+ C_1 C_V - \sum_{n=2}^{N_V} k_{V_n+I}^+ C_{V_n} C_1 \\ & - k_{I-v}^- C_1 - k_{D+I}^+ C_1 - k_{S+I}^+ C_1, \end{aligned} \quad (\text{A1})$$

$$\begin{aligned} \frac{dC_{I_2}}{dt} = & G_{I_2} + \alpha_1^+ C_1^2 + k_{I_3+v}^+ C_V C_{I_3} + \alpha_3^- C_{I_3} + \sum_{n=3}^{N_1} \beta_n^- C_{I_n} + \beta_4^- C_{I_4} + k_{I-v}^- C_1 \\ & - \alpha_2^+ C_1 C_{I_2} - \sum_{n=1}^{N_1} \beta_n^+ C_{I_2} C_{I_n} - \beta_2^+ C_{I_2}^2 - k_{I_2+v}^+ C_V C_{I_2} - \sum_{n=1}^{N_V} k_{V_n+I_2}^+ C_{V_n} C_{I_2} \\ & - \alpha_2^- C_{I_2} - k_{I_2-v}^- C_{I_2} - k_{D+I_2}^+ C_{I_2} - k_{S+I_2}^+ C_{I_2}, \end{aligned} \quad (\text{A2})$$

$$\begin{aligned} \frac{dC_{I_n}}{dt} \quad 3 \leq n \leq N_1 = & G_{I_n} + \alpha_{n-1}^+ C_1 C_{I_{n-1}} + \beta_{n-2}^+ C_{I_2} C_{I_{n-2}} + k_{I_{n+1}+v}^+ C_V C_{I_{n+1}} + \alpha_{n+1}^- C_{I_{n+1}} \\ & + \beta_{n+2}^- C_{I_{n+2}} + k_{I_{n-1}-v}^- C_{I_{n-1}} - \alpha_n^+ C_1 C_{I_n} - \beta_n^+ C_{I_2} C_{I_n} - k_{I_n+v}^+ C_V C_{I_n} \\ & - \alpha_n^- C_{I_n} - \beta_n^- C_{I_n} - k_{I_n-v}^- C_{I_n}, \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} \frac{dC_{x_i^I}}{dt} \quad N_1+1 \leq i \leq M_1 = & G_{x_i^I} + \frac{1}{x_{i+1}^I - x_{i-1}^I} \left[- \left(F_{x_{i+1}^I} C_{x_{i+1}^I} - F_{x_{i-1}^I} C_{x_{i-1}^I} \right) \right. \\ & \left. + \left(\frac{D_{x_{i+1}^I} C_{x_{i+1}^I} - D_{x_i^I} C_{x_i^I}}{x_{i+1}^I - x_i^I} - \frac{D_{x_i^I} C_{x_i^I} - D_{x_{i-1}^I} C_{x_{i-1}^I}}{x_i^I - x_{i-1}^I} \right) \right], \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} \frac{dC_V}{dt} = & G_V + k_{V_2+I}^+ C_{V_2} C_1 + k_{V_3+I_2}^+ C_{V_3} C_{I_2} + \sum_{n=2}^{N_V} \gamma_n^- C_{V_n} + \gamma_2^- C_{V_2} + \sum_{n=1}^{N_V} k_{I_n-v}^- C_{I_n} \\ & + k_{I+v}^+ C_V^{\text{eq}} C_1^{\text{eq}} - \gamma_1^+ C_V^2 - \sum_{n=1}^{N_V} \gamma_n^+ C_V C_{V_n} - k_{I+v}^+ C_V C_1 - \sum_{n=2}^{N_1} k_{I_n+v}^+ C_V C_{I_n} \\ & - k_{V_1+I_2}^+ C_V C_{I_2} - k_{D+v}^+ C_V - k_{S+v}^+ C_V, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} \frac{dC_{V_n}}{dt} \quad 2 \leq n \leq N_V &= G_{V_n} + \gamma_{n-1}^+ C_V C_{V_{n-1}} + k_{V_{n+1}-1}^+ C_{V_{n+1}} C_1 + k_{V_{n+2}+I_2}^+ C_{V_{n+2}} C_{I_2} \\ &+ \gamma_{n+1}^- C_{V_{n+1}} - \gamma_n^+ C_V C_{V_n} - k_{V_n+1}^+ C_{V_n} C_1 - k_{V_n+I_2}^+ C_{V_n} C_{I_2} - \gamma_n^- C_{V_n}, \end{aligned} \quad (A6)$$

