匠心筑梦 人文情怀

多物理场仿真在电磁场、器件等方面的研究

汇 报 人：　张　云　柯

单　　位：深圳技术大学
张明吉老师课题组

内　容

CONTENTS

1. 等离子体
2. 仪器、设备的仿真
3. 其他仿真案例
4. 致谢

1 等离子体案例

1

解析

1.雪崩理论 Townsend
2.流注理论 Reather

理想工况、
经验解析、
工程速算、

2

微观碰撞

1. 电子碰撞截面
2. CHIANTI数据
3. 等离子体数据交换计划 LXCat
4. Blogsig+

微观机制、
混合体系、
拟合函数、

3

宏观模拟

1. 能斯特-普朗克-泊松方程
2.基于平衡态假设的磁流体动力学方程
3. 重离子、电子能量、电子密度方程

宏观到微观的反馈机制不健全。导致计算结果失真。

4

多尺度-多物理场

1. 以微观粒子反应为数据基础。
2. 以EEDF和**反应速率**为桥梁
3. 兼顾**多物理场电离**机制

方程非线性、
程序收敛性、
实验-仿真结果一致性

反应体系 □ 碰撞截面数据与电子能量分布函数

氩气体系 Ars

- 1: e+Ar=>e+Ar *{eir1}*
- 2: e+Ar=>e+Ars *{eir2}*
- 3: e+Ars=>e+Ar *{eir3}*
- 4: e+Ar=>2e+Ar+ *{eir4}*
- 5: e+Ars=>2e+Ar+ *{eir5}*

CF_4 体系

- 1: CF4: Attachment: e+CF4=>F2+CF2- *{eir1}*
- 2: CF4: Elastic: e+CF4=>e+CF4 *{eir2}*
- 3: CF4: Excitation--0.08 eV: e+CF4=>e+CF4l *{eir3}*
- 4: CF4: Excitation--0.17 eV: e+CF4=>e+CF4m *{eir4}*
- 5: CF4: Excitation--7.57 eV: e+CF4=>e+CF4n *{eir5}*
- 6: CF4: Excitation--12.7 eV: e+CF4=>e+CF4o *{eir6}*
- 7: CF4: Ionization: e+CF4=>2e+CF4+ *{eir7}*

甲烷CH4， 氯气Cl2, 二氧化碳CO2,
铜原子Cu， 氟F2, 氢气H2, 氯化氢HCl
氦气He, 汞蒸汽Hg, 氪Kr
六氟化硫SF6,
硅烷SiH4
氙气Xe

以及上述气体的混合气体。
目前最多可做到100个离子反应方程的
二元、三元气体放电

O_2 体系

- 6: e+O2=>e+O2 *{eir6}*
- 7: e+O2=>O+O- *{eir7}*
- 8: e+O2=>e+O2 *{eir8}*
- 9: e+O2=>e+O2 *{eir9}*
- 10: e+O2=>e+O2 *{eir10}*
- 11: e+O2=>e+O2 *{eir11}*
- 12: e+O2=>e+O2 *{eir12}*
- 13: e+O2=>e+O2 *{eir13}*
- 14: e+O2=>e+O2 *{eir14}*
- 15: e+O2=>e+O2a1d *{eir15}*
- 16: e+O2a1d=>e+O2 *{eir16}*
- 17: e+O2=>e+O2b1s *{eir17}*
- 18: e+O2b1s=>e+O2 *{eir18}*
- 19: e+O2=>e+O245 *{eir19}*
- 20: e+O245=>e+O2 *{eir20}*
- 21: e+O2=>e+O+O *{eir21}*
- 22: e+O2=>e+O+O1d *{eir22}*
- 23: e+O2=>e+O+O1s *{eir23}*
- 24: e+O2=>2e+O2+ *{eir24}*

N_2 体系

- 8: N2: Elastic: e+N2=>e+N2 *{eir8}*
- 9. N2_Excitation_0.02 eV--e+N2=e+N2rot *{eir9}*
- 10. N2_Excitation_0.29 eV--e+N2=e+N2v1res_ *{eir10}*
- 11. N2 Excitation--0.291 eV e+N2=e+N2v1 *{eir11}*
- 12 N2 Excitation--0.59 eV e+N2=e+N2v2 *{eir12}*
- 13 N2 Excitation--0.88 eV e+N2=e+N2v3 *{eir13}*
- 14 N2 Excitation--1.17 eV e+N2=e+N2v4 *{eir14}*
- 15 N2 Excitation--1.47 eV e+N2=e+N2v5 *{eir15}*
- 16 N2 Excitation--1.76 eV e+N2=e+N2v6 *{eir16}*
- 17 N2 Excitation--1.76 eV e+N2=e+N2v7 *{eir17}*
- 18 N2 Excitation--2.35 eV e+N2=e+N2v8 *{eir18}*
- 19 N2 Excitation--6.17 eV e+N2=e+N2A3v0 *{eir19}*
- 20 N2 Excitation--7 eV e+N2=e+N2A3v59 *{eir20}*
- 21 N2 Excitation--7.35 eV e+N2=e+N2B3 *{eir21}*
- 22 N2 Excitation--7.36 eV e+N2=e+N2W3 *{eir22}*
- 23 N2 Excitation--7.8 eV e+N2=e+N2A3v10 *{eir23}*
- 24 N2 Excitation--8.16 eV e+N2=e+N2B32 *{eir24}*
- 25 N2 Excitation--8.4 eV e+N2=e+N2A1 *{eir25}*
- 26 N2 Excitation--8.55 eV e+N2=e+N2A12 *{eir26}*
- 27 N2 Excitation--8.89 eV e+N2=e+N2W12 *{eir27}*
- 28 N2 Excitation--11.03 eV e+N2=e+N2C3 *{eir28}*
- 29 N2 Excitation--11.87 eV e+N2=e+N2E3 *{eir29}*
- 30 N2 Excitation--12.25 eV e+N2=e+N2A13 *{eir30}*
- ***31 N2 Excitation--13.00 eV e+N2=e+N2SUM *{eir31}*
- 32: N2 Ionization--15.6 eV e+N2=>2e+N2+ *{eir32}*

1 等离子体案例

深圳技术大学

反应速率k^f □ 碰撞截面数据 □ 电子能量分布函数

- 微观影响宏观的使者
- 宏观影响微观的媒介

$$k^f = \gamma \int_0^\infty \epsilon \sigma_k(\epsilon) f(\epsilon) d\epsilon$$

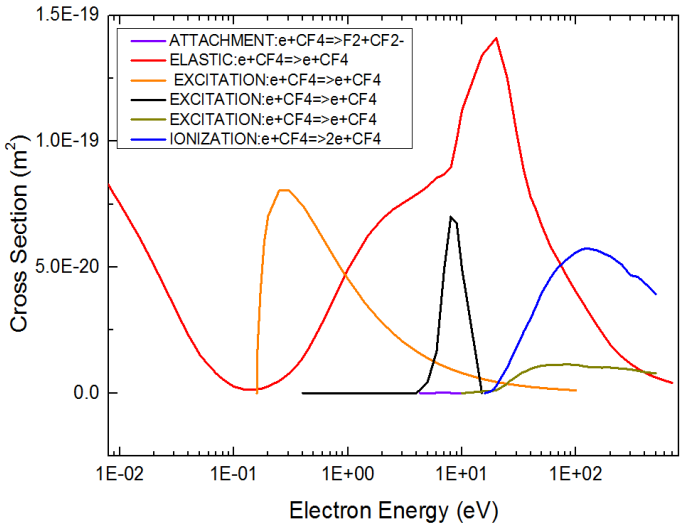
碰撞截面

EEDF

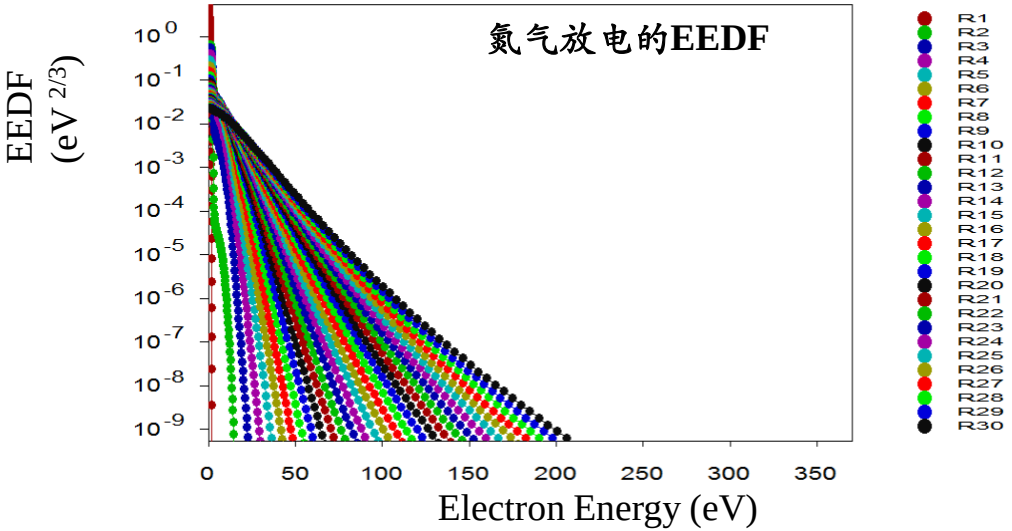
Boltzmann
Maxwellian
Druyvesteyn
Generalized

离子反应速率k^f的四种计算方式

1. 阿伦尼乌斯
2. 常数直接给出
3. 汤森系数或其他插值函数
4. 碰撞截面与EEDF



https://fr.lxcat.net/data/set_type.php

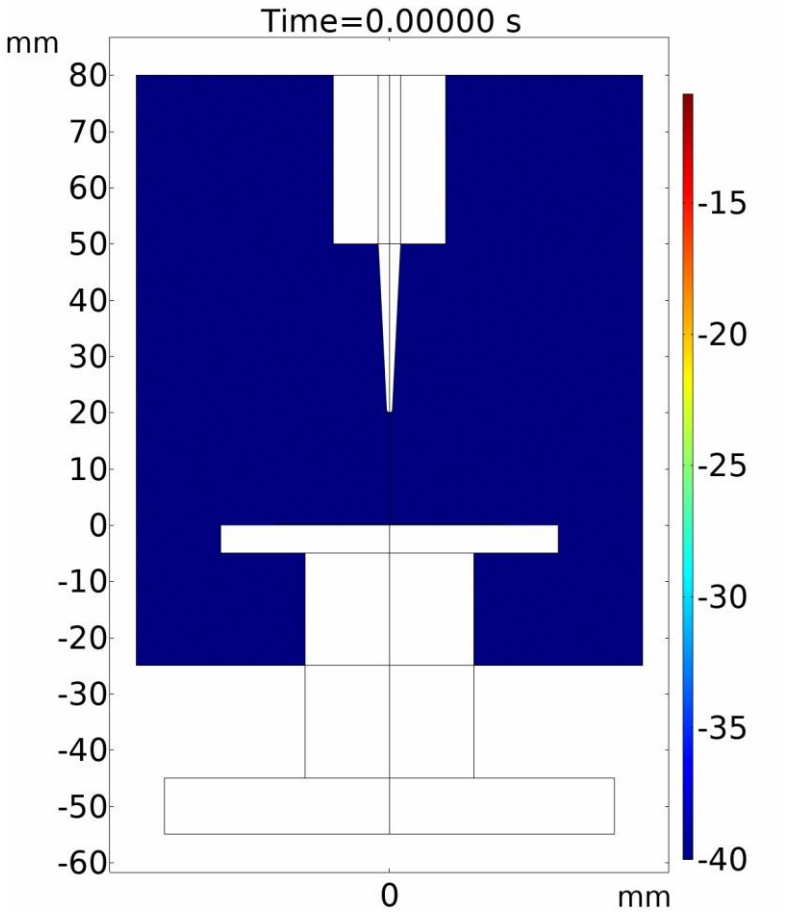


BOLSIG+
Download: https://www.bolsig.laplace.univ-tlse.fr/

1 等离子体案例

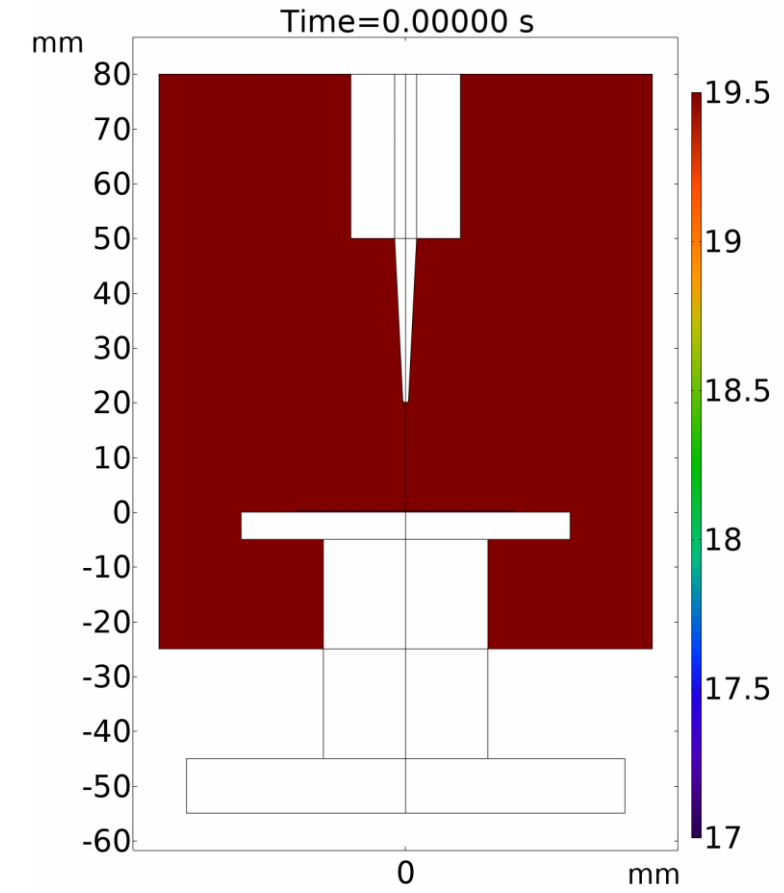
深圳技术大学





$e + N_2 \rightarrow 2e + N_2^+ \ (15.6\ eV)$

电离反应速率(mol/s/m³)对数

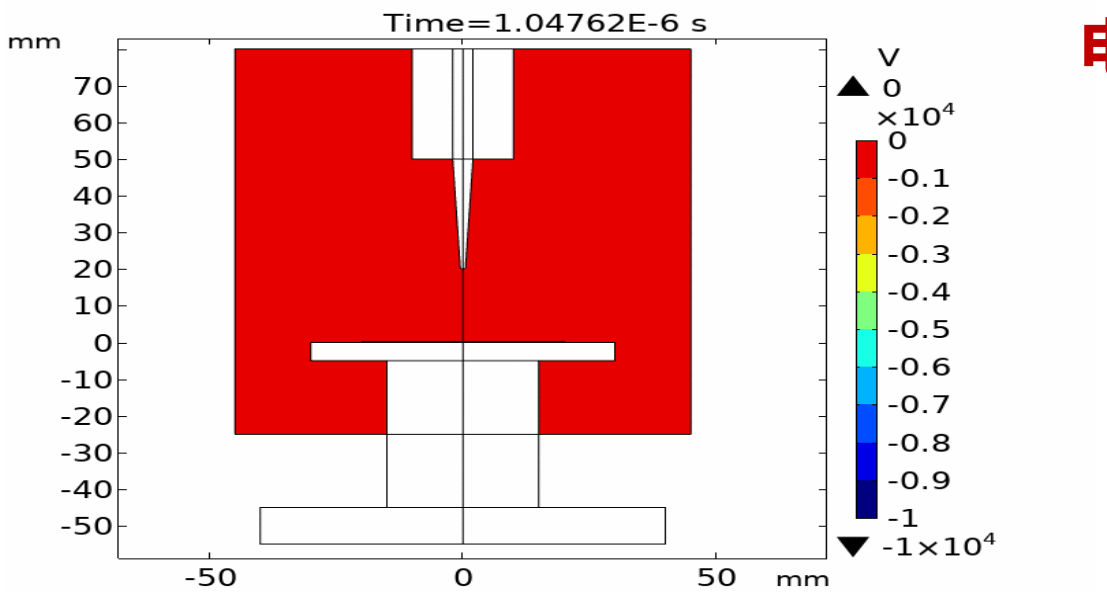


电子数量浓度(1/m³)对数

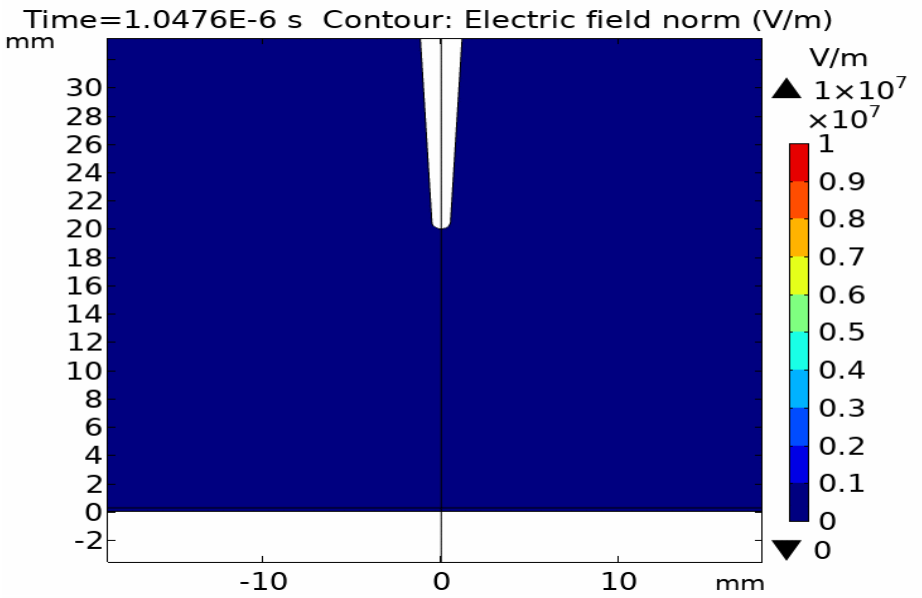
1 等离子体案例

深圳技术大学

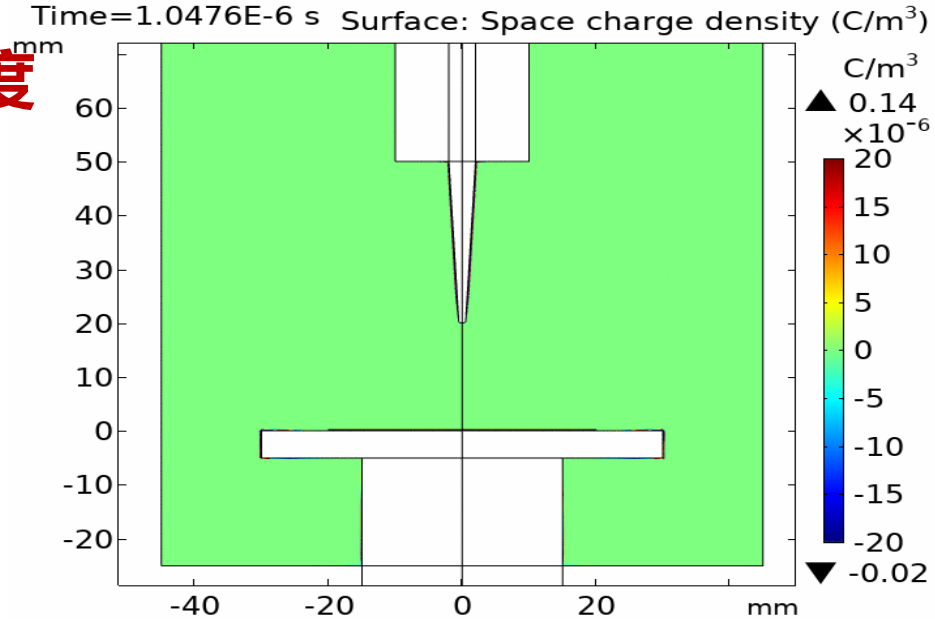
电势



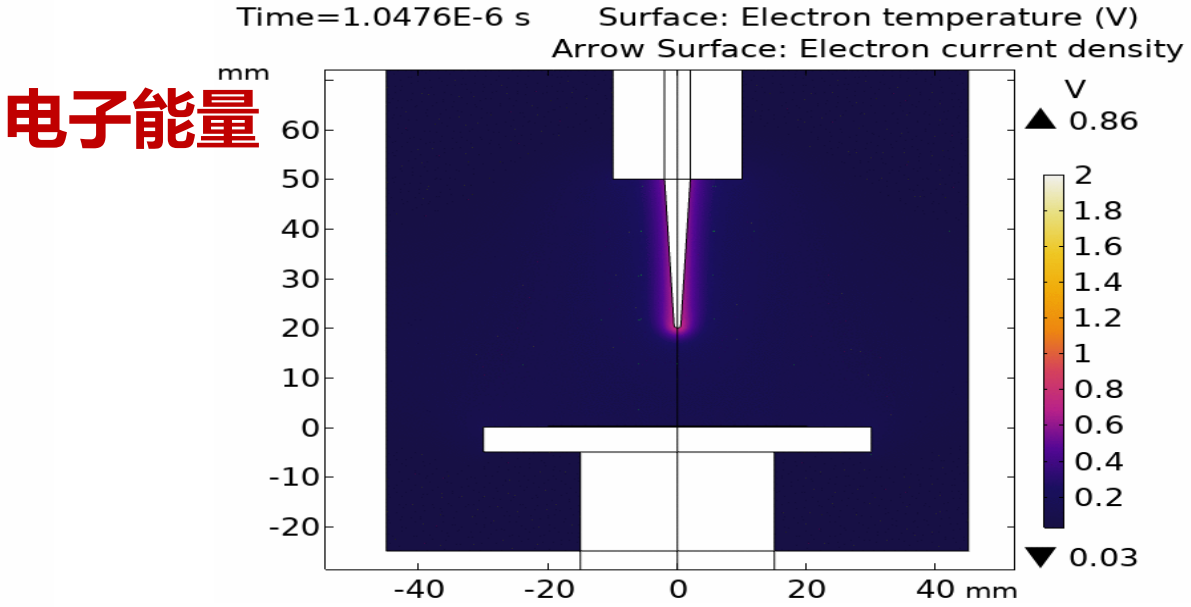
电场



电荷密度

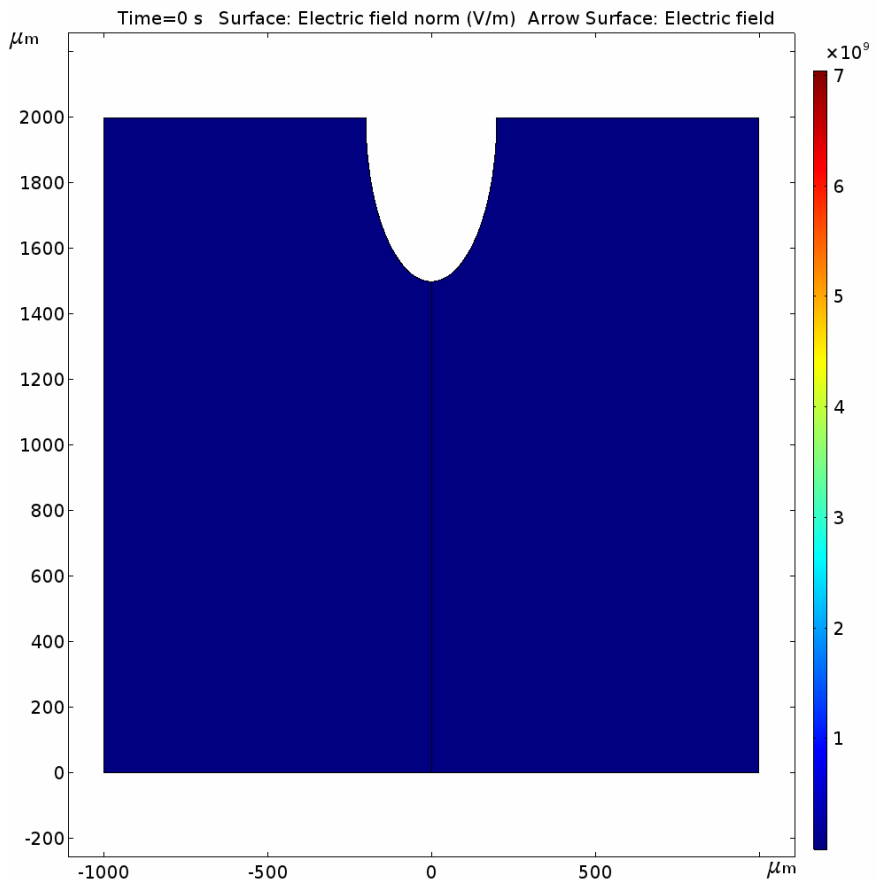


电子能量

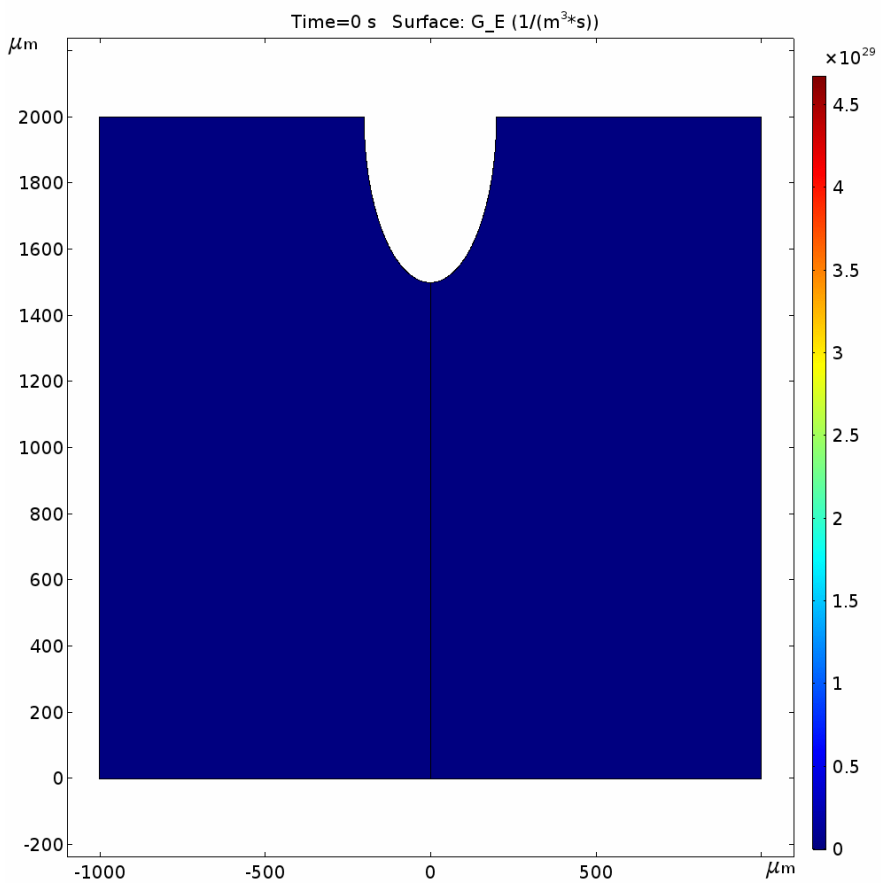


引入光子浓度辅助变量计算光电离速率

电场(V/m)

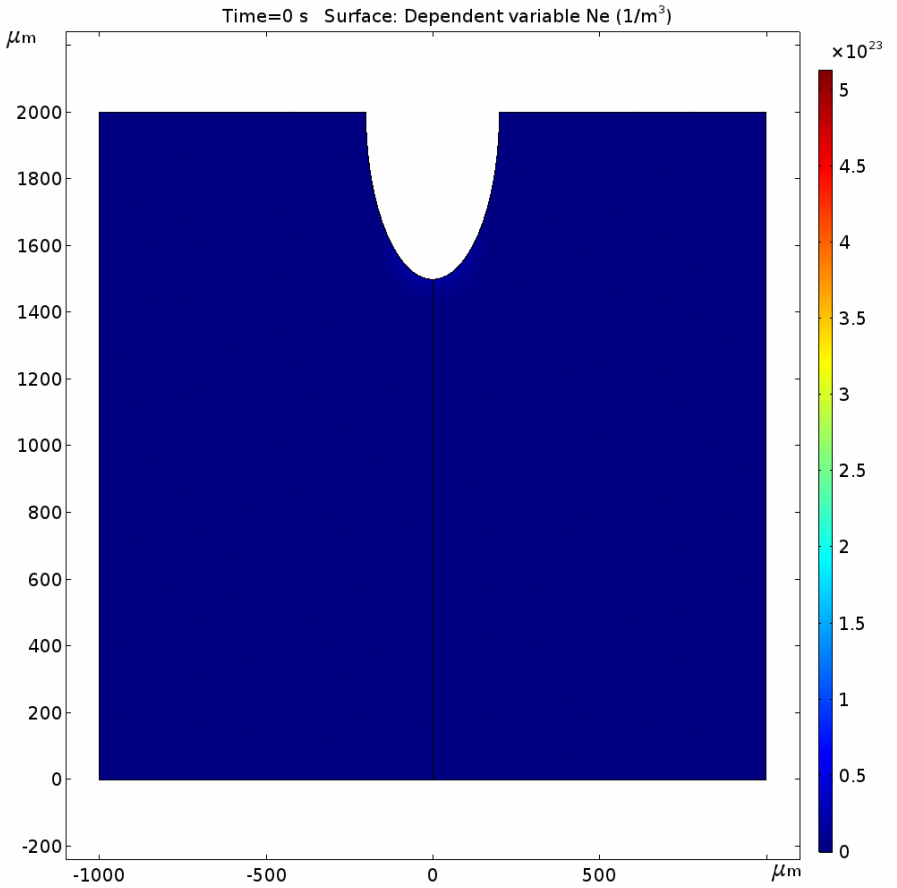


光电子产生速率（1/s/m^3)

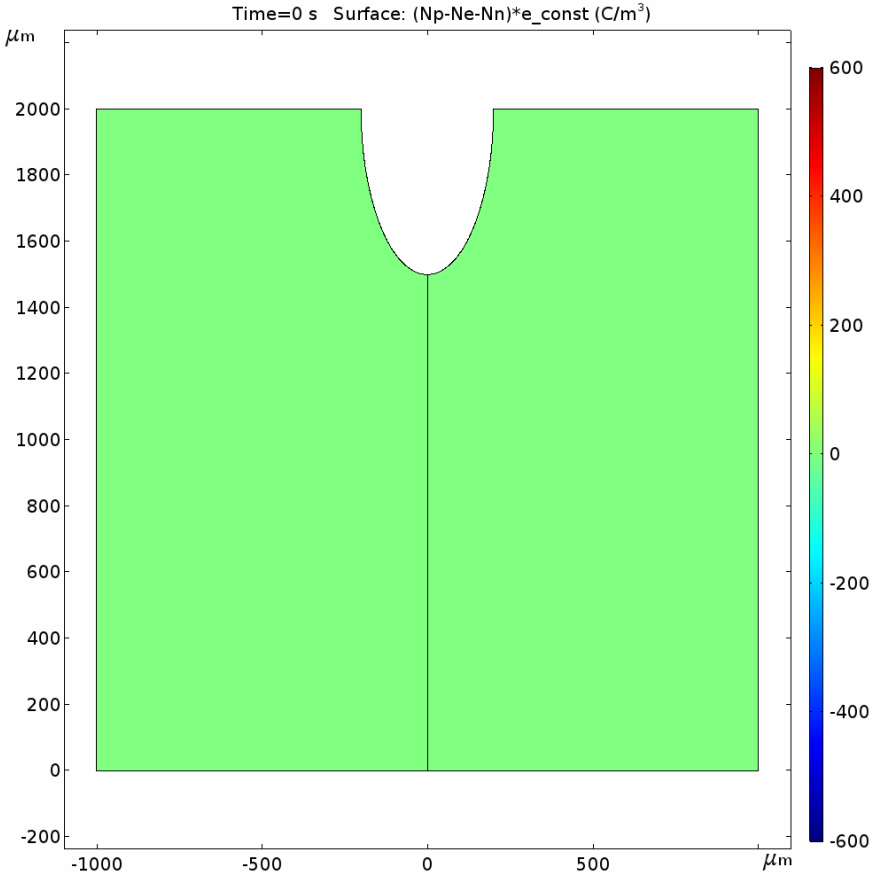


引入光子浓度辅助变量计算光电离速率

电子数量密度(1/ m^3)

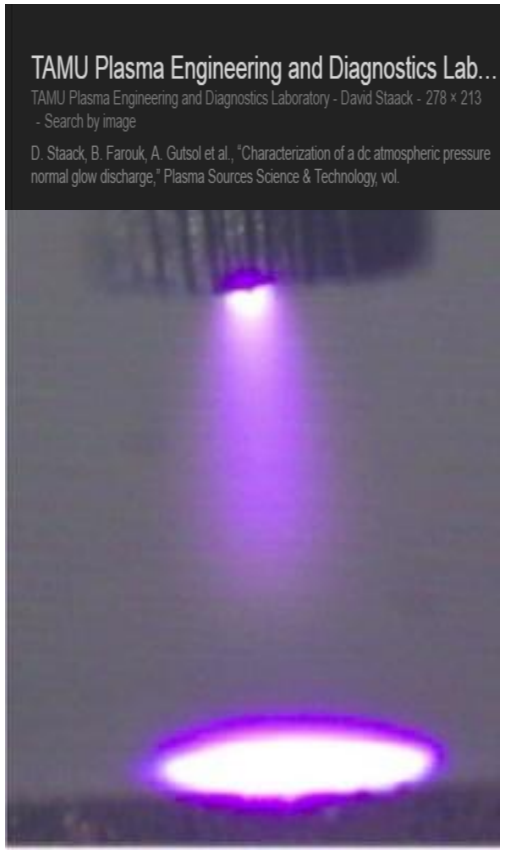


空间电荷密度（C/m^3)

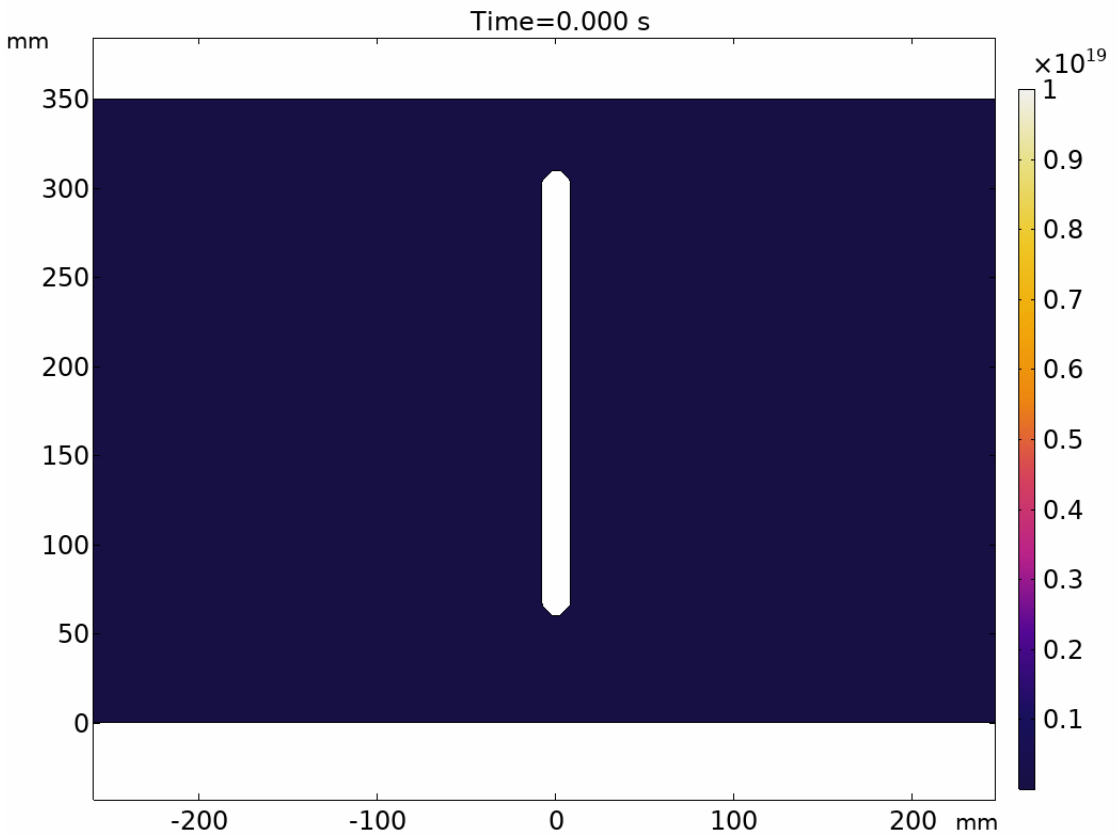


基于实验数据训练模型参数

- 1: e+Ar=>e+Ar
- 2: e+Ar=>e+Ars
- 3: e+Ars=>e+Ar
- 4: e+Ar=>2e+Ar+
- 5: e+Ars=>2e+Ar+
- 6: e+O2=>e+O2
- 7: e+O2=>O+O-
- 8: e+O2=>e+O2
- 9: e+O2=>e+O2
- 10: e+O2=>e+O2
- 11: e+O2=>e+O2
- 12: e+O2=>e+O2
- 13: e+O2=>e+O2
- 14: e+O2=>e+O2
- 15: e+O2=>e+O2a1d
- 16: e+O2a1d=>e+O2
- 17: e+O2=>e+O2b1s
- 18: e+O2b1s=>e+O2
- 19: e+O2=>e+O245
- 20: e+O245=>e+O2
- 21: e+O2=>e+O+O
- 22: e+O2=>e+O+O1d
- 23: e+O2=>e+O+O1s
- 24: e+O2=>2e+O2+
- Species: e
- Species: Ar
- ****MC****Species: Ars
- ****EC****Species: Ar+
- ****MF****Species: O2

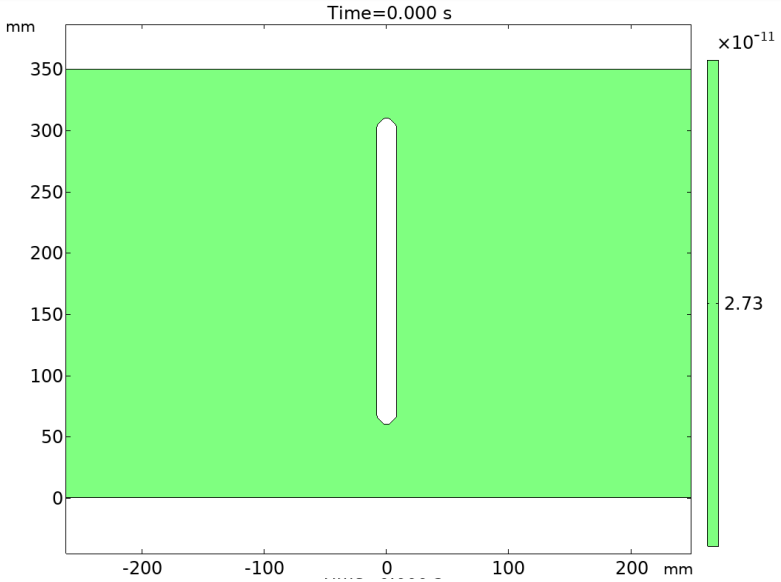


电子数量浓度($1/m^3$)

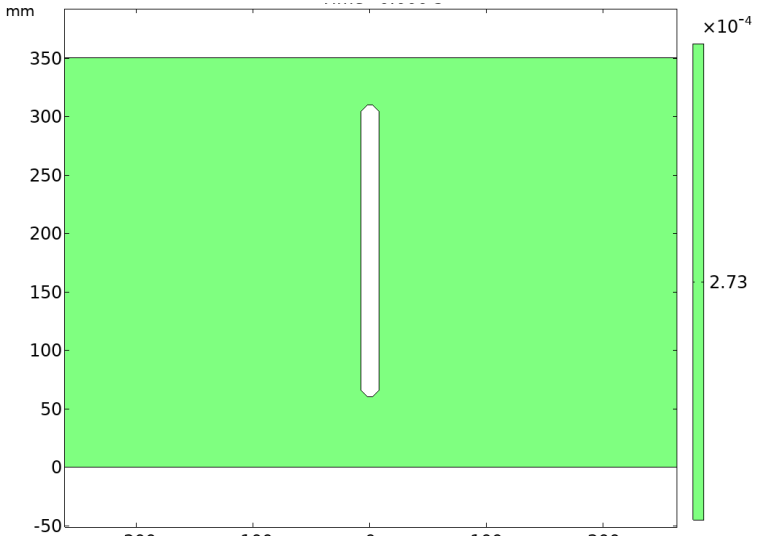


二次电子发射

O^-浓度 (mol/m^3)

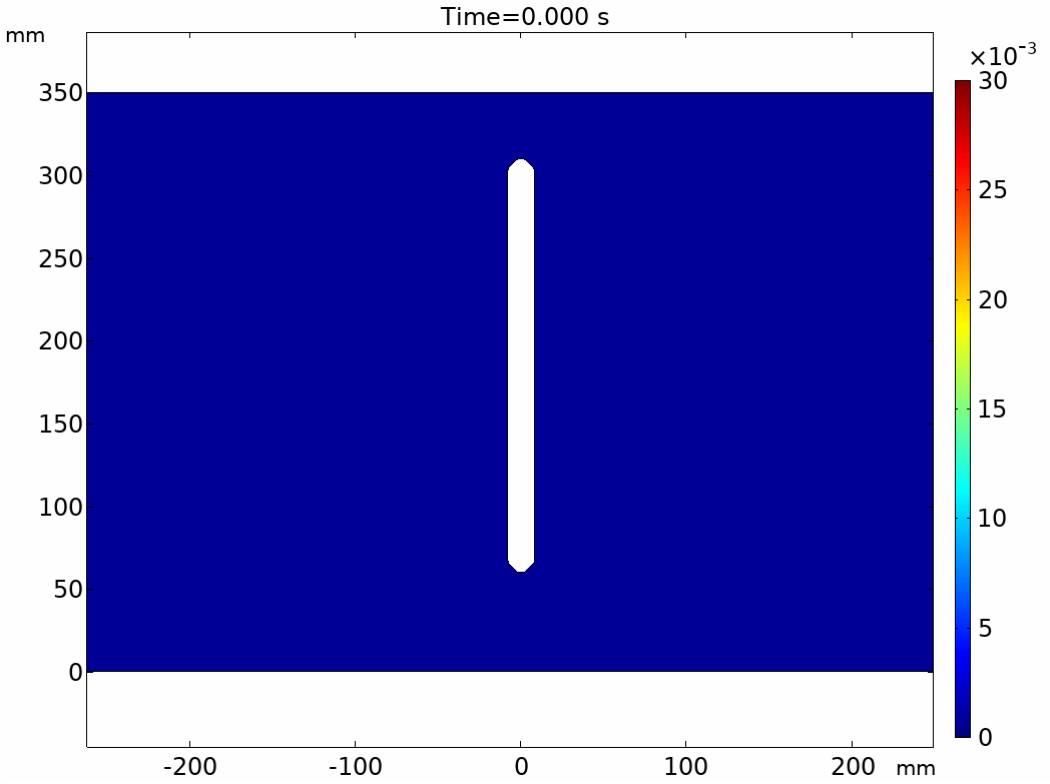


O_2浓度 (mol/m^3)



$e + Ar \rightarrow 2e + Ar^+ \ (15.6\ eV)$

电离反应速率($mol/s/m^3$)



能斯特-普朗克-泊松方程 □ 归一化

基本思想：

归一化正离子、负离子、电子；
半定性-半定量考虑产生、吸附、复合、中和等反应过程，
结合电场高斯定理，考虑了离子分布对空间电场的影响。

$$\frac{\partial N_e}{\partial t} + \nabla \cdot (-D_e \nabla N_e) + \beta_e \cdot \nabla N_e = f_e$$

$$\frac{\partial N_n}{\partial t} + \nabla \cdot (-D_n \nabla N_n) + \beta_n \cdot \nabla N_n = f_n$$

$$\frac{\partial N_p}{\partial t} + \nabla \cdot (-D_p \nabla N_p) + \beta_p \cdot \nabla N_p = f_p$$

$$\mathbf{E} = \nabla V$$

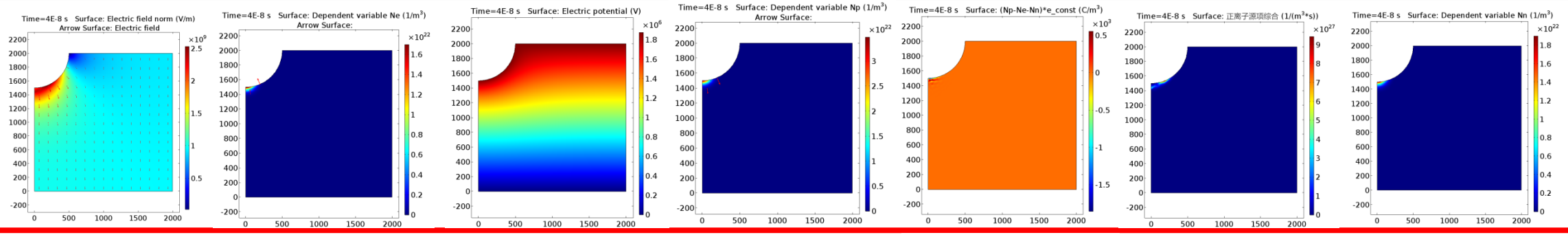
$$\nabla \cdot \nabla V = \frac{\rho_v}{\varepsilon_0}$$

$$\rho_v = e(N_p - N_e - N_n)$$

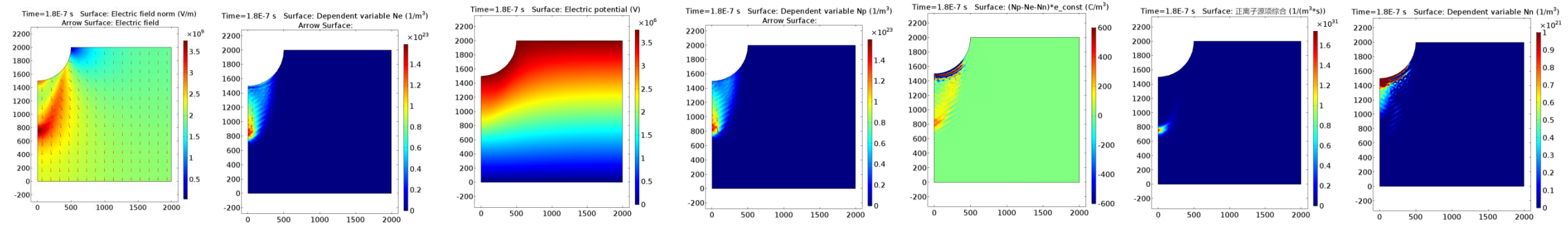
1 等离子体案例——PDE

流注放电　　口 能斯特-普朗克-泊松方程

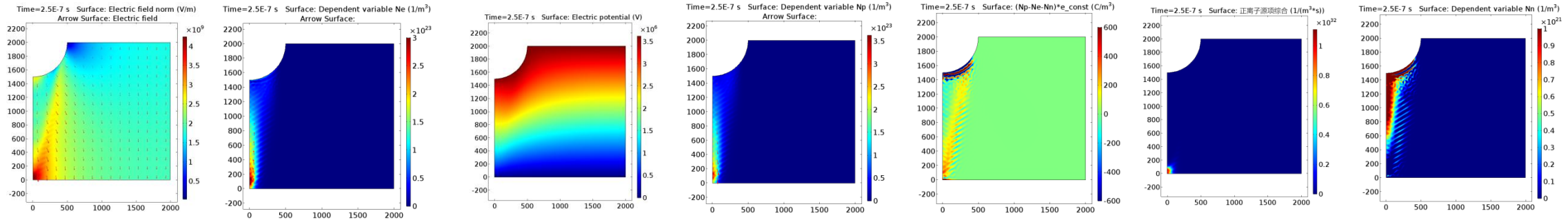
起晕



发展



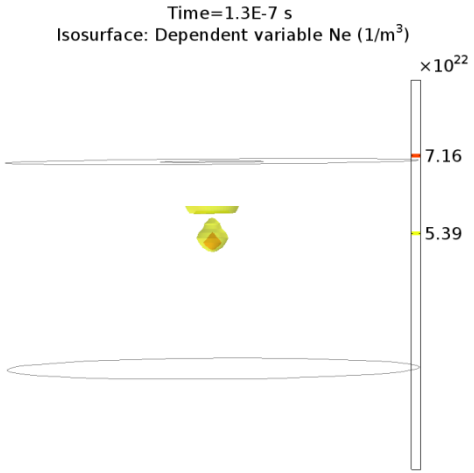
击穿

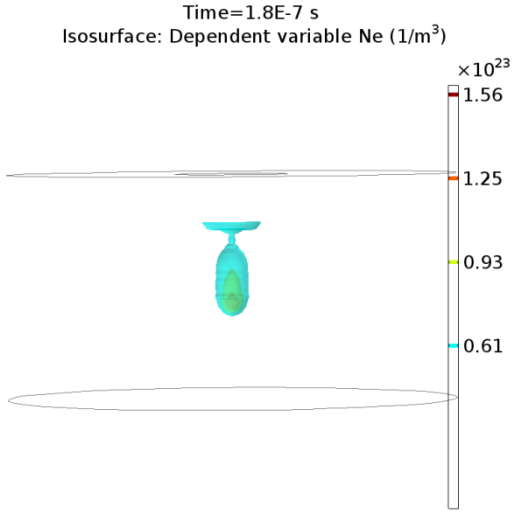


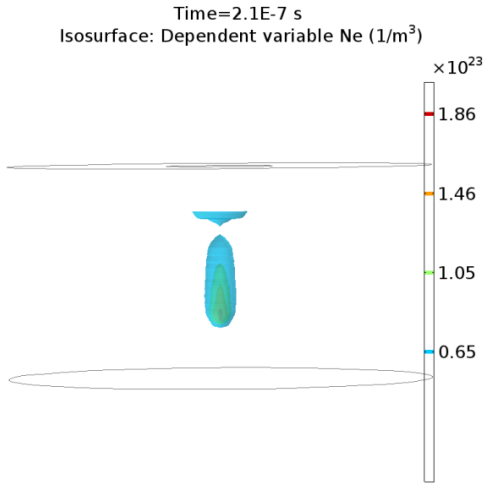
电场　　电子数量密度　　电势　　正离子数量密度　　空间电荷密度　　电离源项　　负离子数量密度