$$\begin{aligned} \frac{dC_{x_i^V}}{dt} \quad N_V+1 \leq i \leq M_V &= G_{x_i^V} + \frac{1}{x_{i+1}^V - x_{i-1}^V} \left[- \left(F_{x_{i+1}^V} C_{x_{i+1}^V} - F_{x_{i-1}^V} C_{x_{i-1}^V} \right) \right. \\ &\left. + \left(\frac{D_{x_{i+1}^V} C_{x_{i+1}^V} - D_{x_i^V} C_{x_i^V}}{x_{i+1}^V - x_i^V} - \frac{D_{x_i^V} C_{x_i^V} - D_{x_{i-1}^V} C_{x_{i-1}^V}}{x_i^V - x_{i-1}^V} \right) \right]. \end{aligned} \quad (A7)$$

2. 结合能及位错环捕获偏置因子表达式^[1]

缺陷与可移动缺陷反应的结合能（使用毛细管近似）：

$$E_{I_n}^f = E_{I_{n-1}}^f + E_1^f - E_{I_{n-1}}^b, \quad (A8)$$

$$E_{I_{n-1}}^b = E_1^f + \frac{E_{I_2}^b - E_1^f}{2^{2/3} - 1} \left[n^{2/3} - (n-1)^{2/3} \right], \quad (A9)$$

$$E_{I_{n-2}}^b = 2E_1^f - E_{I_2}^b + \frac{E_{I_2}^b - E_1^f}{2^{2/3} - 1} \left[(n+1)^{2/3} - (n-1)^{2/3} \right], \quad (A10)$$

$$E_{I_{n-V}}^b = E_V^f + \frac{E_1^f - E_{I_2}^b}{2^{2/3} - 1} \left[n^{2/3} - (n-1)^{2/3} \right], \quad (A11)$$

$$E_{V_n-V}^b = E_V^f + \frac{E_{V_2}^b - E_V^f}{2^{2/3} - 1} \left[n^{2/3} - (n-1)^{2/3} \right]. \quad (A12)$$

间隙位错环捕获偏置因子：

$$Z_{I_n}^I = Z_D^I \max \left[\frac{2\pi}{\ln(4r_{I_n}/b)}, 1 \right], \quad (A13)$$

$$Z_{I_n}^{I_2} = Z_D^I \max \left[\frac{2\pi}{\ln(4r_{I_n}/b)}, 1 \right], \quad (A14)$$

$$Z_{I_n}^V = Z_D^V \max \left[\frac{2\pi}{\ln(4r_{I_n}/b)}, 1 \right]. \quad (A15)$$

表 A1 本研究模型使用的纯钨参数
Table A1. Tungsten parameters used in this research model.

参数	单位	数值	描述	参考文献
a	nm	0.317	晶格常数	[3]
b	nm	0.274	伯格矢量大小	[2]
G	GPa	161	纯钨剪切模量	[4]
r_{IV}	nm	0.465	复合半径	[2]
E_I^f	eV	9.466	间隙原子形成能	[2]
E_V^f	eV	3.20	空位形成能	[5]
E_I^m	eV	0.013	间隙原子迁移能	[7]
E_I^m	eV	0.024	双间隙原子迁移能	[7]
E_V^m	eV	1.66	空位迁移能	[7]
E_{I2}^b	eV	2.12	SIA-SIA 结合能	[2]
E_{V2}^b	eV	0.6559	Vac-Vac 结合能	[2]
D_I^0	m ² /s	8.77×10^{-8}	间隙原子扩散前置系数	[7]
D_{I2}^0	m ² /s	7.02×10^{-8}	双间隙原子扩散前置系数	[7]
D_V^0	m ² /s	1.77×10^{-6}	空位扩散前置系数	[7]
Z_D^I	—	1.20	位错捕获间隙原子偏置因子	[2]
Z_D^{I2}	—	1.20	位错捕获双间隙原子偏置因子	[1]
Z_D^V	—	1.00	位错捕获空位偏置因子	[2]
$\bar{\gamma}$	eV/Å ²	0.235	空洞平均表面能密度	[8]
E_{111}	eV/Å	0.827	位错环平均线能量前对数因子	[8]
ρ_W	g/m ³	1.935×10^7	纯钨密度	—
N_A	mol ⁻¹	6.02×10^{23}	阿伏伽德罗常数	—
M_W	g/mol	183.85	纯钨摩尔质量	—

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