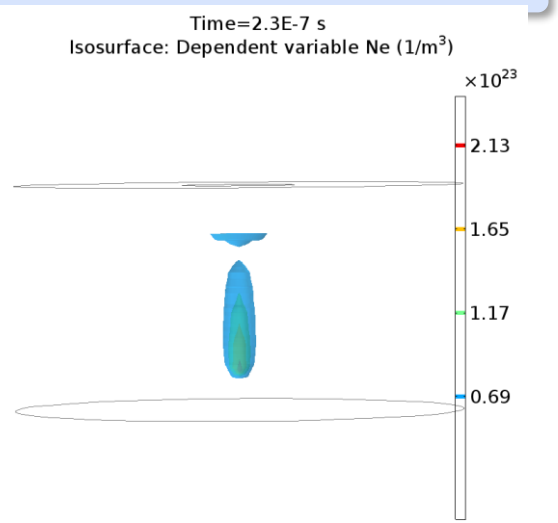
放电区域的形成发展和湮灭

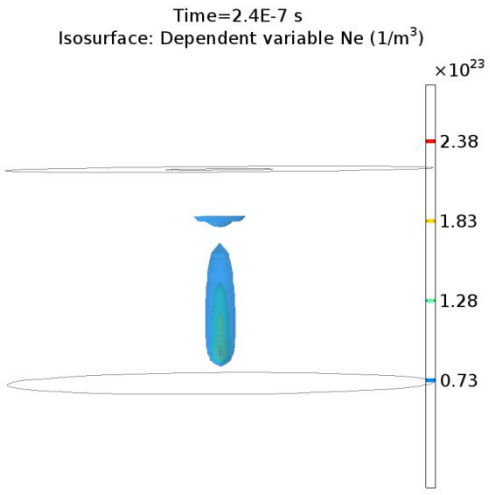
□ 能斯特-普朗克-泊松方程

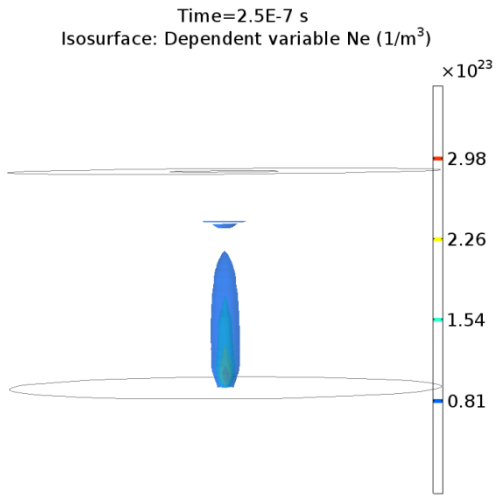


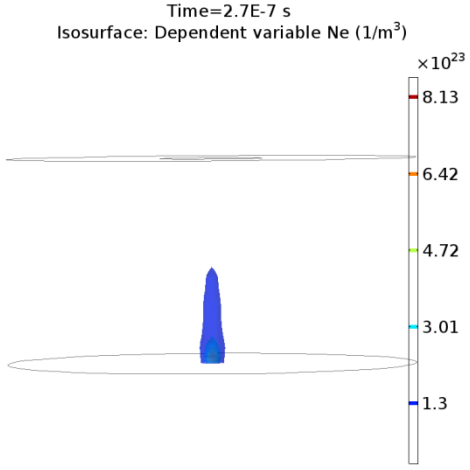


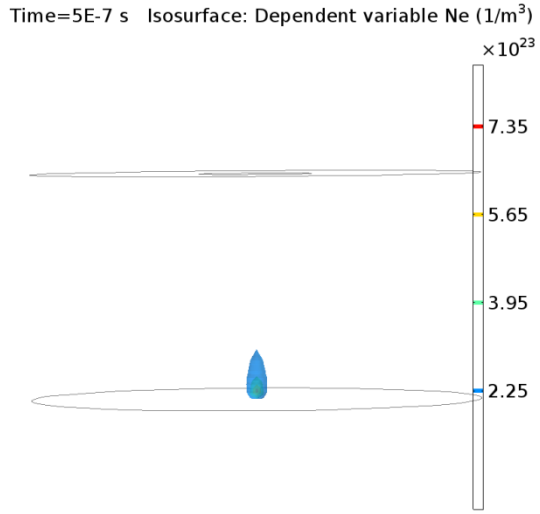






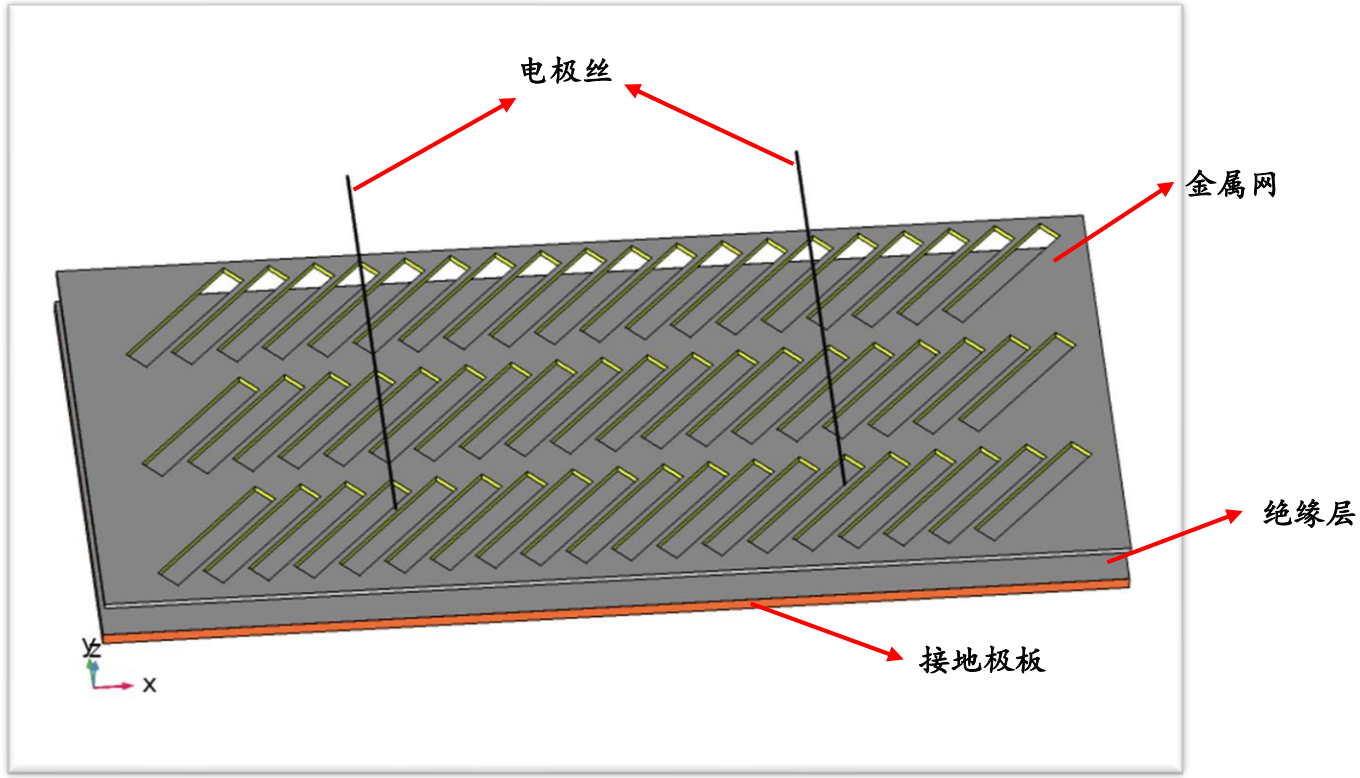


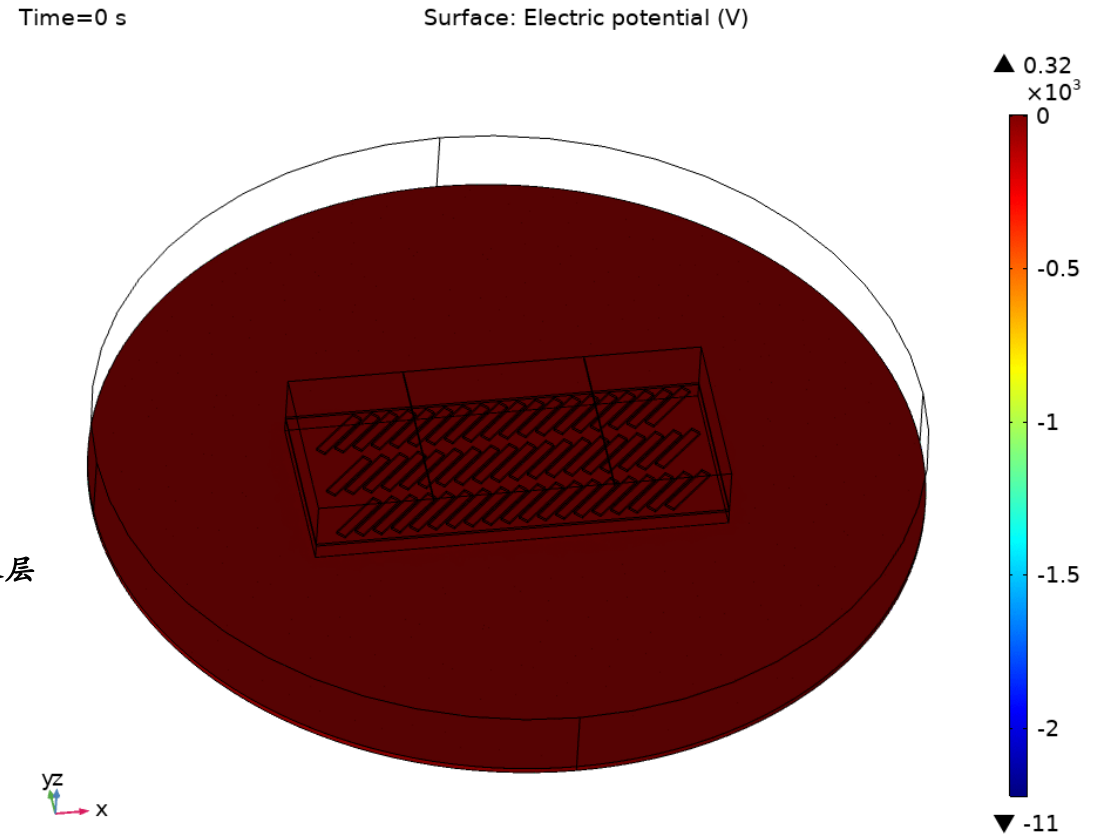




离子沉积加工过程模拟

几何结构

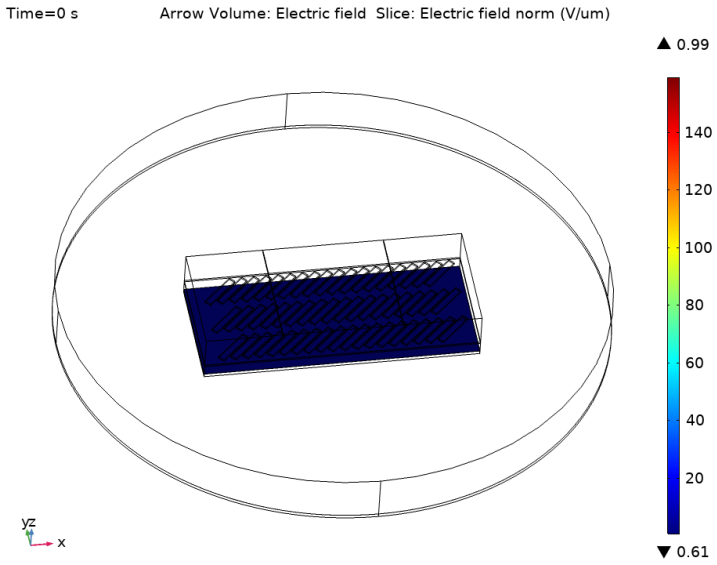




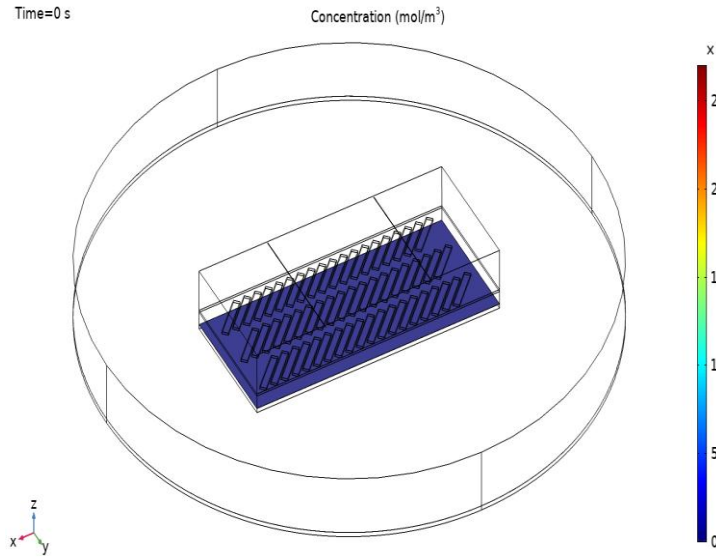
电势变化动图(0–100s)

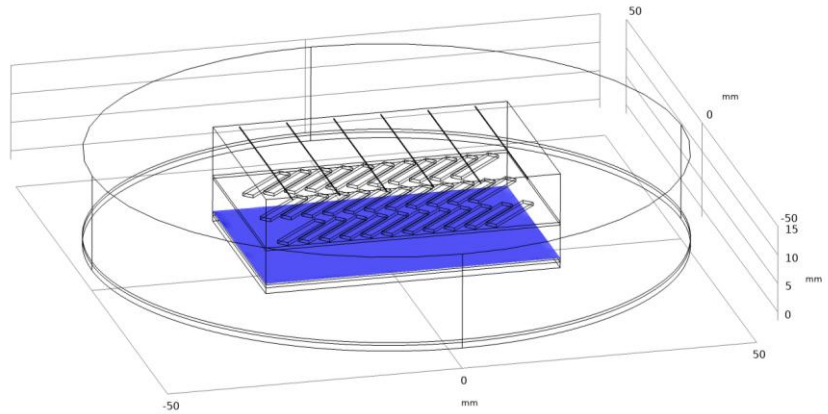
1 等离子体案例——PDE

深圳技术大学



电场变化动图(0-100s)

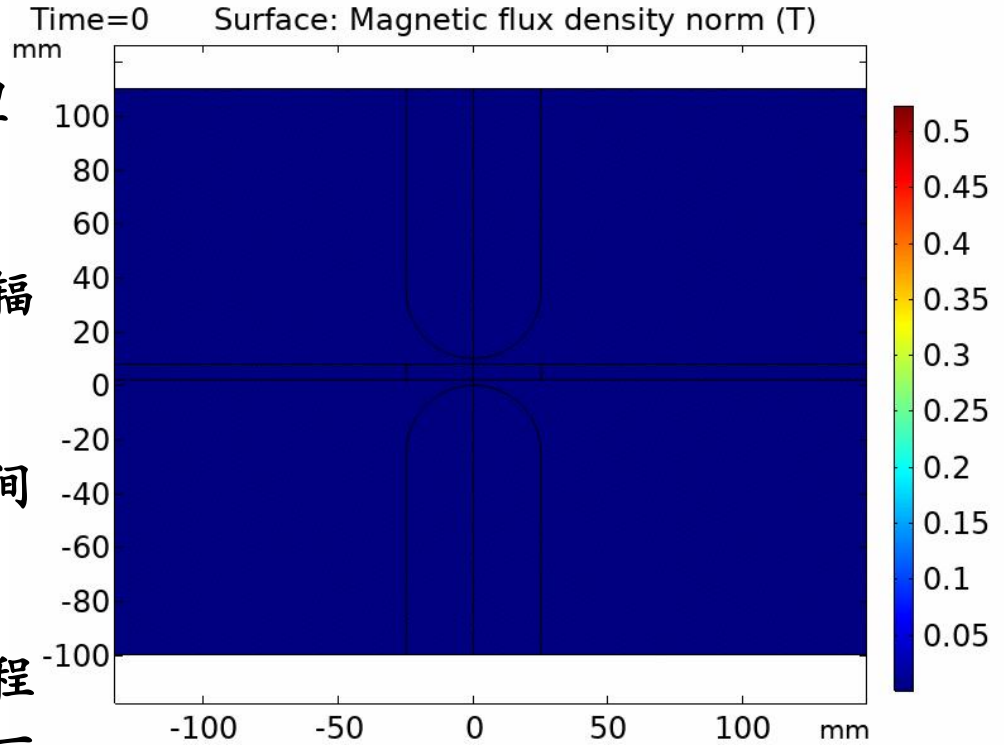


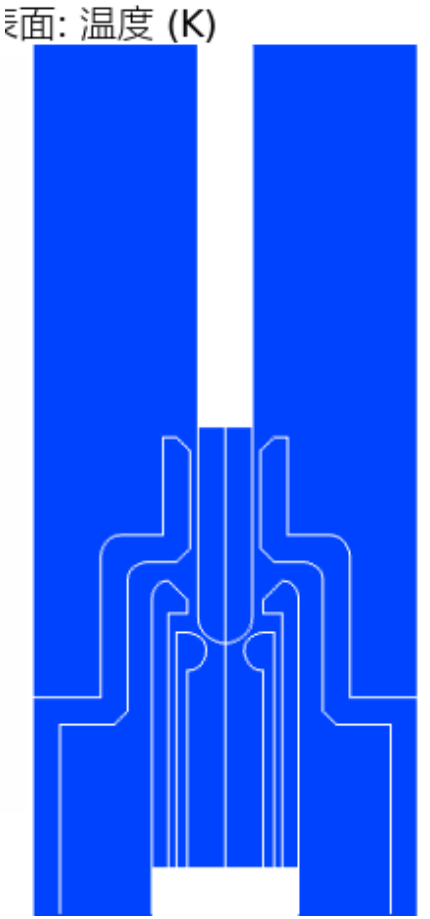


电子浓度动图(0-100s)

继电器分离过程电弧模拟

- 以温度表征等离子体的电离程度
- 基于MHD（Magnetohydrodynamics）理论
- 通过离子电导率-温度实验数据+温度电离辐射数据与实验建立联系
- 适用于等离子体已经形成、并且在一段时间内达到自持状态
- 或者适用于准自持放电问题：即，放电过程的某个阶段离子体系达到短时间的平衡。一般来说，这种假设适用于放电时间在几十微妙以上的问题。

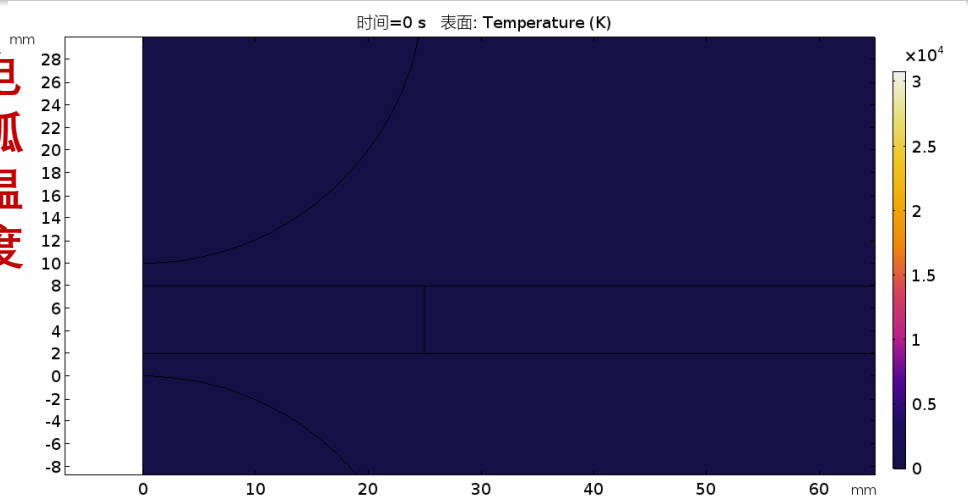




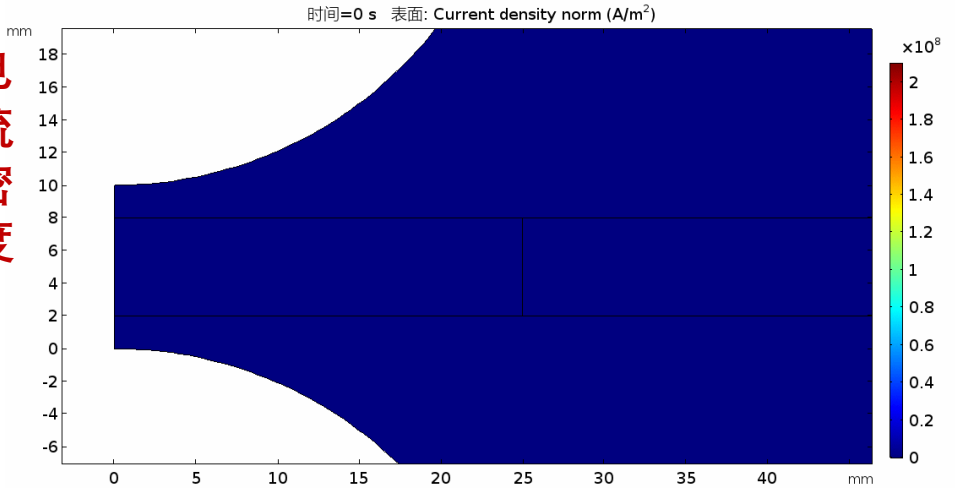
[1]P. F. a. E. P. Maher I. Boulos, Thermal Plasmas Fundamentals and Application-Volume-1. New York and London: Plenum Press, 1994.

继电器分离过程电弧模拟

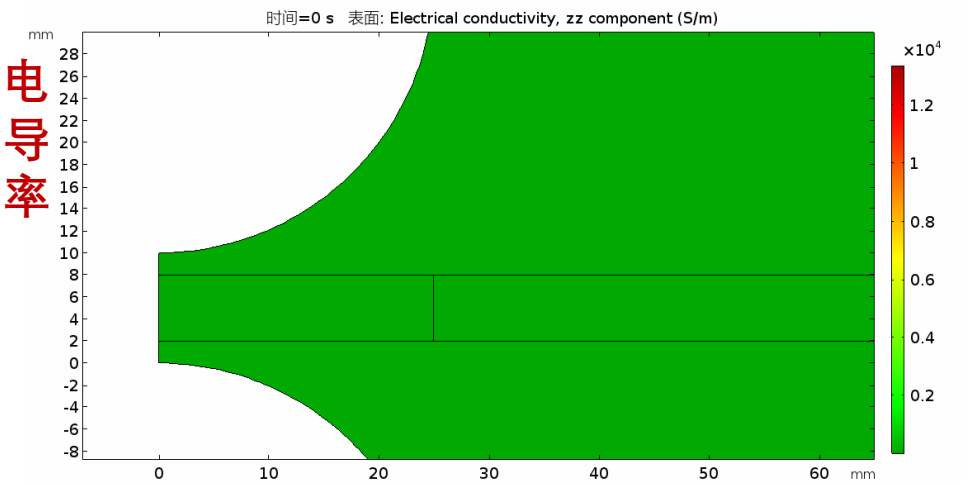
电弧温度



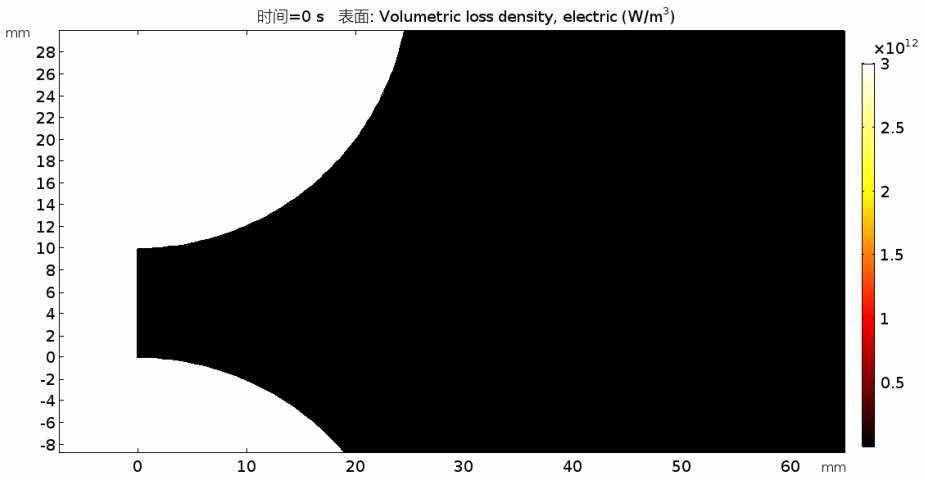
电流密度



电导率

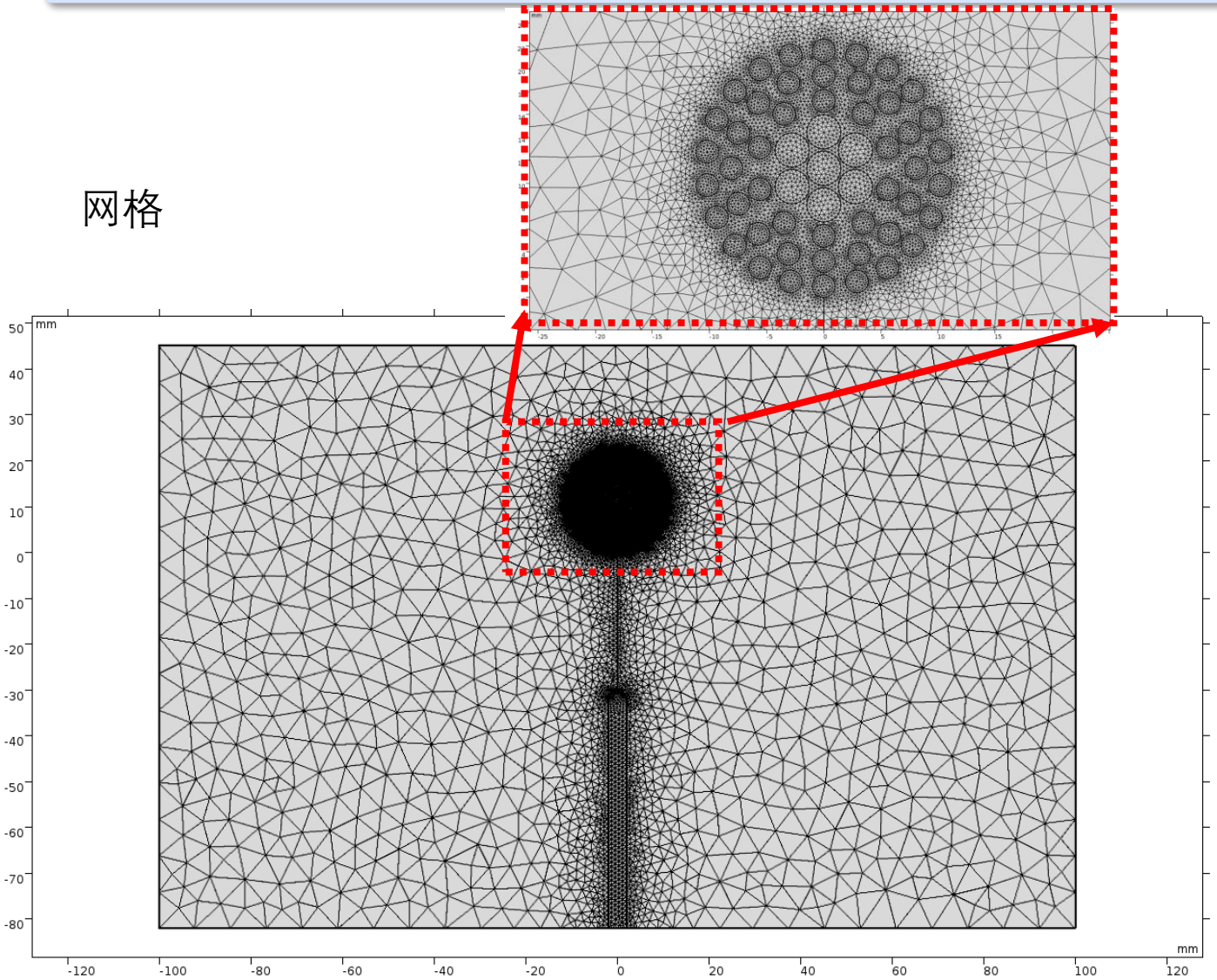


能量密度



模拟电弧对导线灼烧

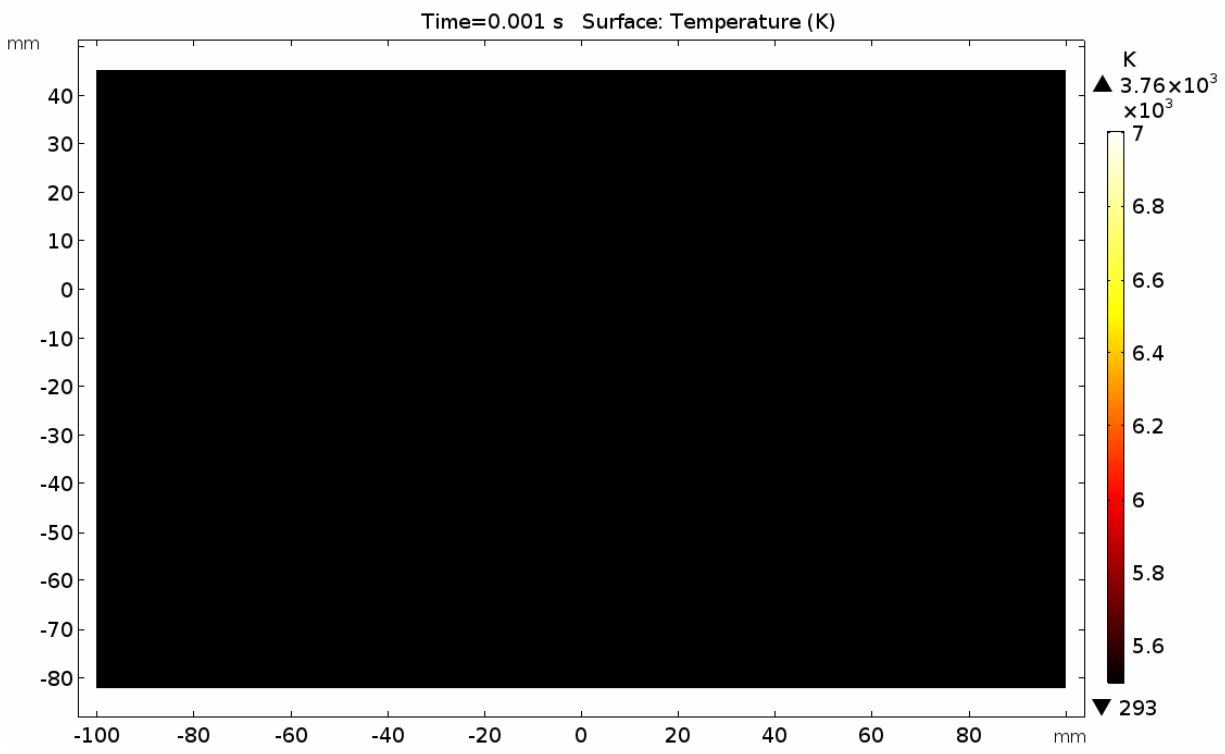
网格



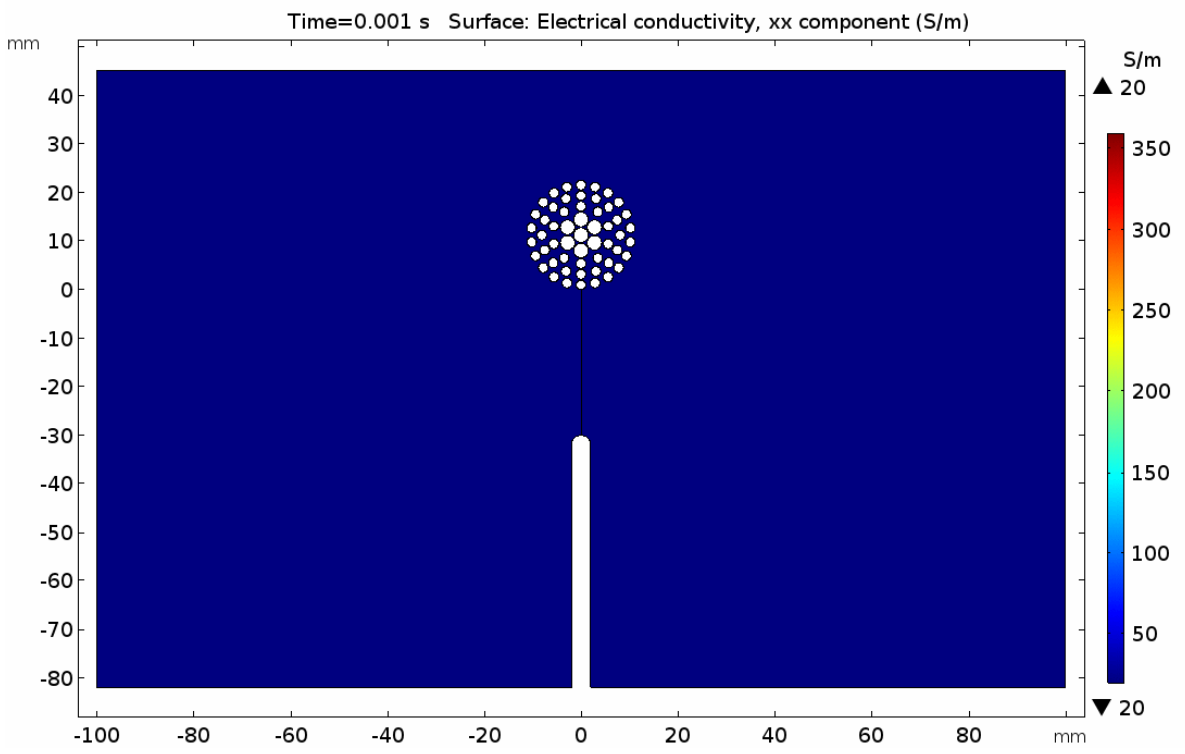
物理场

- Electric Currents *(ec)*
  - Current Conservation 1
  - Electric Insulation 1
  - Initial Values 1
  - 棒电极接地
  - Terminal 1
- Heat Transfer in Fluids *(ht)*
  - Fluid 1
  - Initial Values 1
  - Thermal Insulation 1
  - Solid 1
  - 竖直对流
  - Heat Flux 2
  - Heat Flux 3
- Multiphysics
  - Equilibrium Discharge Heat Source 1 *(phs1)*
  - Temperature Coupling 1 *(tc1)*
  - Equilibrium Discharge Boundary Heat Source 1 *(bphs1)*

1 (准）平衡态等离子体仿真



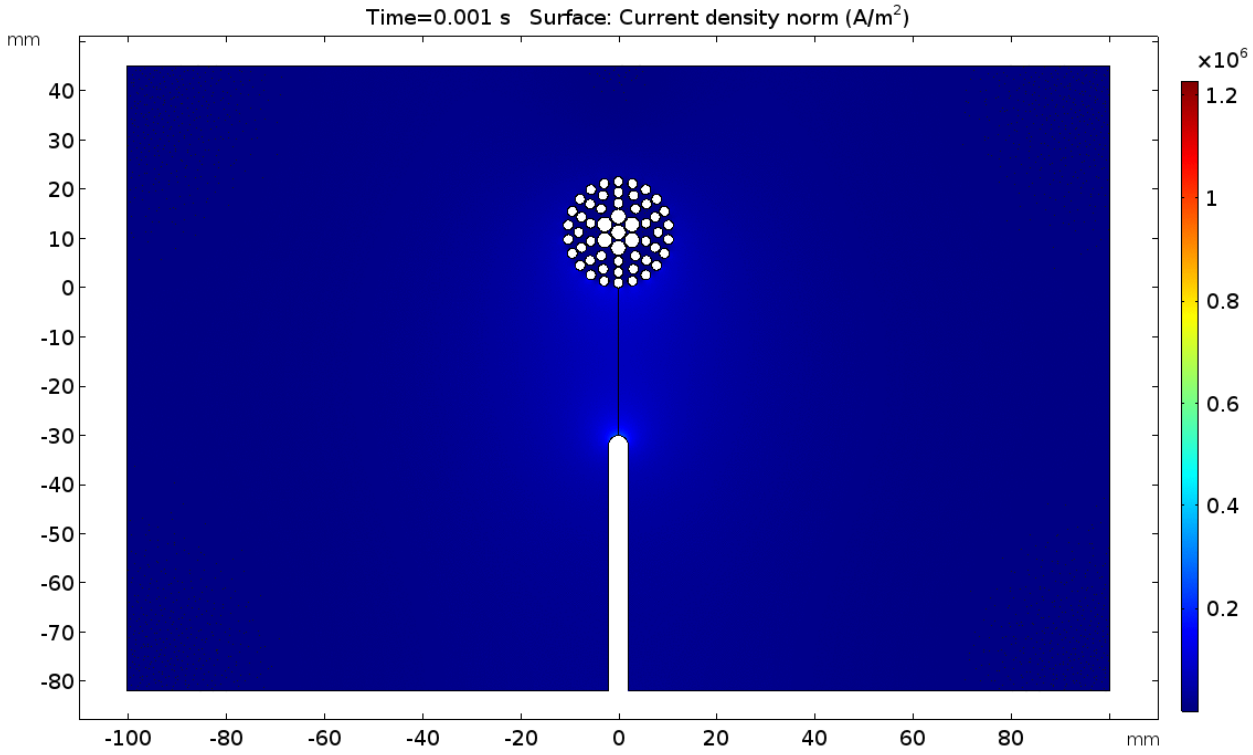
温度



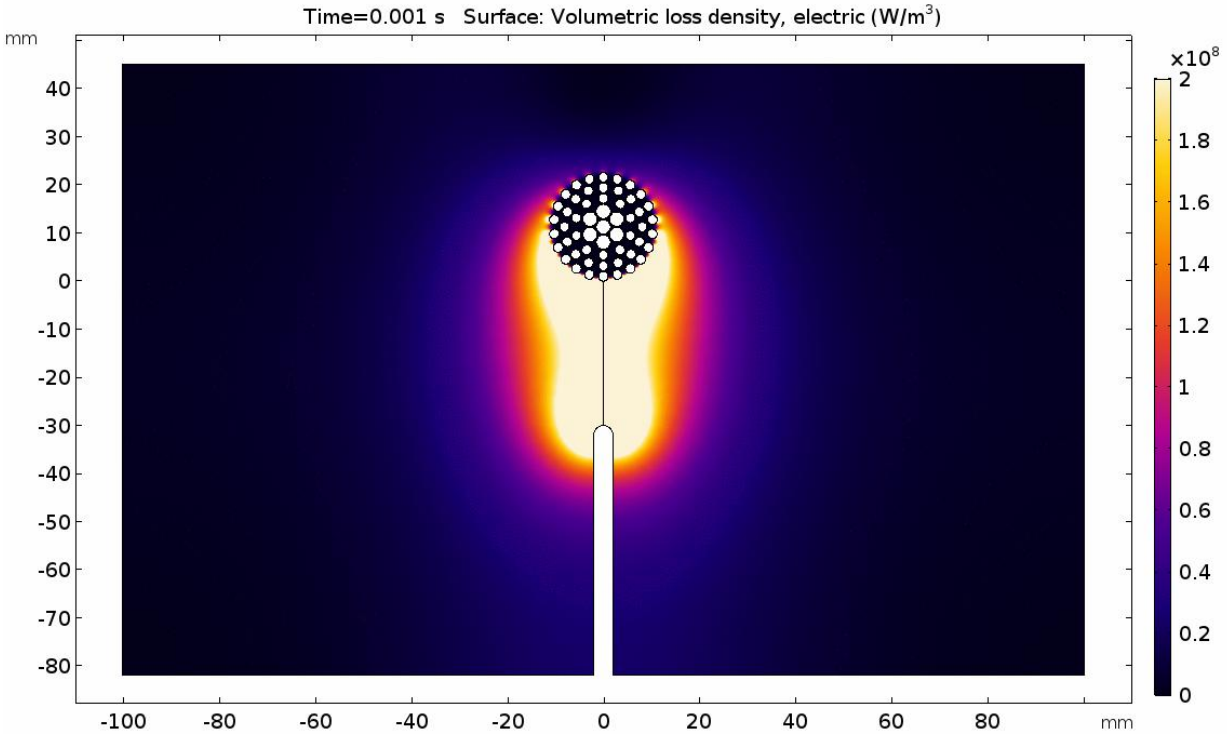
电导率

1 (准）平衡态等离子体仿真

深圳技术大学



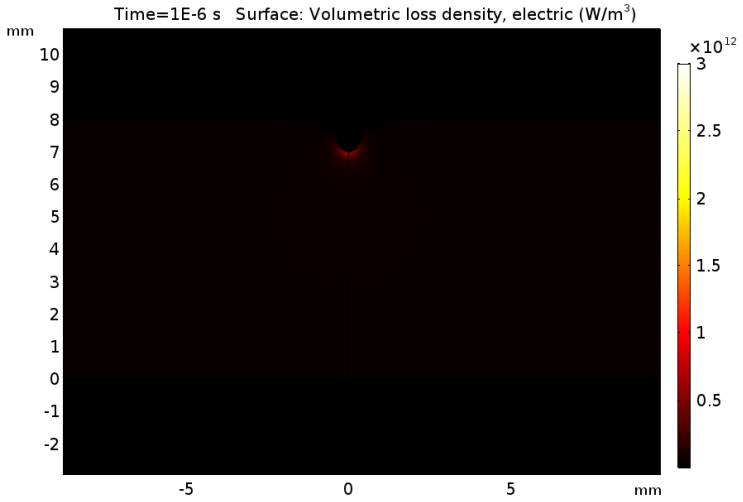
电流密度

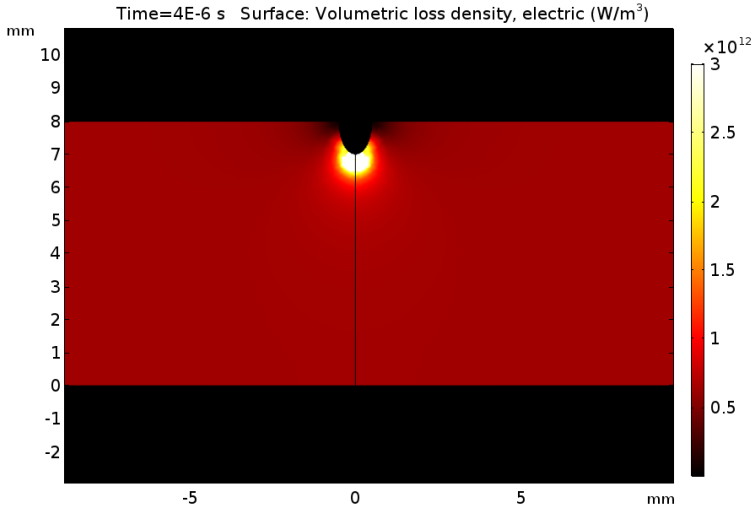


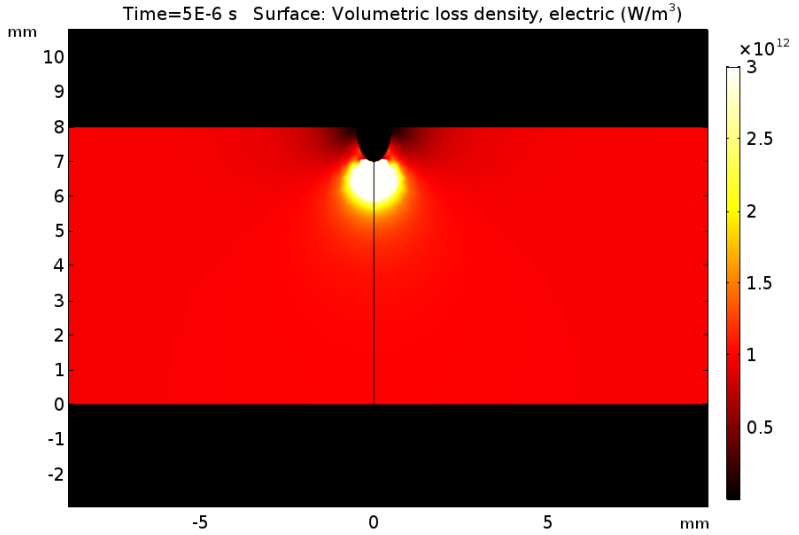
发热量

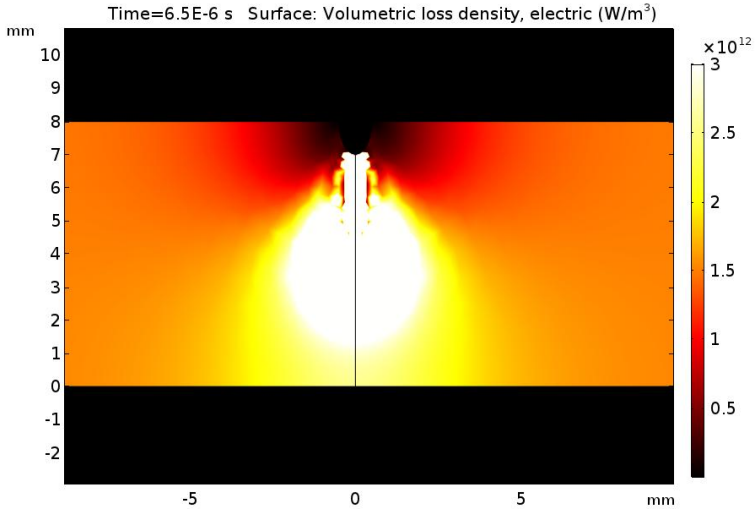
基于平衡态等离子体理论的流注放电过程模拟

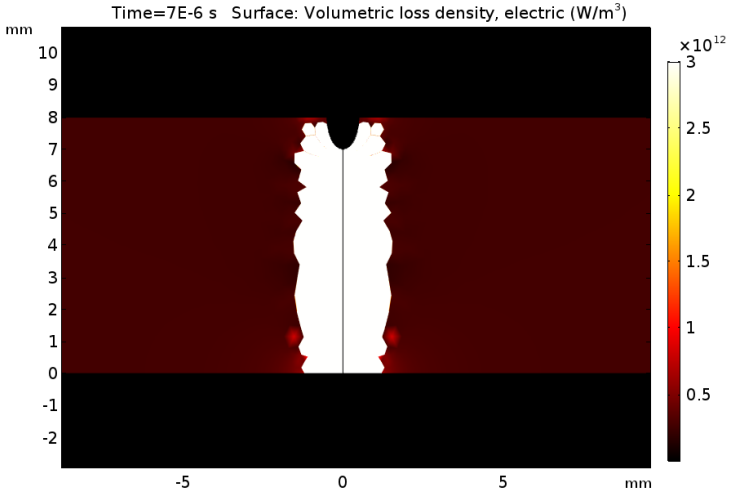
口 能量密度

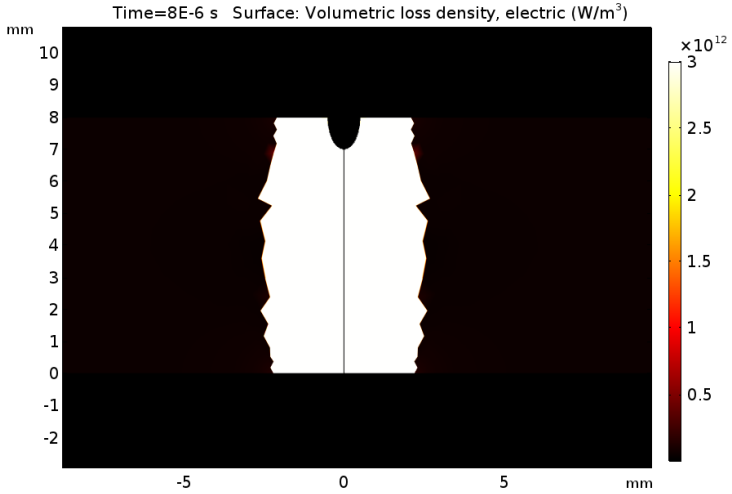






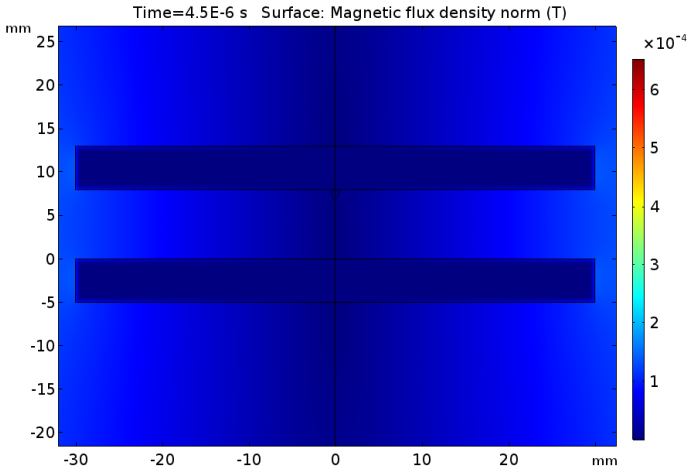


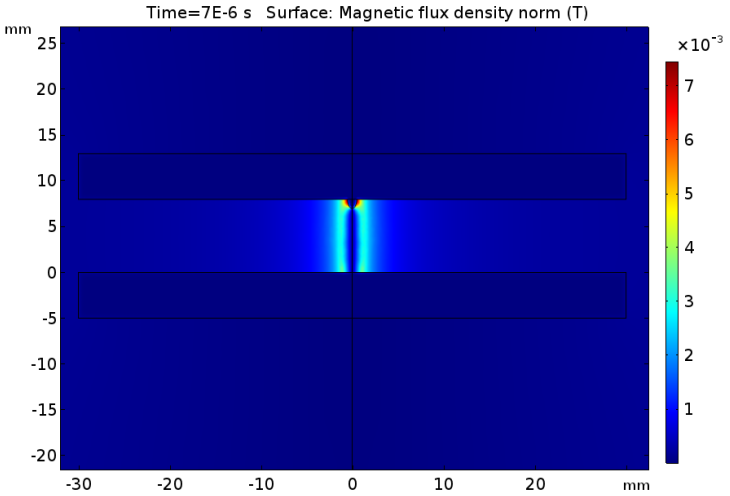


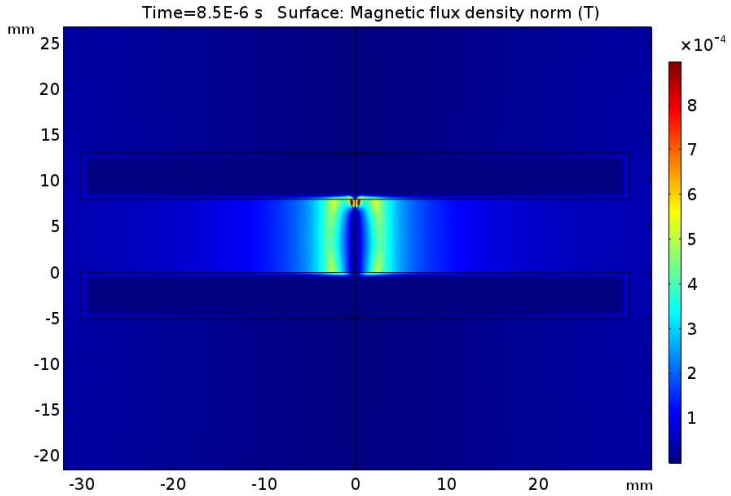


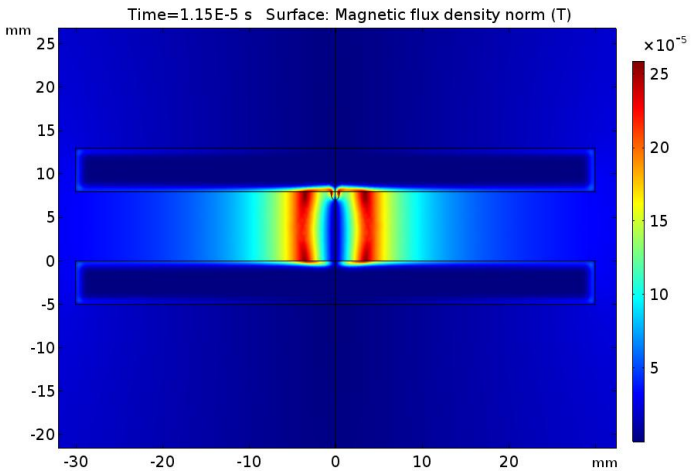
基于平衡态等离子体理论的流注放电过程模拟

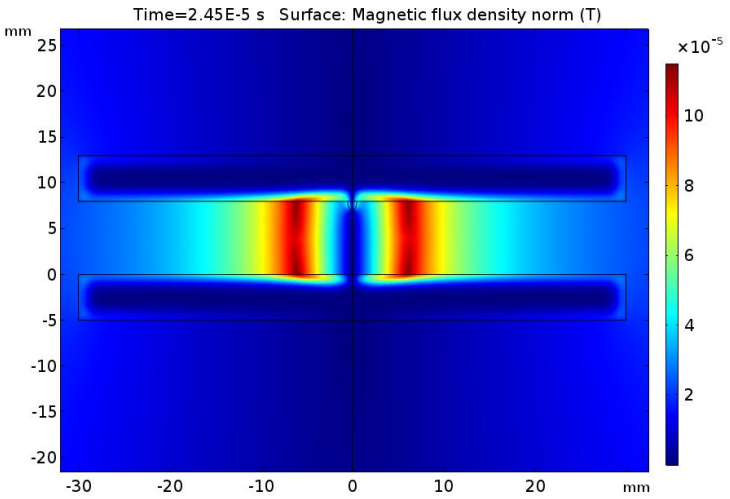
口 磁场

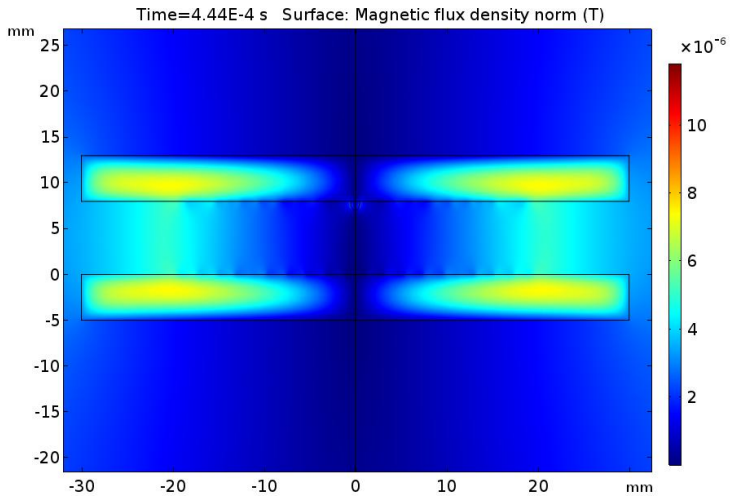






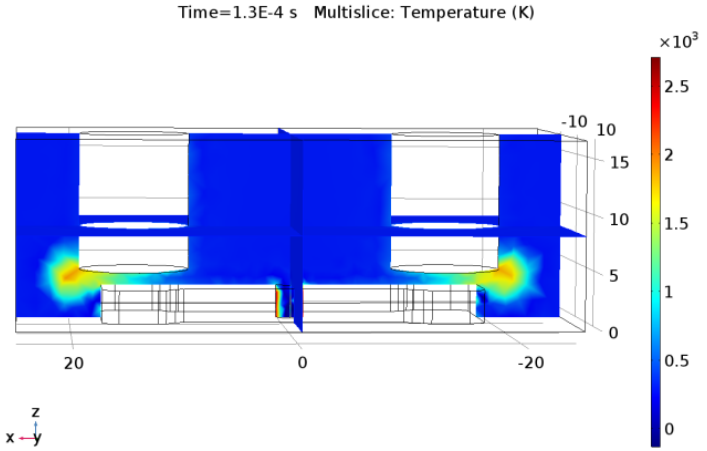


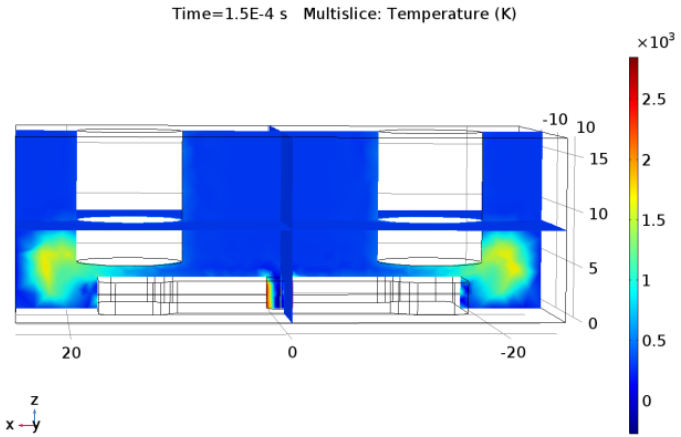


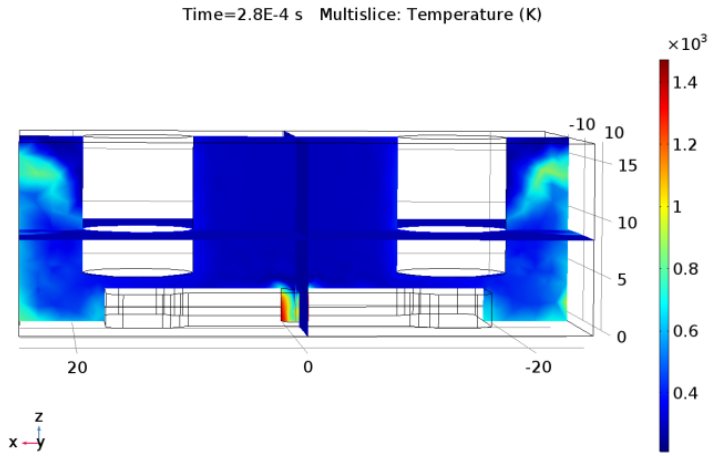


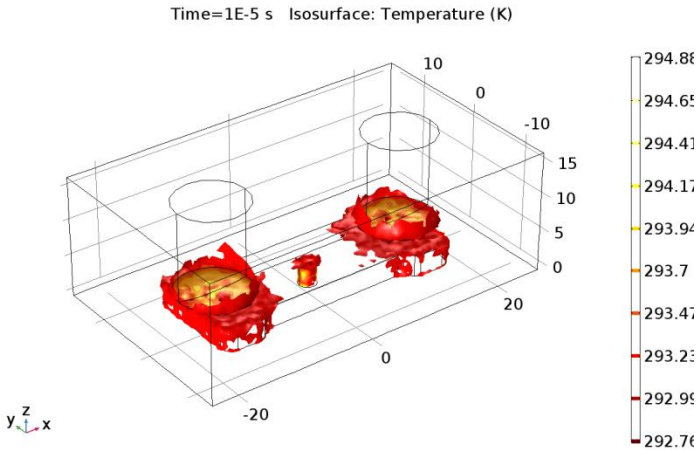
（准）平衡态等离子体仿真

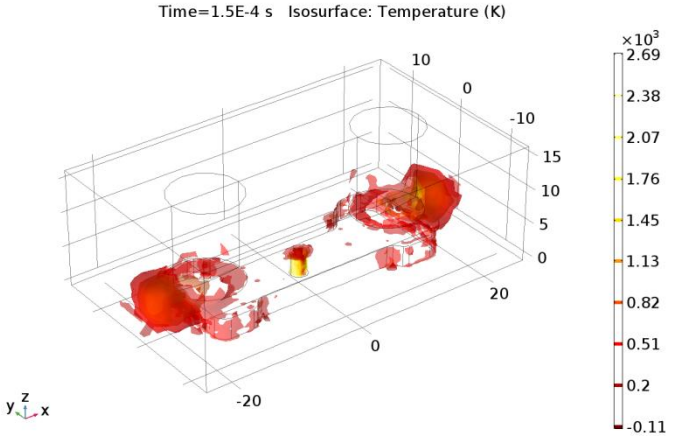
磁控灭弧

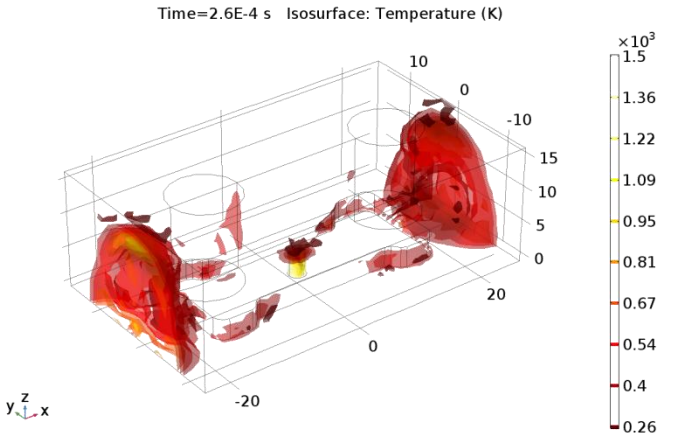






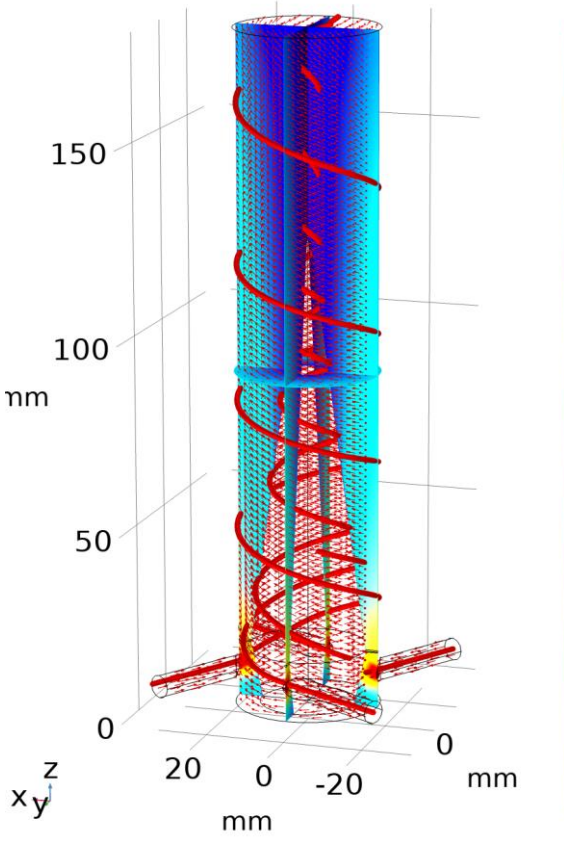




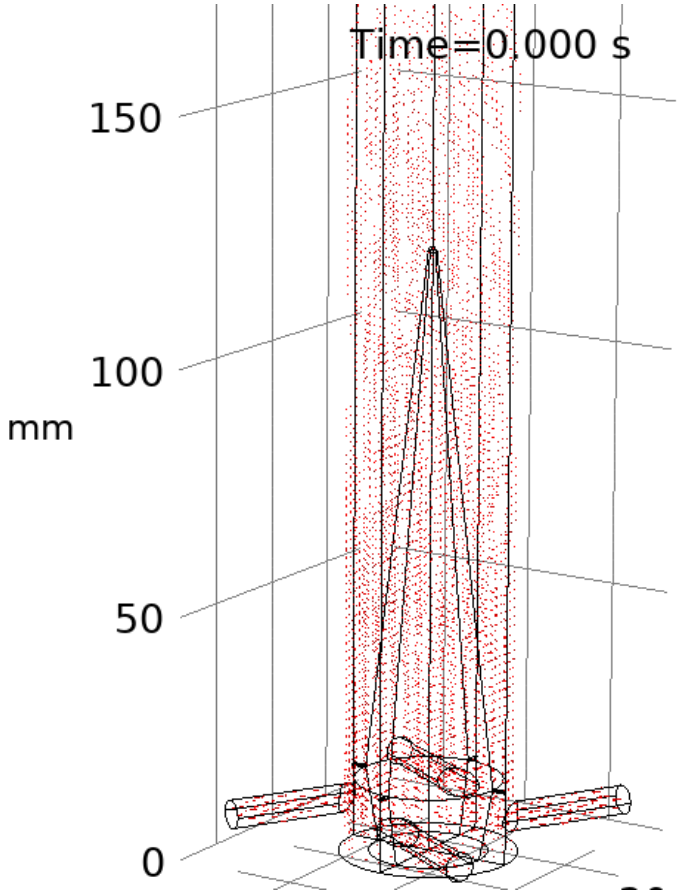


模拟高速流体中棒-筒电极中的电弧滑移过程

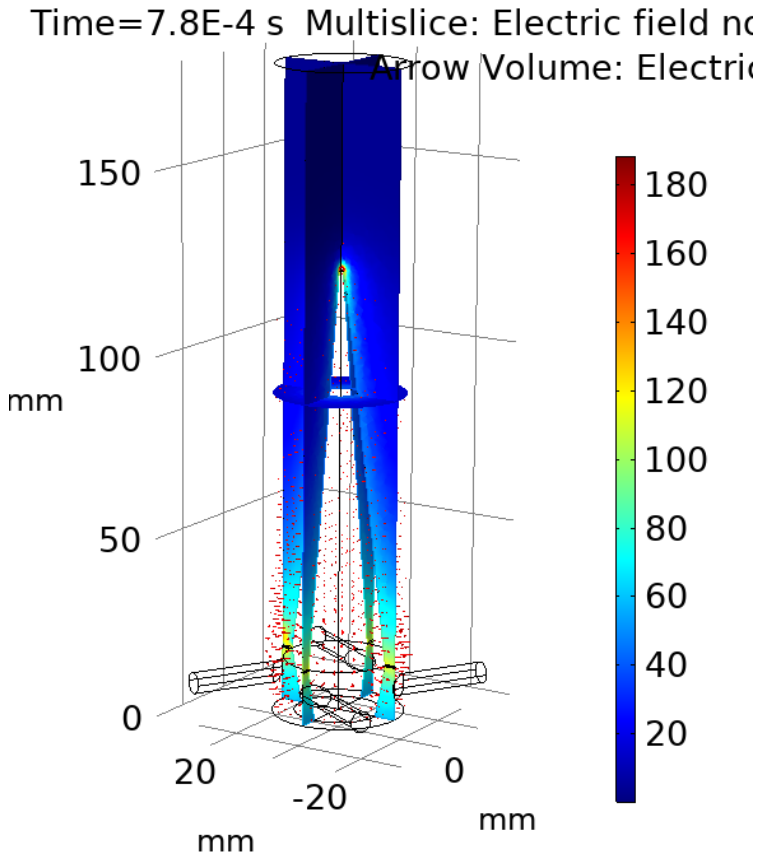
流场|u|单位m/s，及其流线



电子密度（1/m³）

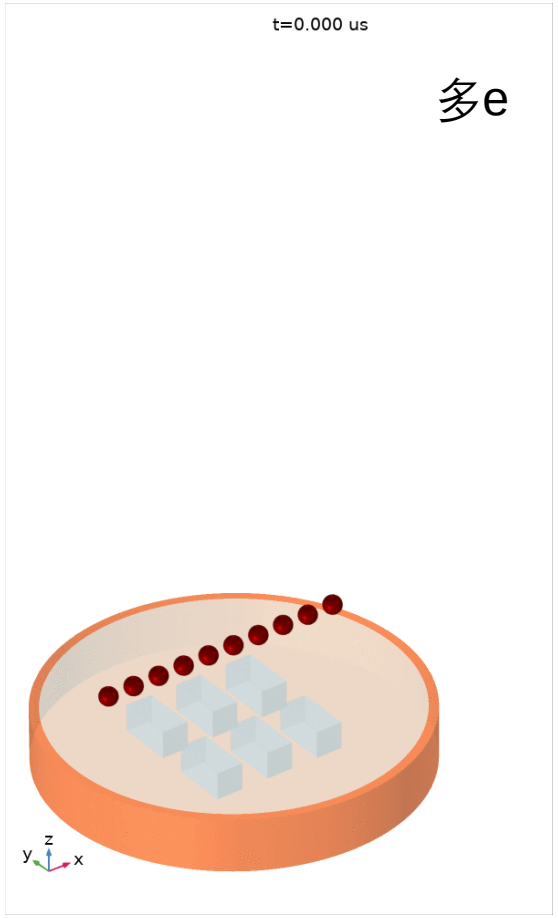


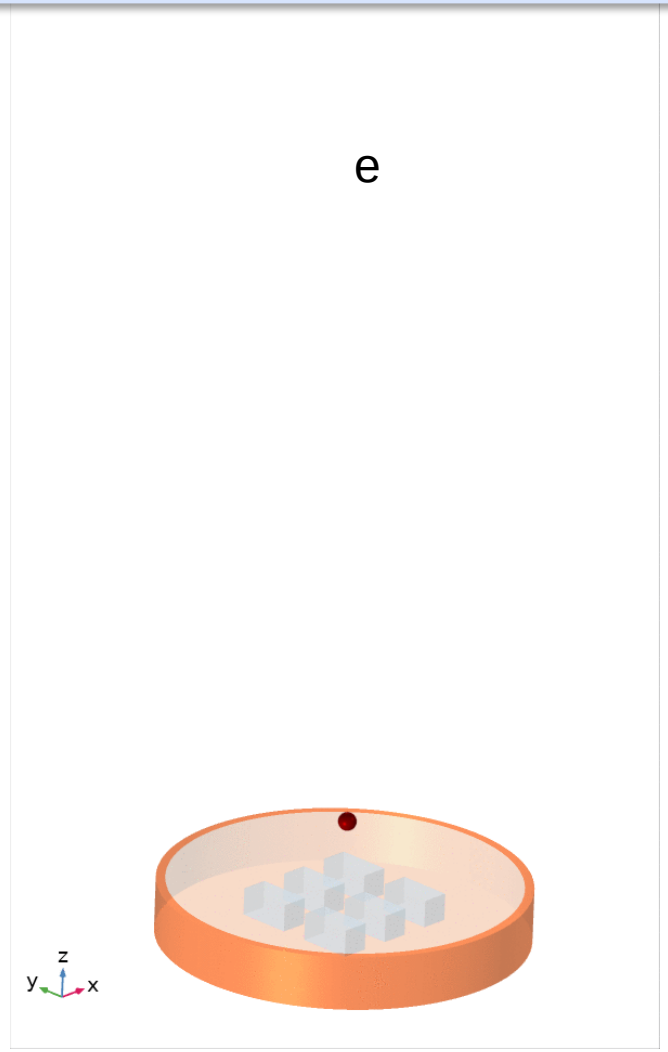
电场|E|单位V/m

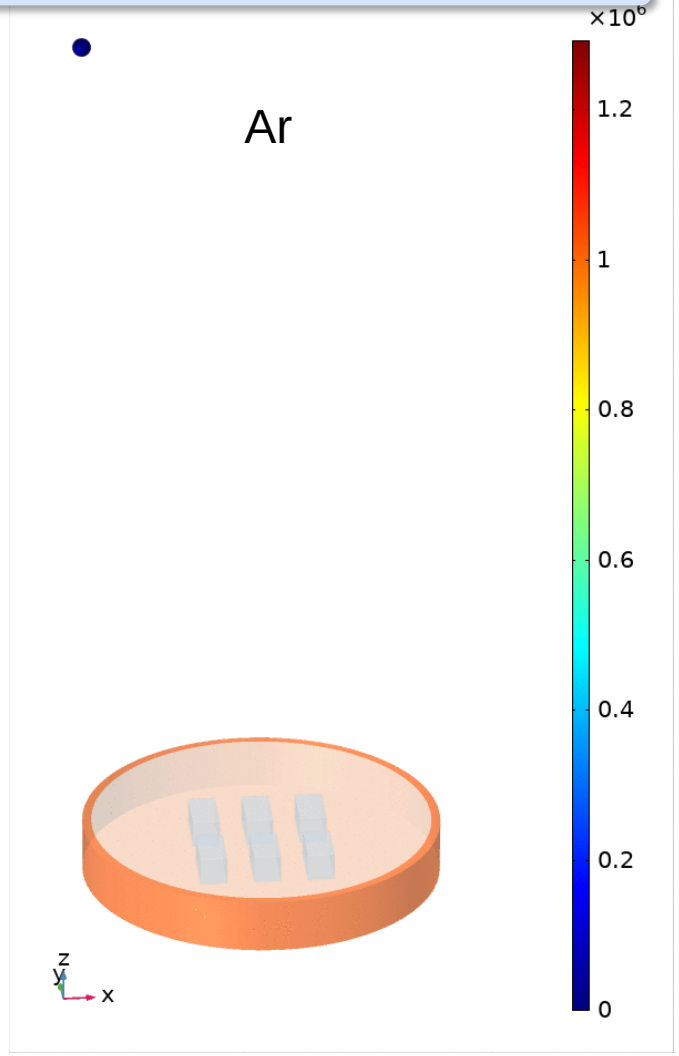


磁控离子倍增

□ 粒子-粒子相互作用

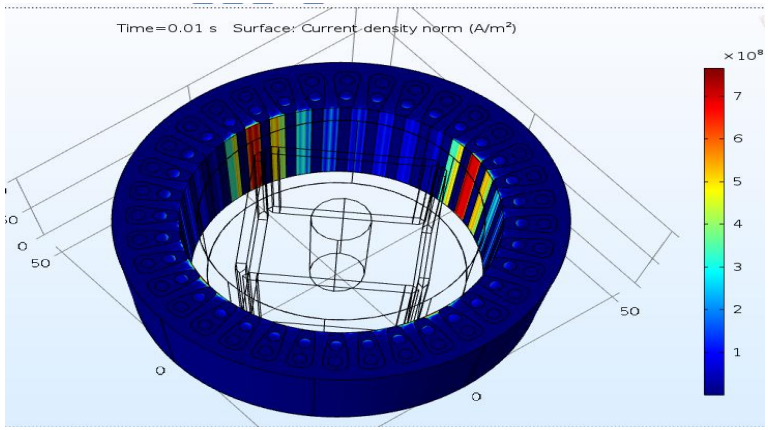




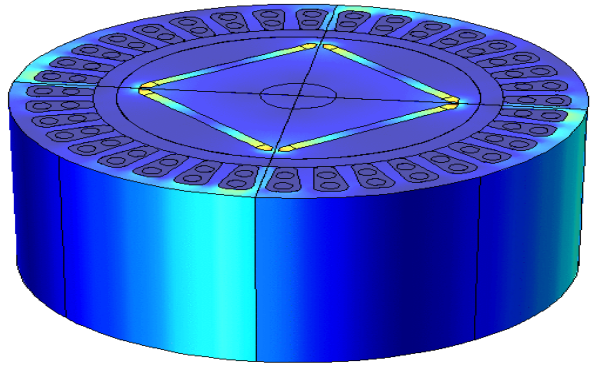


计算永磁同步电机在工作过程中的磁场、涡流、损耗、受力、反向电动势等关键性能指标。

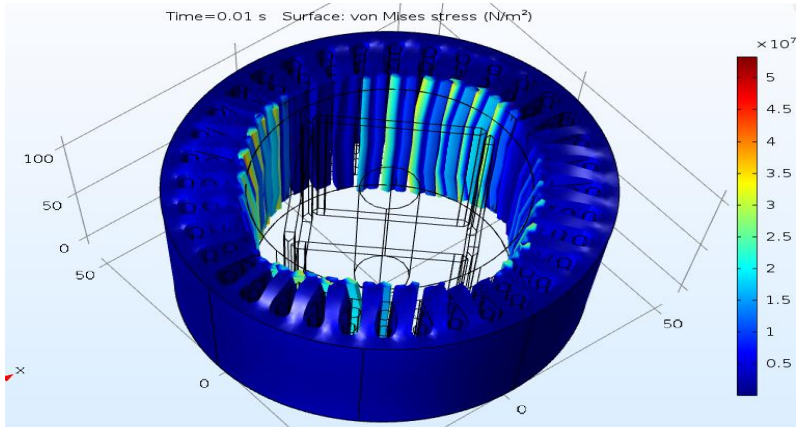
转动涡流



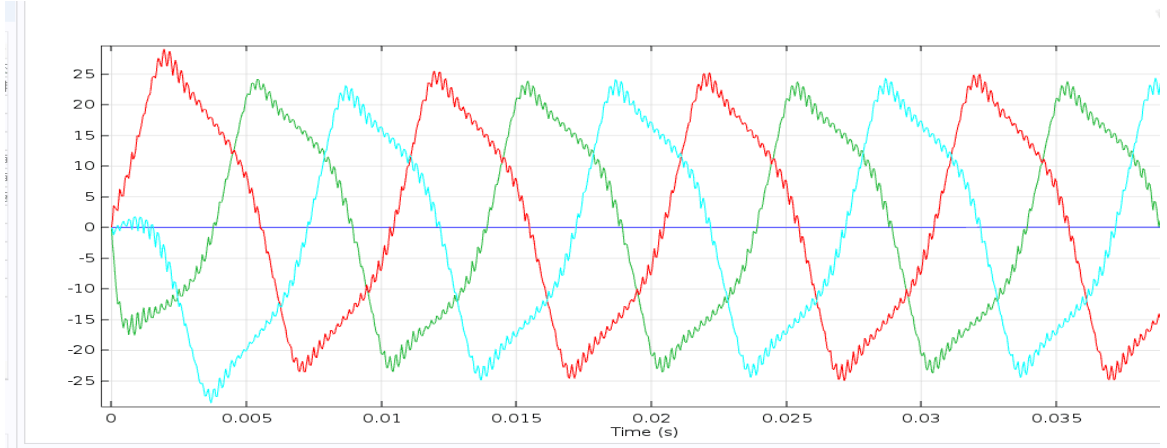
磁场



转动应力/应变

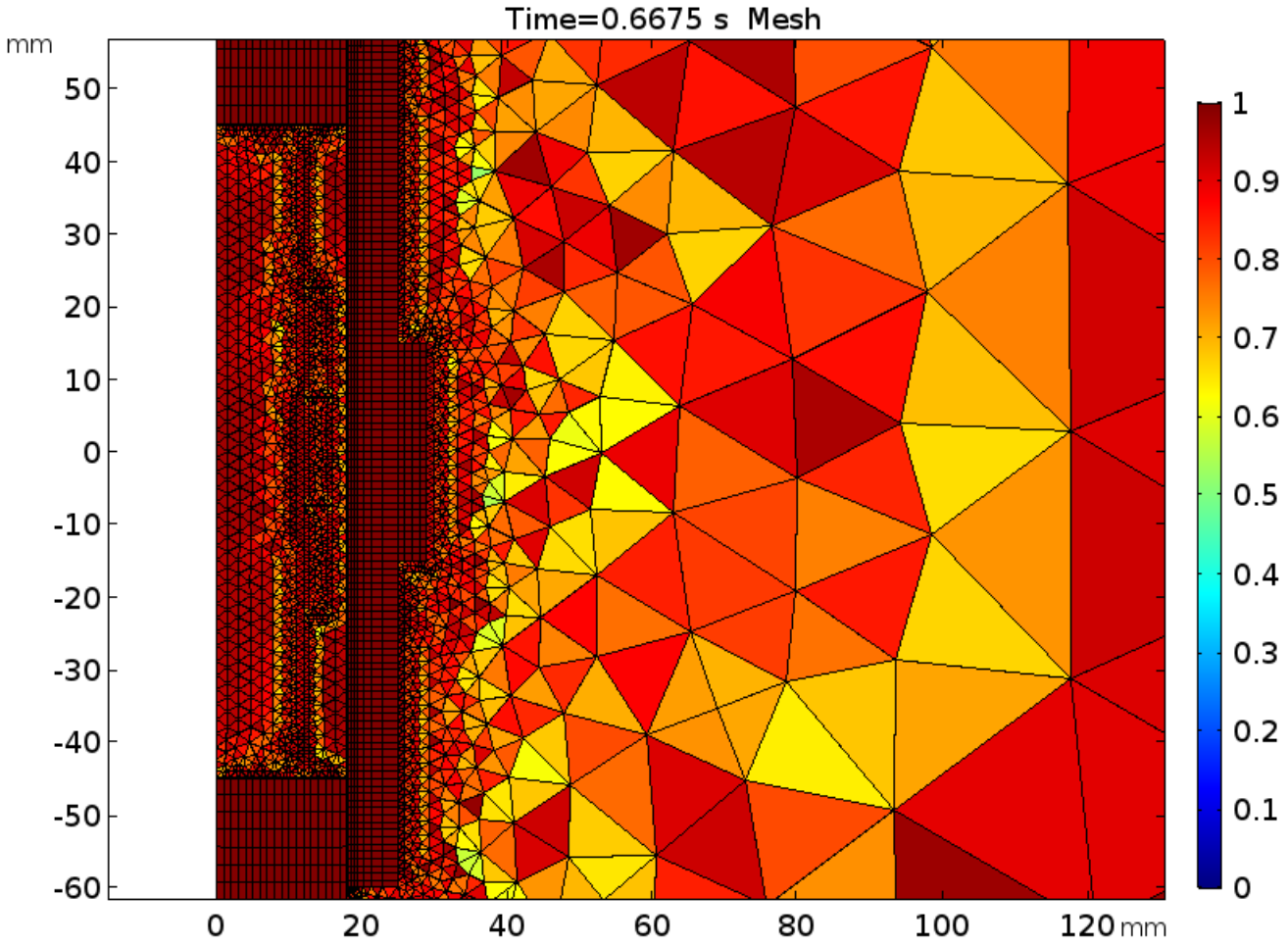


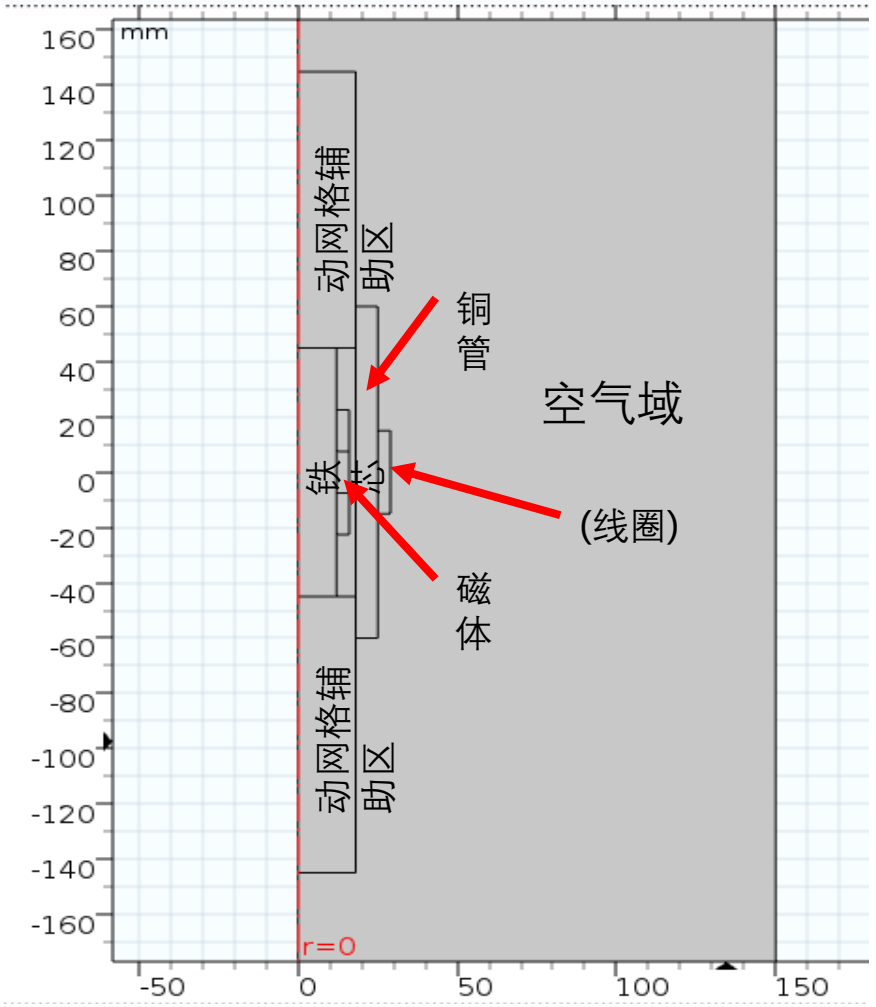
反电动势

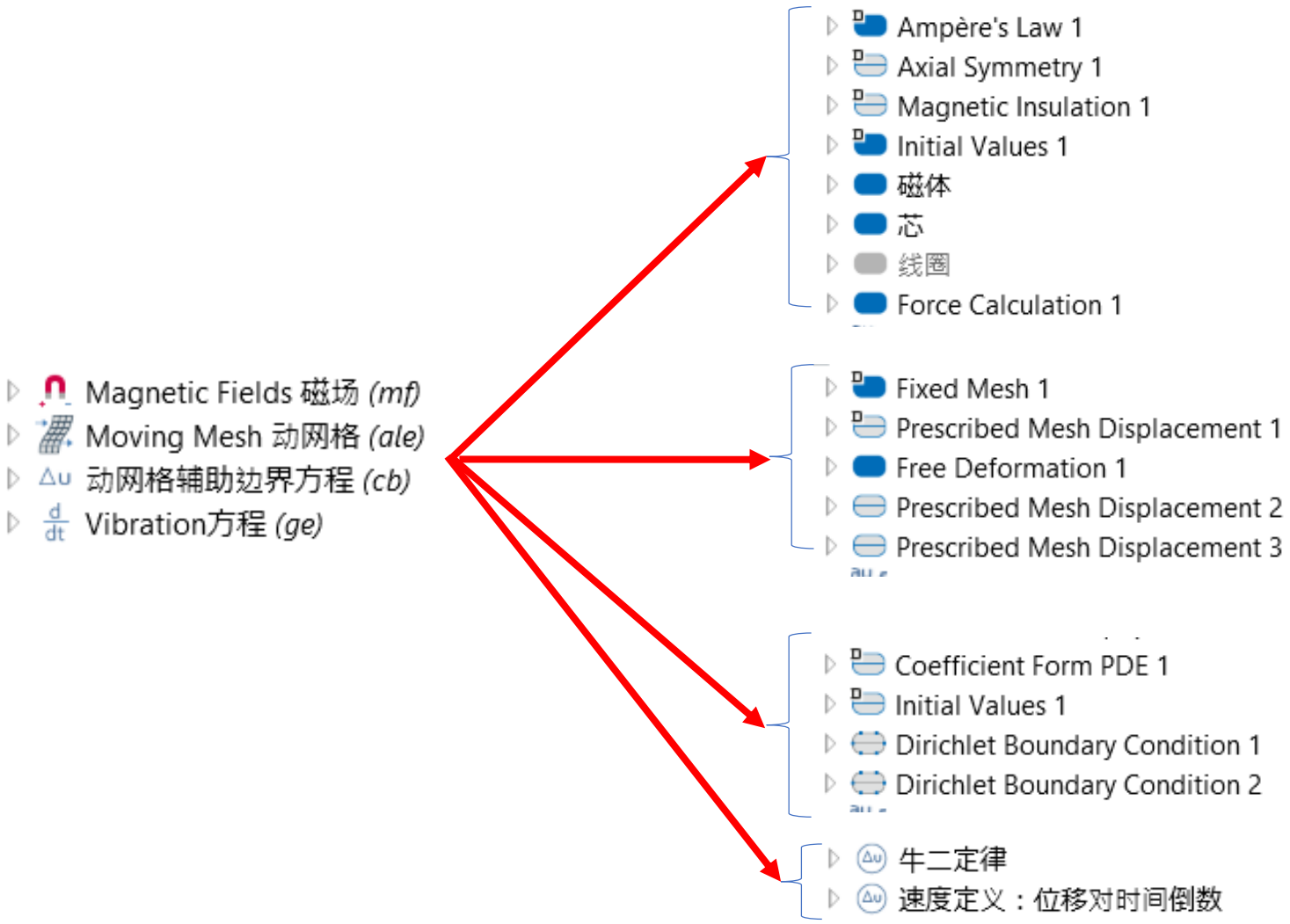


2 电磁阻尼器

电磁阻尼器的工作原理是：当磁体与导体发生相对运动时，会在导体内部产生涡流(涡流产生的磁场方向与磁体磁场方向相反)，并受到与运动速度相反的电磁力的作用。经过一段时间，动能以涡流发热的形式发生转换，从而实现“阻尼”效果。



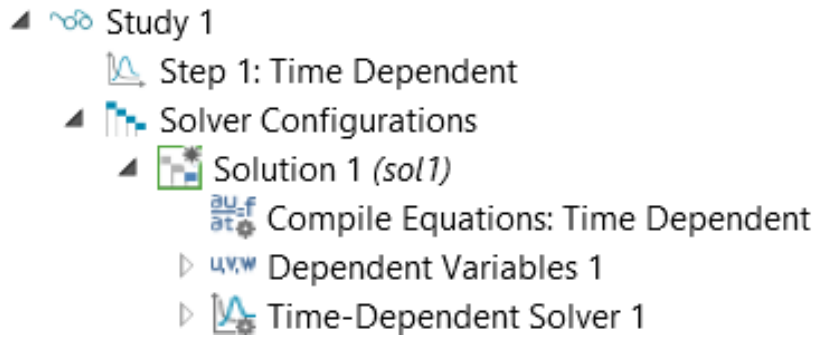


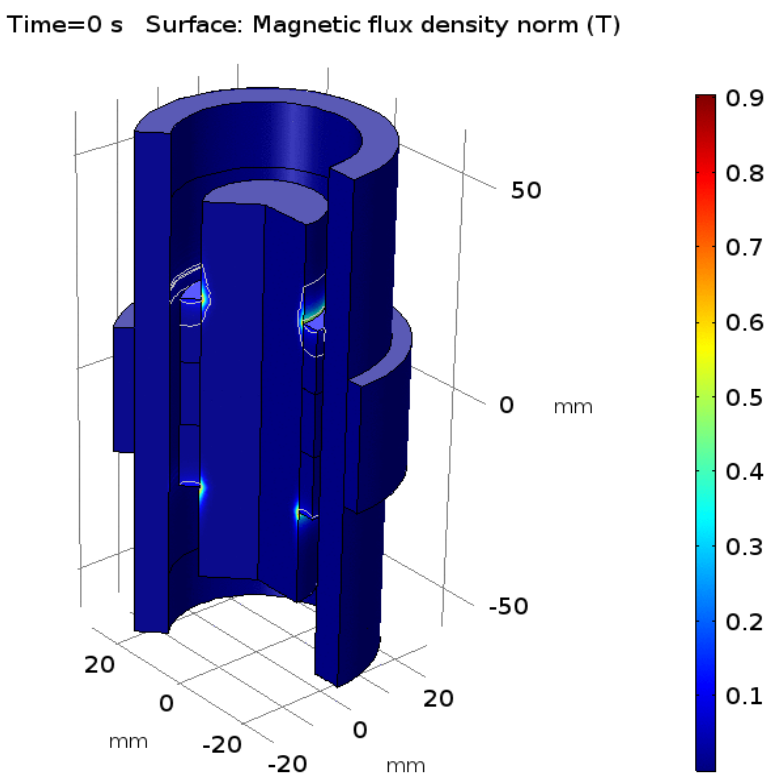

Magnetic Fields 磁场 (mf)
Moving Mesh 动网格 (ale)
动网格辅助边界方程 (cb)
Vibration方程 (ge)
Ampère's Law 1
Axial Symmetry 1
Magnetic Insulation 1
Initial Values 1
磁体
芯
线圈
Force Calculation 1
Fixed Mesh 1
Prescribed Mesh Displacement 1
Free Deformation 1
Prescribed Mesh Displacement 2
Prescribed Mesh Displacement 3
Coefficient Form PDE 1
Initial Values 1
Dirichlet Boundary Condition 1
Dirichlet Boundary Condition 2
牛二定律
速度定义：位移对时间倒数

网格序列

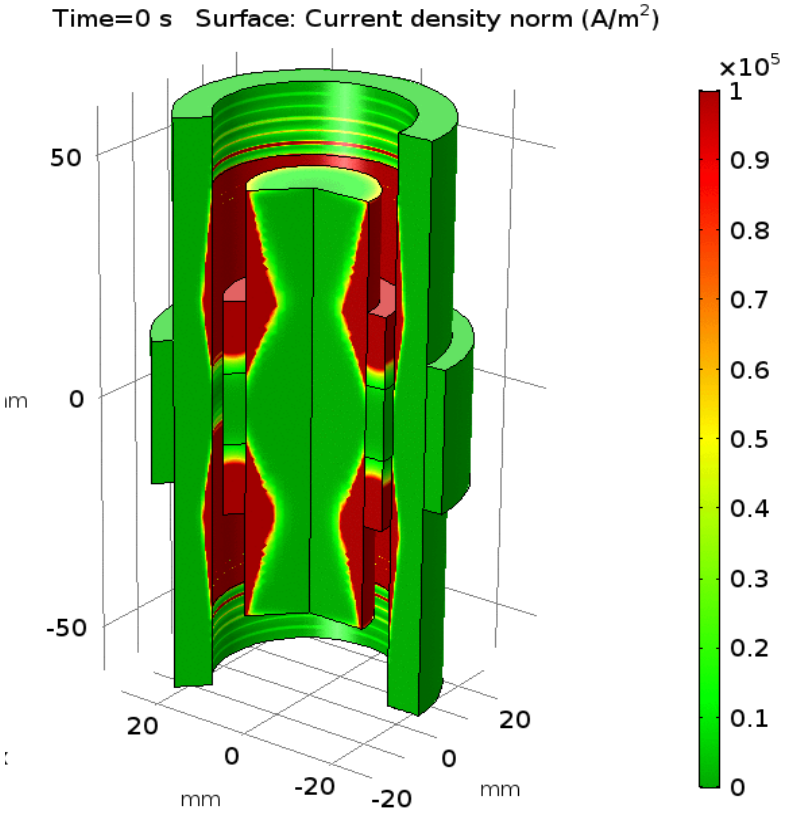

Mesh 1
Size
Edge 1
Mapped 1
Free Triangular 1
Mapped 2
Free Triangular 3

求解器

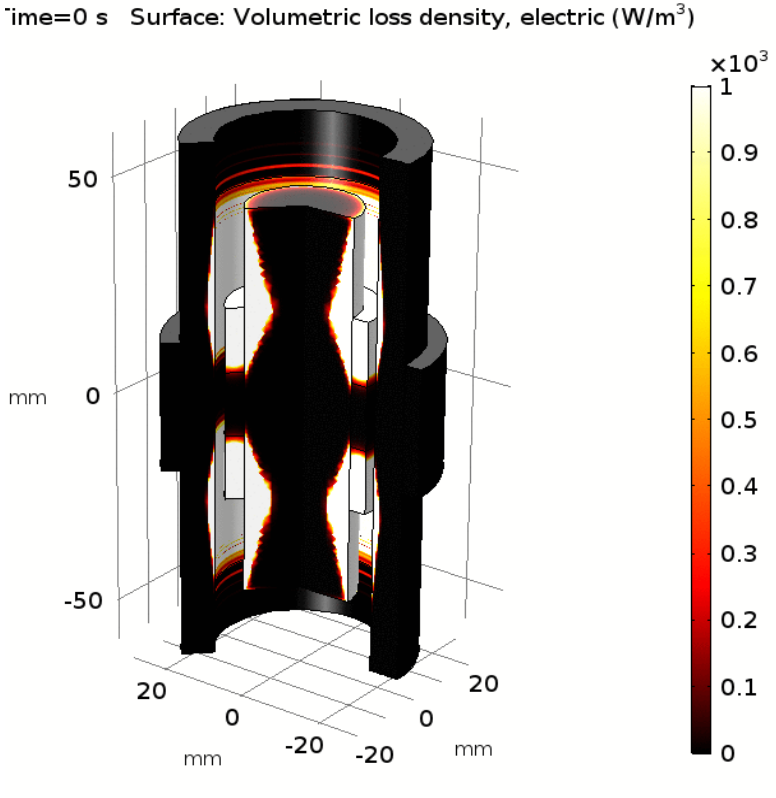

Study 1
Step 1: Time Dependent
Solver Configurations
Solution 1 (sol1)
Compile Equations: Time Dependent
Dependent Variables 1
Time-Dependent Solver 1


Time=0 s Surface: Magnetic flux density norm (T)
50
0
-50
mm
20
0
-20
mm
20
0
-20
mm
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
z
x

磁场


Time=0 s Surface: Current density norm (A/m²)
50
0
-50
mm
20
0
-20
mm
20
0
-20
mm
×10⁵
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

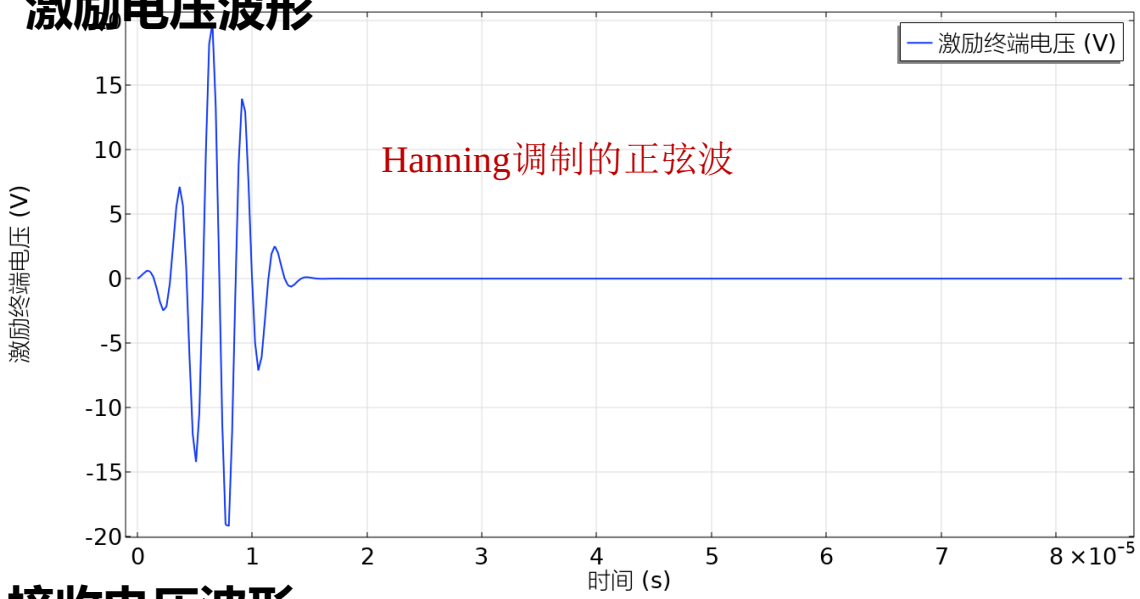
涡流


ime=0 s Surface: Volumetric loss density, electric (W/m³)
50
0
-50
mm
20
0
-20
mm
20
0
-20
mm
×10³
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

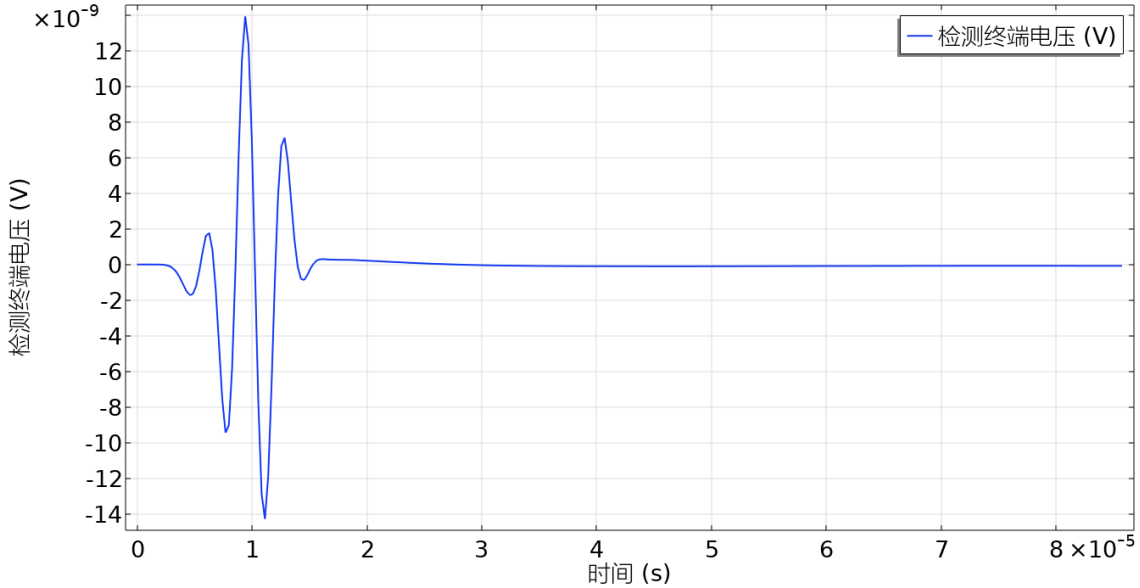
损耗

2 压电效应

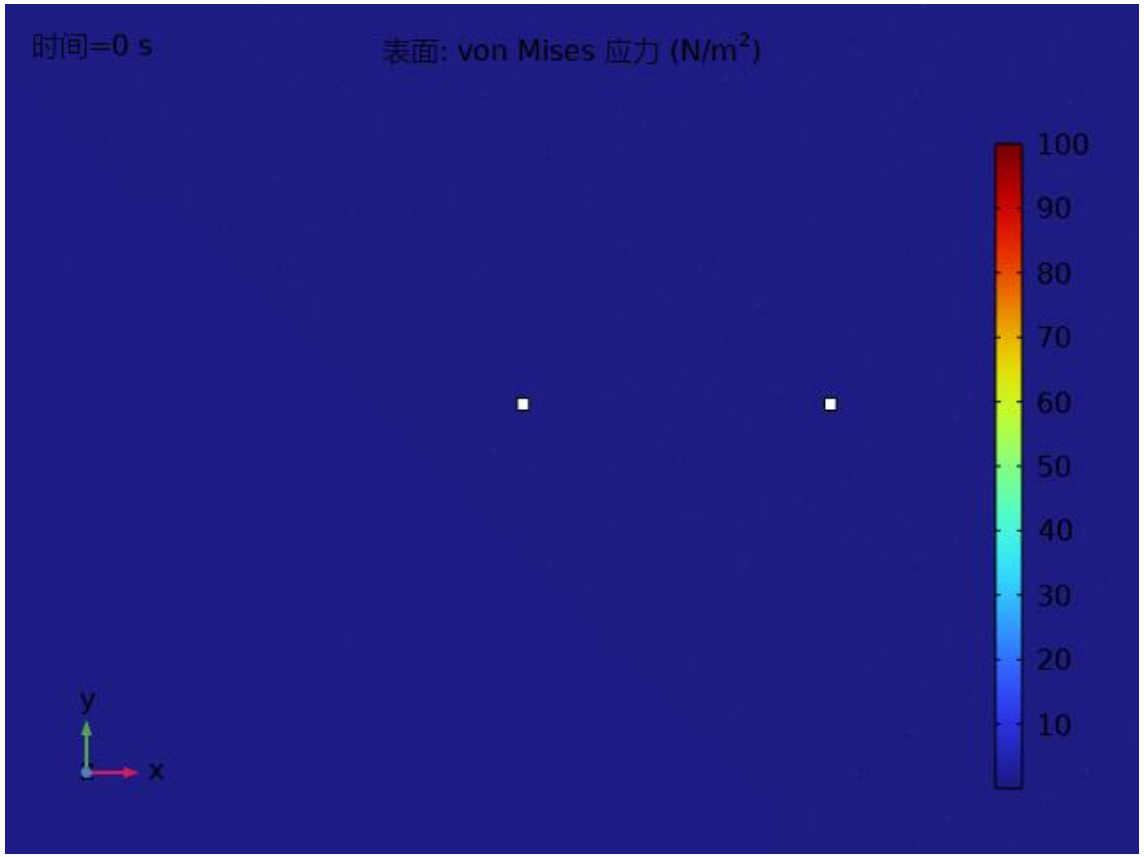
激励电压波形



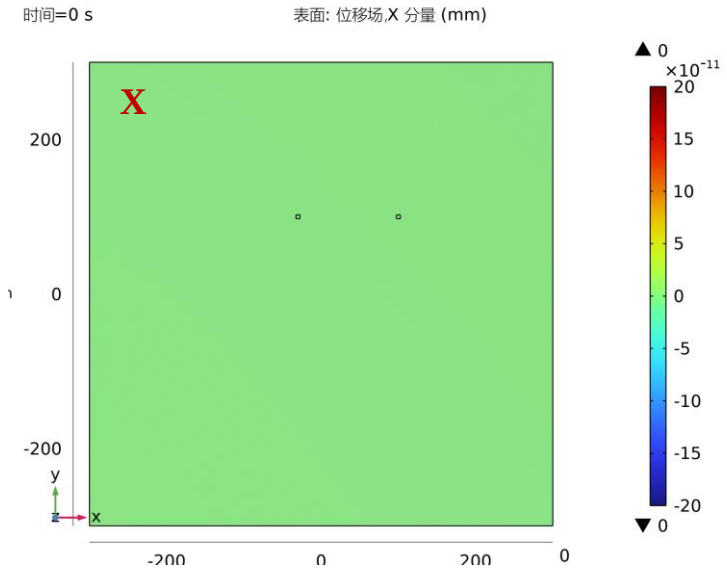
接收电压波形

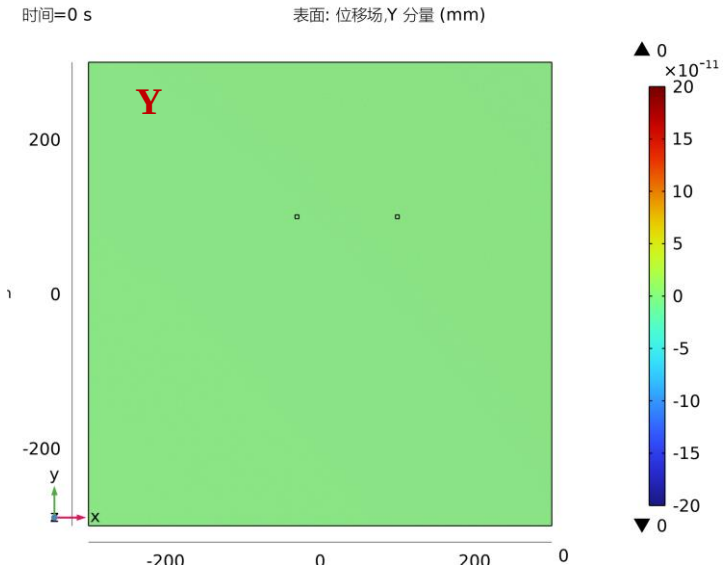


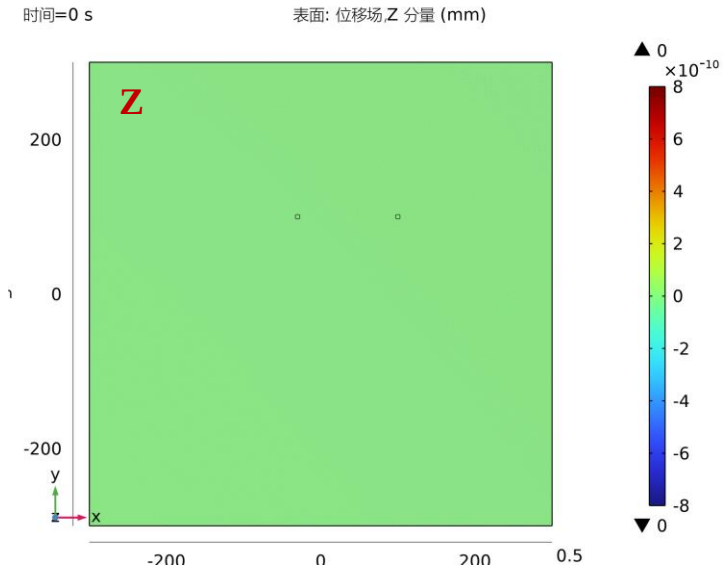
应力波



直角坐标系位移分布

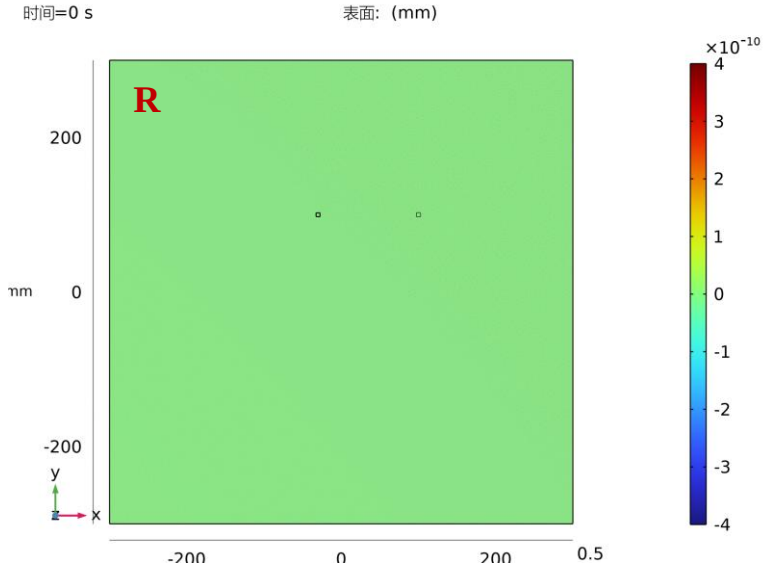


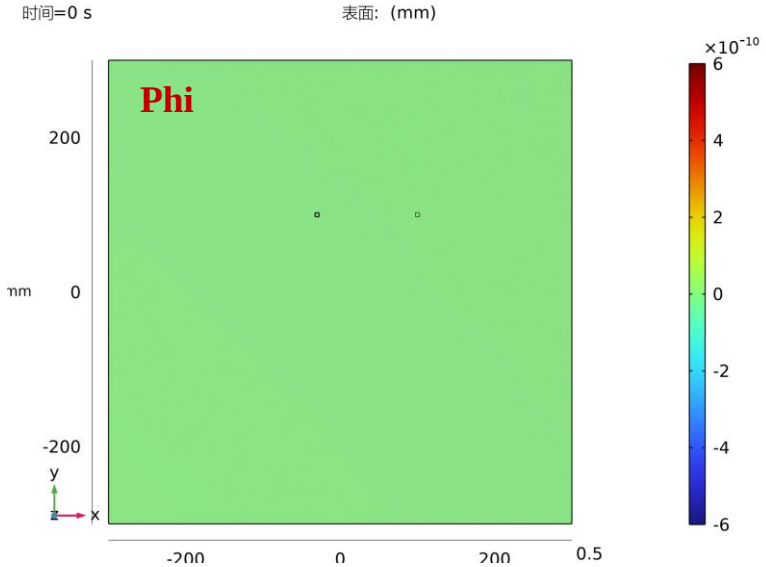


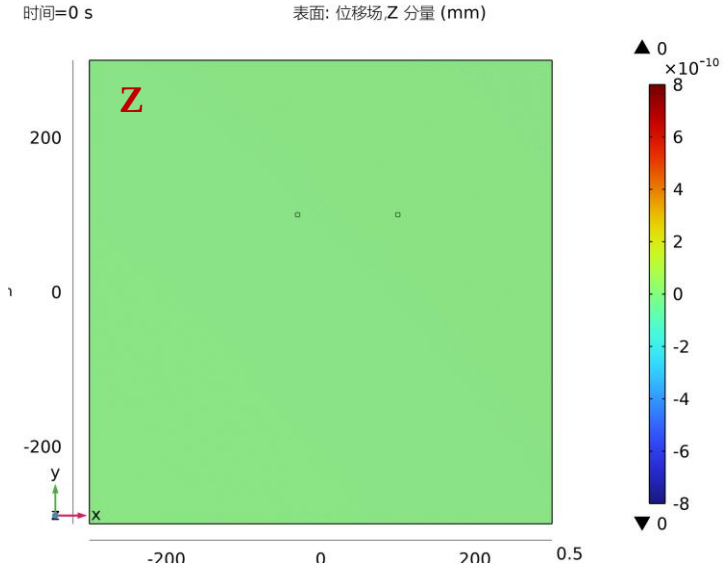


激励频率 350[kHz]

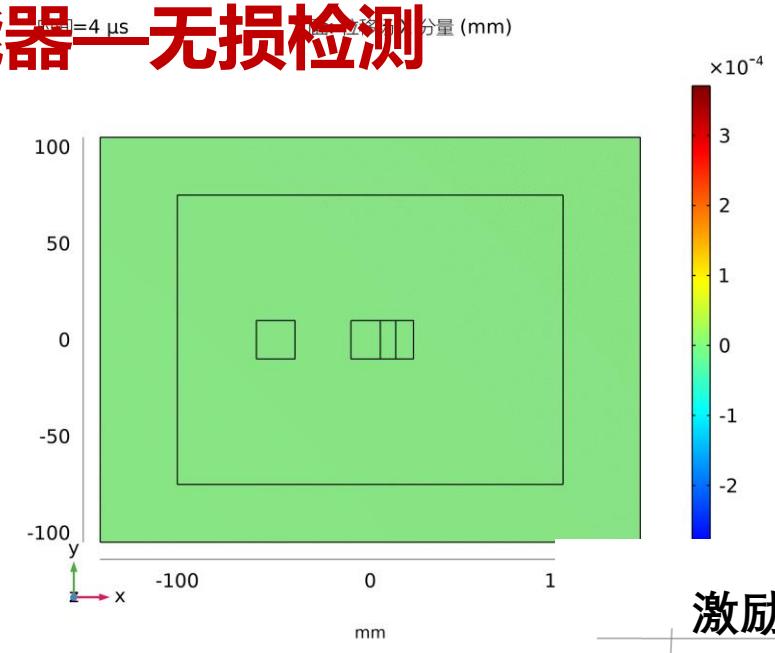
柱坐标系位移分布

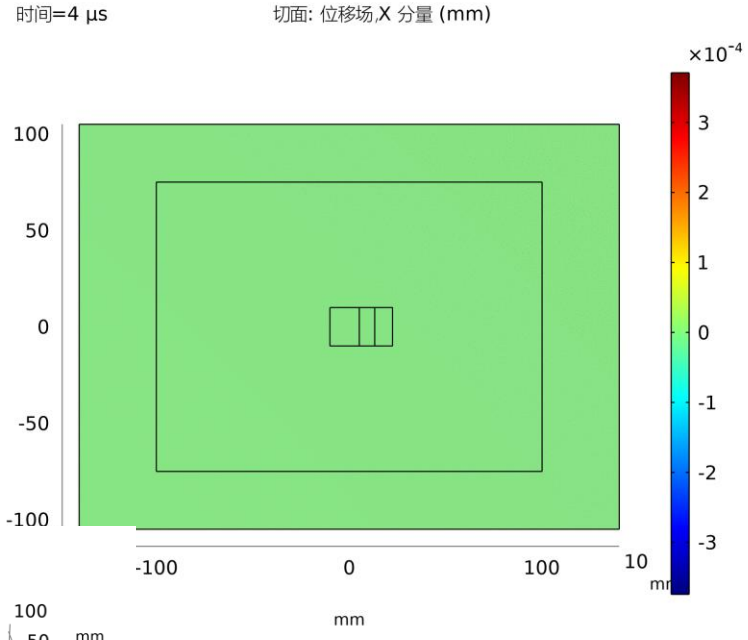




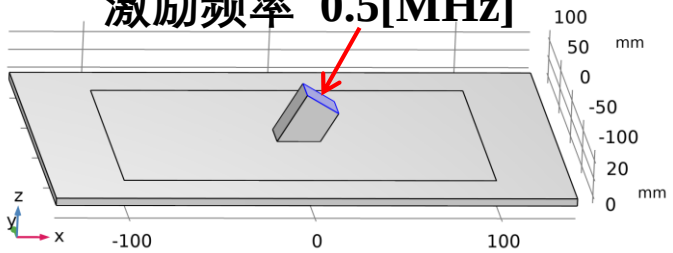


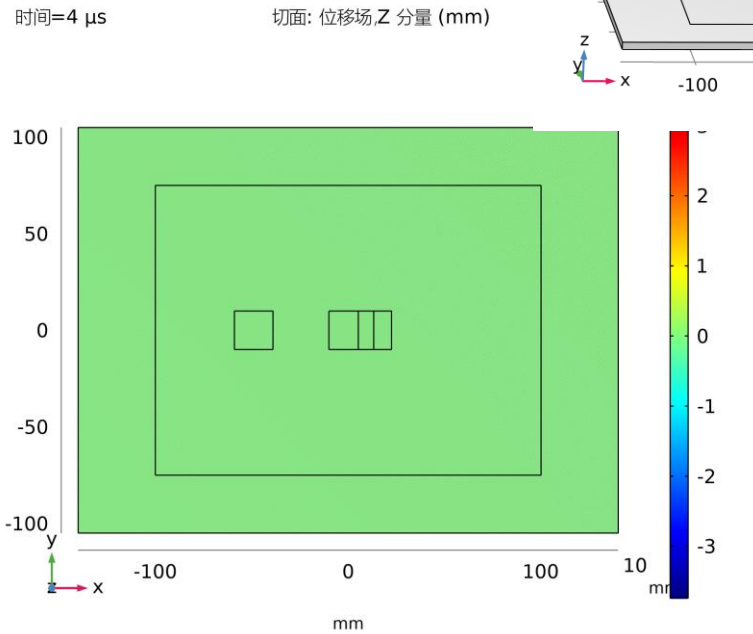
导波换能器—无损检测

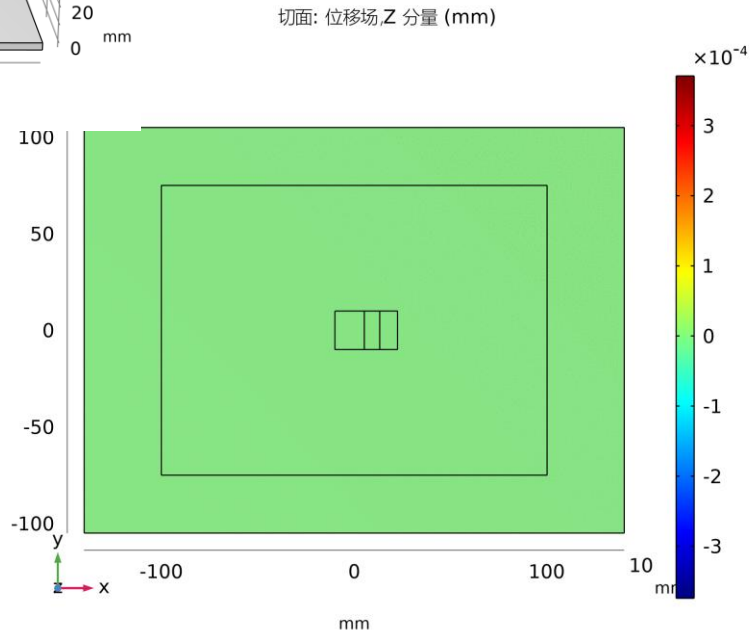




激励频率 0.5[MHz]







2 压电直线电机

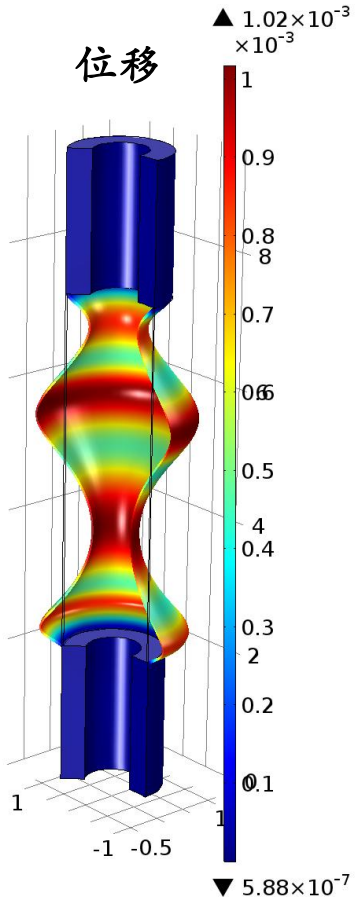
深圳技术大学

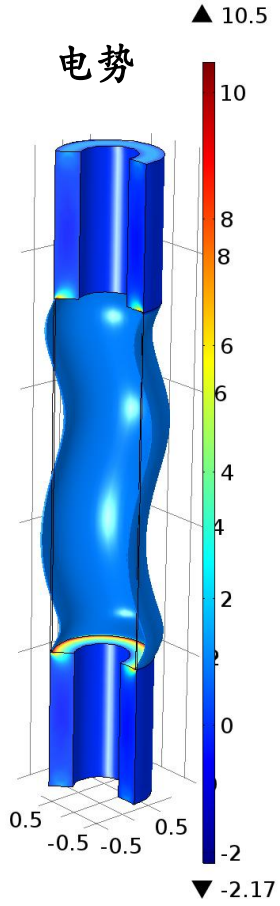
基本原理：压电材料作为电极夹在弹性材料两端，通过对压电材料施加一定时序的电压，并产生位移位移作用于中间的弹性材料，产生蠕动。类似于毛毛虫的爬动效果，构成“直线电机”

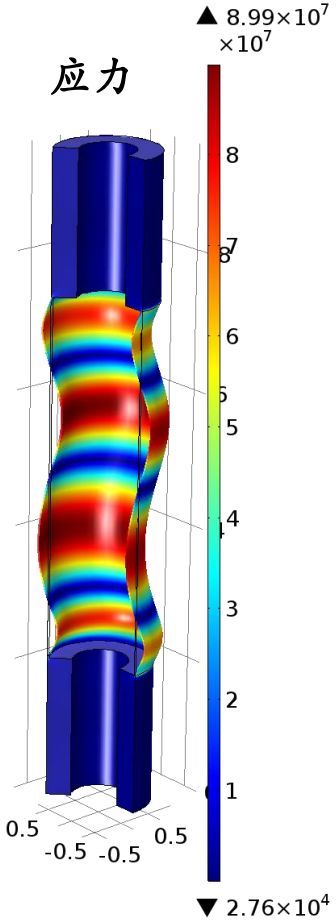


Custom piezoelectric SQUIGG motor offers 0.5 µm resolutic up to 2 mm of travel.

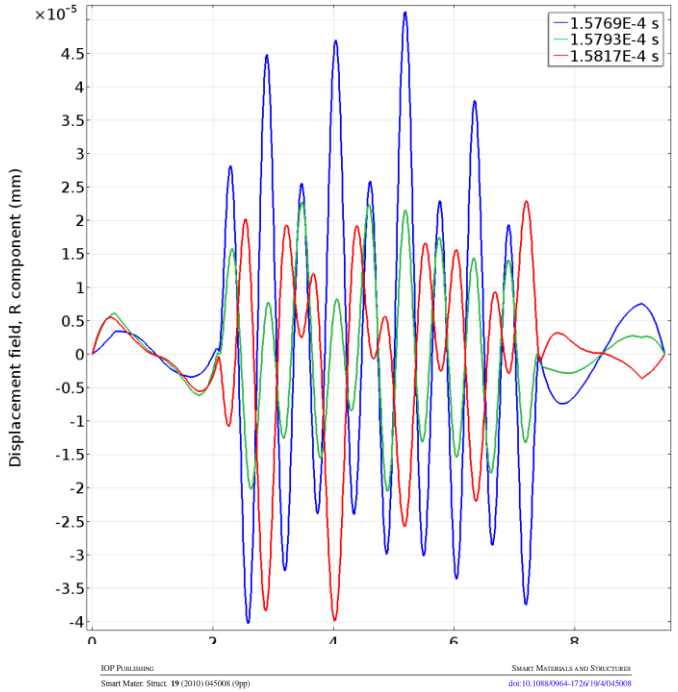
http://www.newscaletech.cc /technology/motors-for-oen specials.php







不同时刻的形变产生爬行

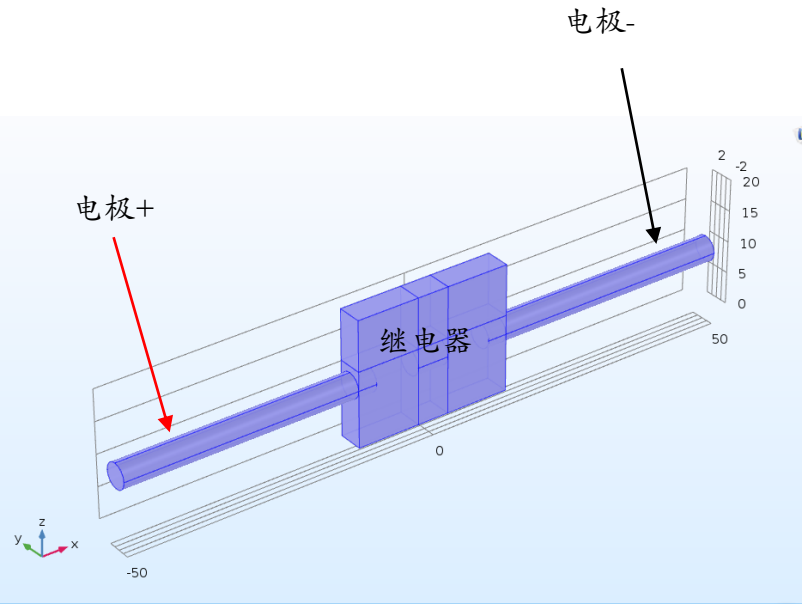


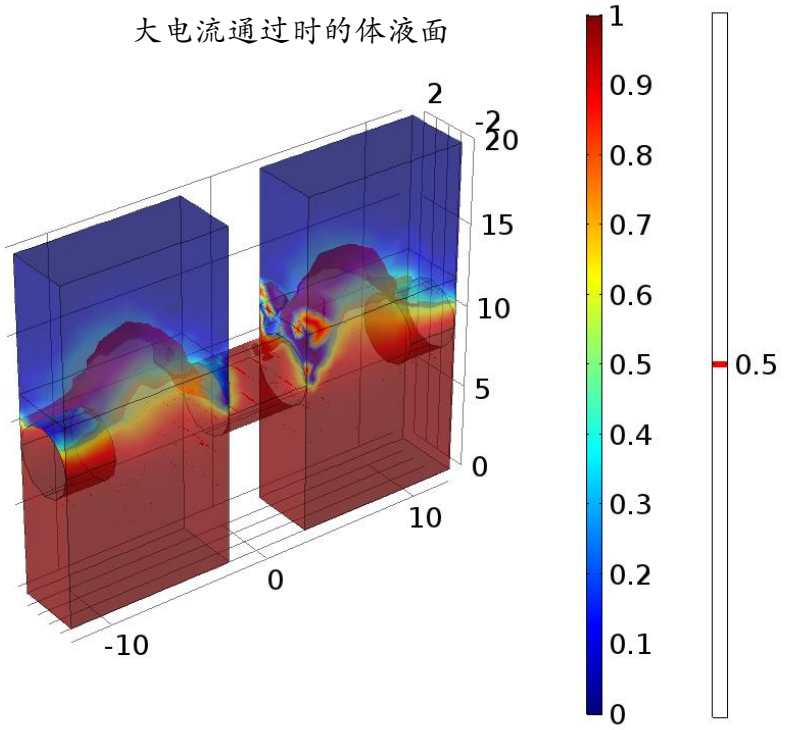
IOP Publishing — Smart Materials and Structures
Smart Mater. Struct. 19 (2010) 045008 (9pp) — doi:10.1088/0964-1726/19/4/045008

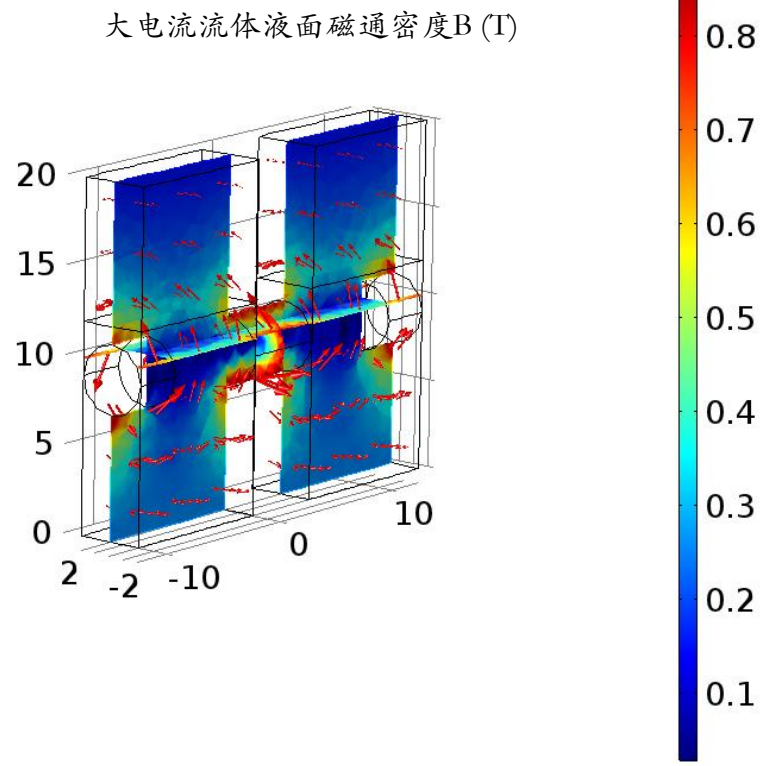
A piezoelectric linear ultrasonic motor with the structure of a circular cylindrical stator and slider

2 液态自恢复继电器

基本原理：对液态金属施加电流，由于电流的作用会在液态金属内部产生感应磁场，感应磁场与之前的电流密度共同产生作用在液态金属上的洛伦兹力，在洛伦兹力的驱动下，液态金属发生形变，之后液态金属内部的电场和磁场也产生变化，这是一个电磁场和流场（两相流）的双向耦合问题。大电流过载后，流体形变导致断路。电流消失后，金属在重力作用下自动恢复原有形貌，继续导通。

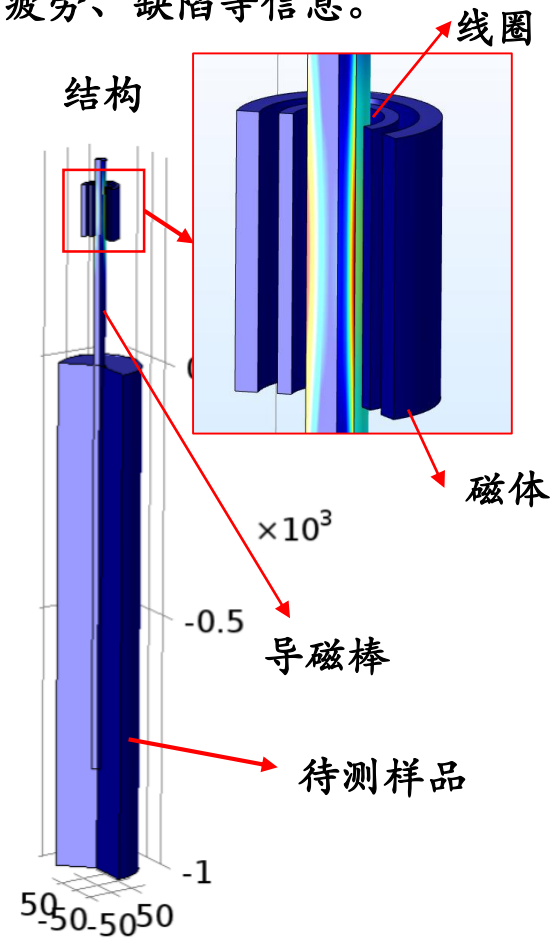


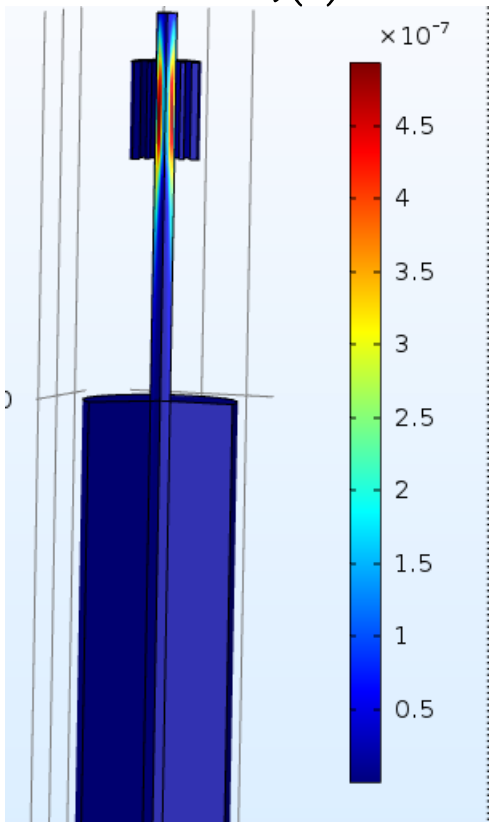


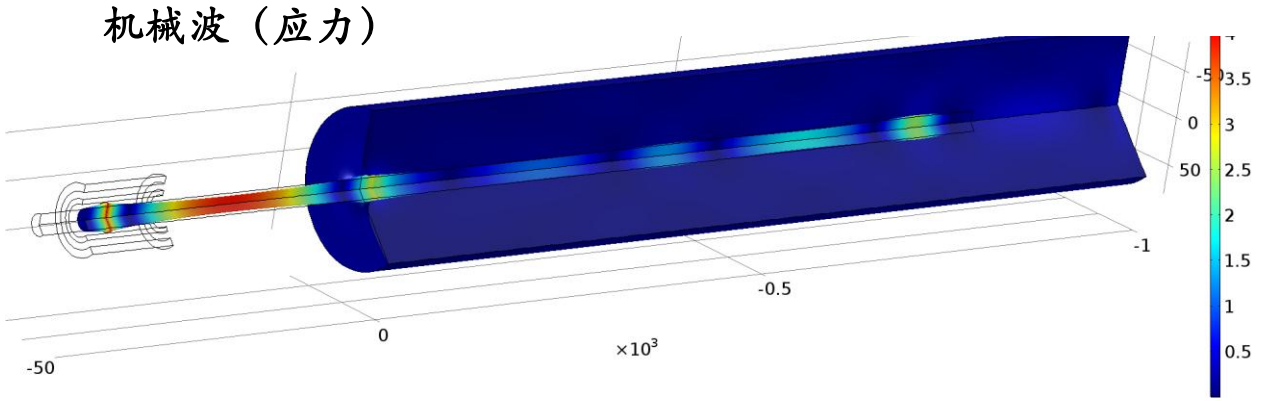


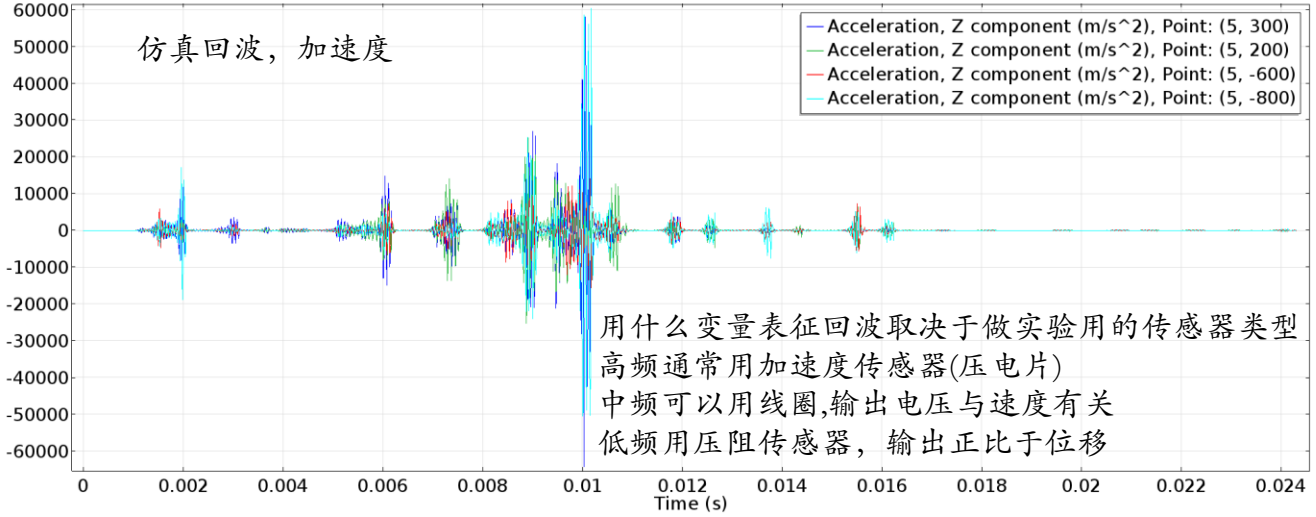
2 电磁超声换能器

基本原理：永磁体产生静磁场偏置，提供最佳静态工作点。AC电流激励线圈产生交变磁场，交变磁场在导电样品中产生涡流，涡流与静磁场作用产生洛伦兹力，洛伦兹力驱动样品内部产生横波。除此之外，取决于待测样品材料，磁致伸缩效应会产生纵波。横波/纵在样品传递中，如果遇到缺陷、腐蚀的情况会产生不同的反射回波，通过检测反射回波，可以判定样品的厚度、疲劳、缺陷等信息。









用什么变量表征回波取决于做实验用的传感器类型
高频通常用加速度传感器(压电片)
中频可以用线圈,输出电压与速度有关
低频用压阻传感器，输出正比于位移

技术路线

稳态

- 稳态：地下水饱和状态、流场分布对矿物溶质反应及浓度分布的影响。
- 瞬态：微生物生长死亡影响地下系统多孔介质渗透率，从而影响饱和度。

瞬态

Richards Equation

$$\nabla \cdot (\rho \mathbf{u}) = Q_m$$

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p + \rho \mathbf{g})$$

微生物浓度影响渗透率 X_i

Partial Differential Equation

$$X_i$$

$$\frac{\partial X}{\partial t} = v_{max} \times IT \times \frac{C_1}{K_{s1} + C_1} \times \frac{C_2}{K_{s2} + C_2} \times X_i - v_{dec} \times X_i$$

速度 $\mathbf{u}$

非饱和状态 $dl.un$

物质源 S_i

弥散 $D_{D,i}$

吸附 c_P

扩散 $D_{e,i}$

The Transport of Diluted Species in Porous Media

$$C_i$$

$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i + S_i$$

$$\mathbf{J_i} = -(D_{D,i} + D_{e,i})\nabla c_i$$

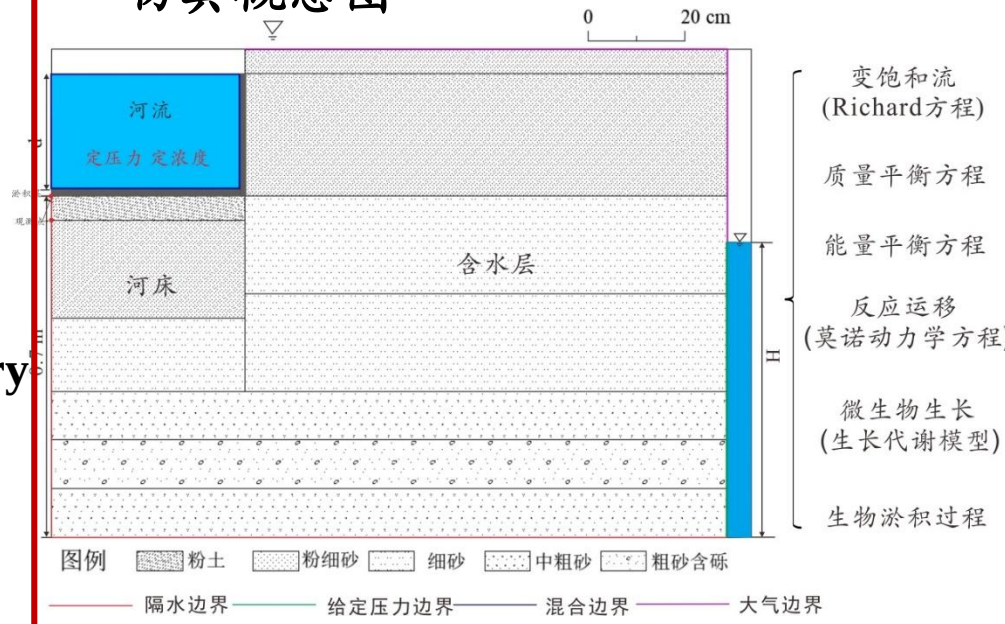
化学反应 R_i

反应物/生成物浓度 c_i

Chemistry

A+B→C+D

仿真概念图



由**饱和度控制的反应速率**作用下，化学反应对生成物、反应物浓度的影响。

反应类型	反应方程
好氧呼吸	$CH_2O+O_2 \rightarrow CO_2+H_2O$
Fe^{2+}氧化	$4Fe^{2+}+O_2+10H_2O \rightarrow 4Fe(OH)_3+8H^+$
反硝化	$5CH_2O+4NO_3^-+4H^+ \rightarrow 5CO_2+2N_2+7H_2O$
Mn(IV)还原	$CH_2O+2MnO_2+4H^+ \rightarrow 2Mn^{2+}+3H_2O+CO_2$
Mn^{2+}氧化	$2Mn^{2+}+O_2+2H_2O=2MnO_2+4H^+$
SO_4^{2-}还原	$2CH_2O+SO_4^{2-}+H^+ \rightarrow HS^-+2H_2O+2CO_2$
Fe(III)还原	$CH_2O+4Fe(OH)_3+8H^+ \rightarrow 4Fe^{2+}+11H_2O+CO_2$

反应速率与饱和度状态的关系

$H_p < 0$，非饱和

$H_p \geq 0$，饱和

$$\begin{cases} r_{CH_2O/O_2} = k_{O_2} c_{CH_2O} \dfrac{c_{O_2}}{K_{O_2}+c_{O_2}} + \alpha_0 \left(\dfrac{c_{O_2}}{H} - c_{DO}\right) & H_p < 0 \\ r_{CH_2O/O_2} = k_{O_2} c_{CH_2O} \dfrac{c_{O_2}}{K_{O_2}+c_{O_2}} & H_p \geq 0 \end{cases}$$

$$\begin{cases} r_{CH_2O/Fe} = k_{Fe^{2+}} \dfrac{c_{Fe^{2+}}}{K_{Fe^{2+}}+c_{Fe^{2+}}} \dfrac{c_{O_2}}{K_{O_2}+c_{O_2}} & H_p < 0 \\ 0 & H_p \geq 0 \end{cases}$$

$$\begin{cases} r_{CH_2O/NO_3} = k_{NO_3}\ c_{CH_2O}^{0}\ \dfrac{c_{NO_3}}{K_{NO_3}+c_{NO_3}}\ \dfrac{K_{i,O_2}}{K_{i,O_2}+c_{O_2}} & H_p < 0 \\ & H_p \geq 0 \end{cases}$$

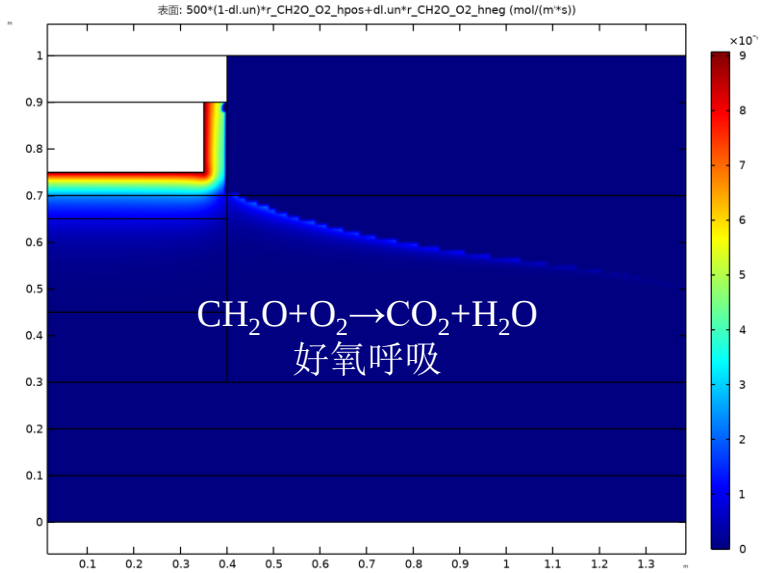
$$\begin{cases} r_{CH_2O/Mn} = k_{Mn} c_{CH_2O}^{0} \dfrac{c_{MnO_2}}{K_{Fe(OH)_3}+c_{MnO_2}} \dfrac{K_{i,O_2}}{K_{i,O_2}+c_{O_2}} \dfrac{K_{i,NO_3}}{K_{i,NO_3}+c_{NO_2}} & H_p < 0 \\ & H_p \geq 0 \end{cases}$$

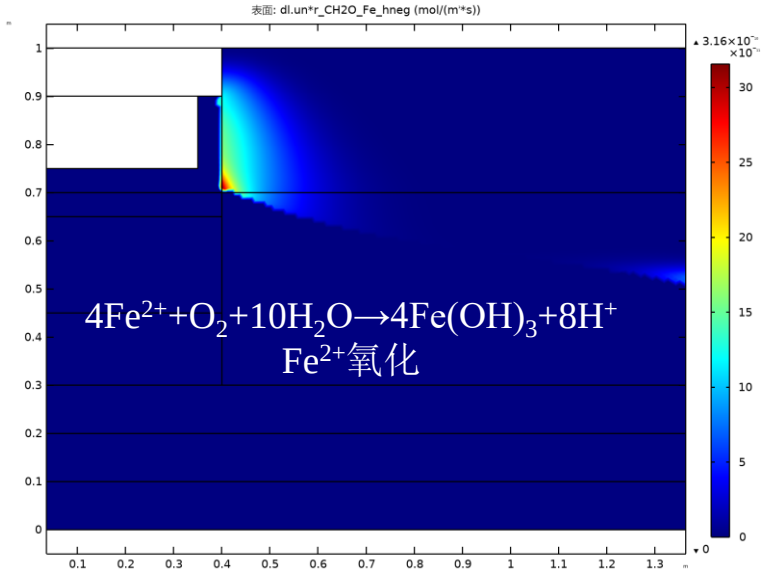
$$\begin{cases} r_{CH_2O/Mn} = k_{Mn^{2+}} \dfrac{c_{Mn^{2+}}}{K_{Mn^{2+}}+c_{Mn^{2+}}} \dfrac{c_{O_2}}{K_{O_2}+c_{O_2}} & H_p < 0 \\ 0 & H_p \geq 0 \end{cases}$$

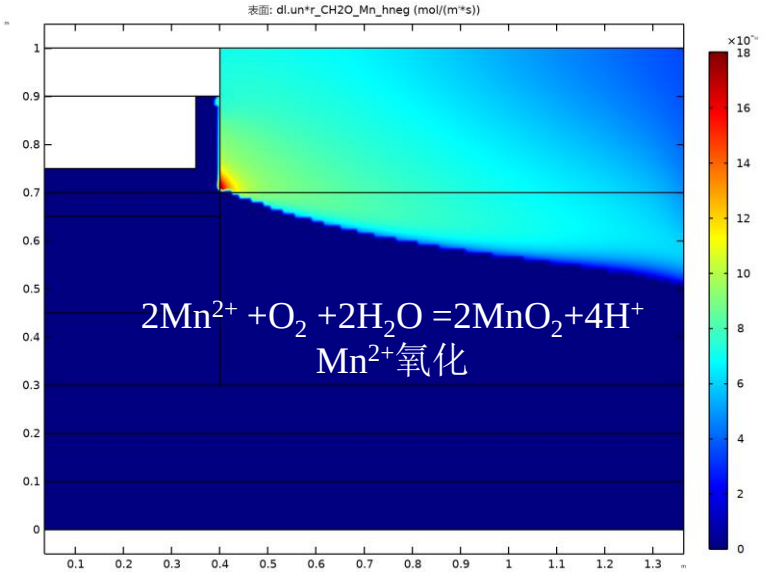
$$\begin{cases} r_{CH_2O/SO_4} = k_{SO_4} c_{CH_2O}^{0} \dfrac{c_{SO_4}}{K_{SO_4}+c_{SO_4}} \dfrac{K_{i,O_2}}{K_{i,O_2}+c_{O_2}} \dfrac{K_{i,NO_3}}{K_{i,NO_3}+c_{NO_2}} \dfrac{K_{i,MnO_2}}{K_{i,MnO_2}+c_{MnO_2}} \dfrac{c_{Fe(OH)_3}}{K_{Fe(OH)_3}+c_{Fe(OH)_3}} & H_p < 0 \\ & H_p \geq 0 \end{cases}$$

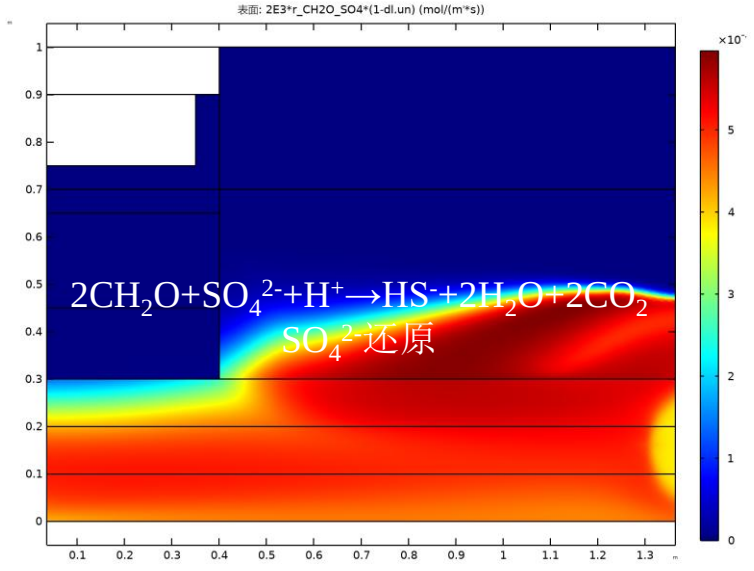
$$\begin{cases} r_{CH_2O/Fe} = k_{Fe} c_{CH_2O}^{0} \dfrac{c_{Fe(OH)_3}}{K_{Fe(OH)_3}+c_{Fe(OH)_3}} \dfrac{K_{i,O_2}}{K_{i,O_2}+c_{O_2}} \dfrac{K_{i,NO_3}}{K_{i,NO_3}+c_{NO_2}} \dfrac{K_{i,MnO_2}}{K_{i,MnO_2}+c_{MnO_2}} & H_p < 0 \\ & H_p \geq 0 \end{cases}$$

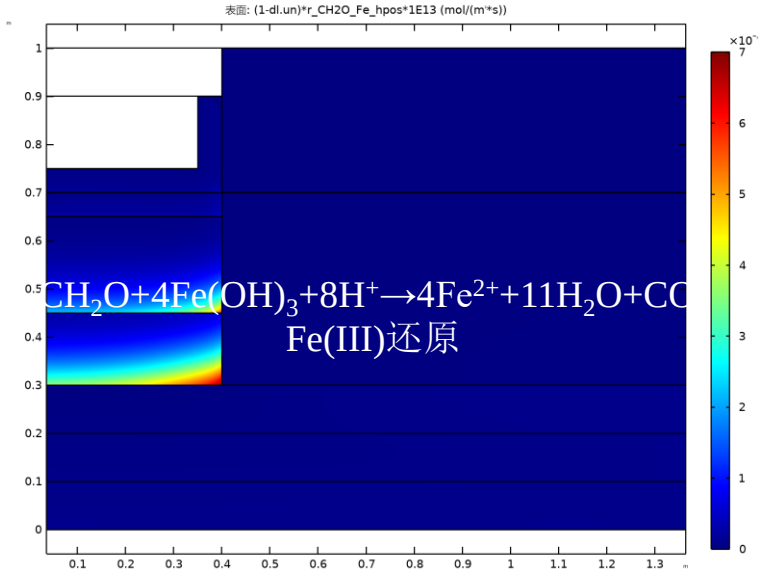
各化学反应反应速率

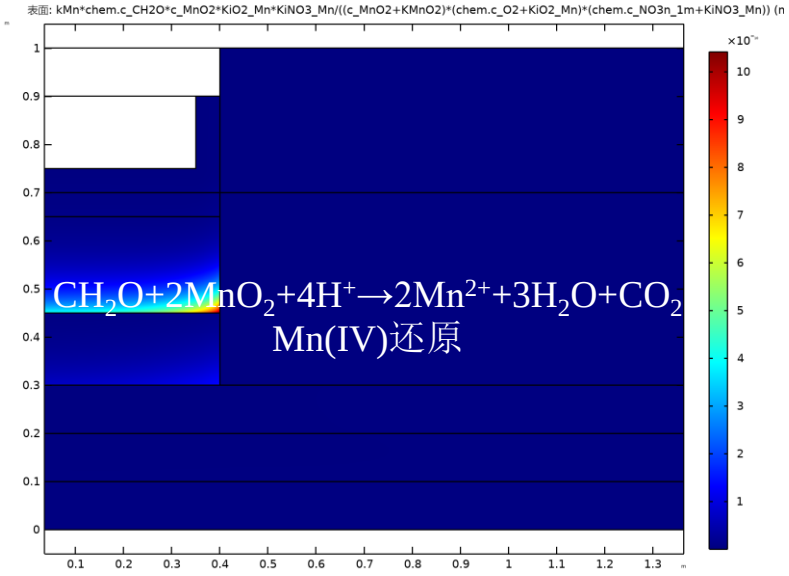

表面: 500*(1-dl.un)*r_CH2O_O2_hpos+dl.un*r_CH2O_O2_hneg (mol/(m³*s))
$CH_2O+O_2 \rightarrow CO_2+H_2O$
好氧呼吸


表面: dl.un*r_CH2O_Fe_hneg (mol/(m³*s))
$4Fe^{2+}+O_2+10H_2O \rightarrow 4Fe(OH)_3+8H^+$
Fe^{2+}氧化


表面: dl.un*r_CH2O_Mn_hneg (mol/(m³*s))
$2Mn^{2+}+O_2+2H_2O=2MnO_2+4H^+$
Mn^{2+}氧化


表面: 2E3*r_CH2O_SO4*(1-dl.un) (mol/(m³*s))
$2CH_2O+SO_4^{2-}+H^+ \rightarrow HS^-+2H_2O+2CO_2$
SO_4^{2-}还原


表面: (1-dl.un)*r_CH2O_Fe_hpos*1E13 (mol/(m³*s))
$CH_2O+4Fe(OH)_3+8H^+ \rightarrow 4Fe^{2+}+11H_2O+CO$
Fe(III)还原


表面: kMn*chem.c_CH2O*c_MnO2*KiO2_Mn*KiNO3_Mn/((c_MnO2+KMnO2)*(chem.c_O2+KiO2_Mn)*(chem.c_NO3n_1m+KiNO3_Mn)) (n
$CH_2O+2MnO_2+4H^+ \rightarrow 2Mn^{2+}+3H_2O+CO_2$
Mn(IV)还原

偏微分方程物理场（PDE）编译

Double莫诺动力学方程、微生物衰减一阶速率方程

模拟微生物生长死亡过程，求解各微生物浓度分布。

$$e_a\frac{\partial^2\mathbf{u}}{\partial t^2}+d_a\frac{\partial\mathbf{u}}{\partial t}+\nabla\cdot(-c\nabla\mathbf{u}-\alpha\mathbf{u}+\gamma)+\beta\nabla\cdot\mathbf{u}+a\mathbf{u}=f$$

莫诺动力学方程

$$\frac{\partial X}{\partial t}=v_{max}\times IT\times\frac{C_1}{K_{s1}+C_1}\times\frac{C_2}{K_{s2}+C_2}\times X$$

微生物死亡方程

$$\frac{\partial X}{\partial t}=-v_{dec}\times X$$

好氧微生物

$$\frac{\partial X_i}{\partial t}=Y\left(1-\frac{X_i}{\rho_{X_i}(\varepsilon_0-\theta_r)}\right)V_iX_i\frac{C_{DOC}}{K_{DOC}+C_{DOC}}\frac{C_{DO}}{K_{DO}+C_{DO}}$$

硝酸盐还原微生物

$$\frac{\partial X_i}{\partial t}=Y\left(1-\frac{X_i}{\rho_{X_i}(\varepsilon_0-\theta_r)}\right)V_iX_i\frac{C_{DOC}}{K_{DOC}+C_{DOC}}\frac{C_{NO3-}}{K_{NO3-}+C_{NO3-}}$$

铁锰还原微生物

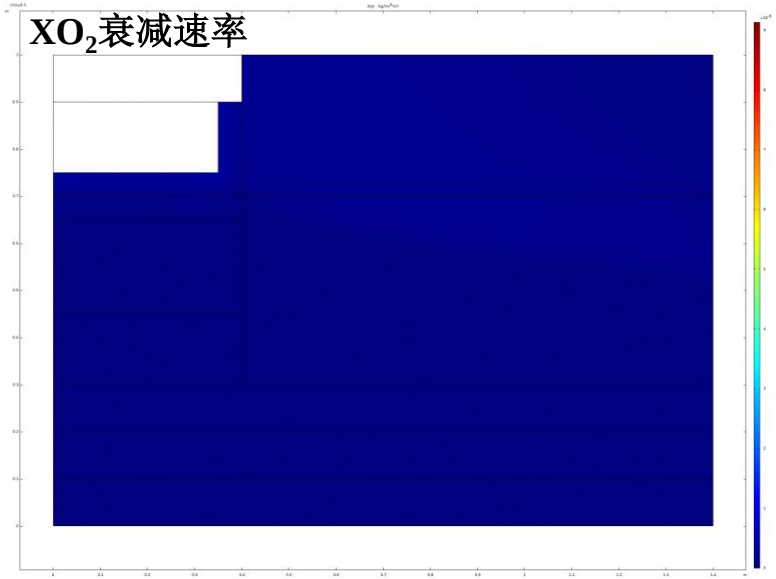
$$\frac{\partial X_i}{\partial t}=Y\left(1-\frac{X_i}{\rho_{X_i}(\varepsilon_0-\theta_r)}\right)V_iX_i\frac{C_{DOC}}{K_{DOC}+C_{DOC}}\frac{C_{Fe(OH)3}}{K_{Fe(OH)3}+C_{Fe(OH)3}}\frac{C_{MnO2}}{K_{MnO2}+C_{MnO2}}$$

硫酸盐还原微生物

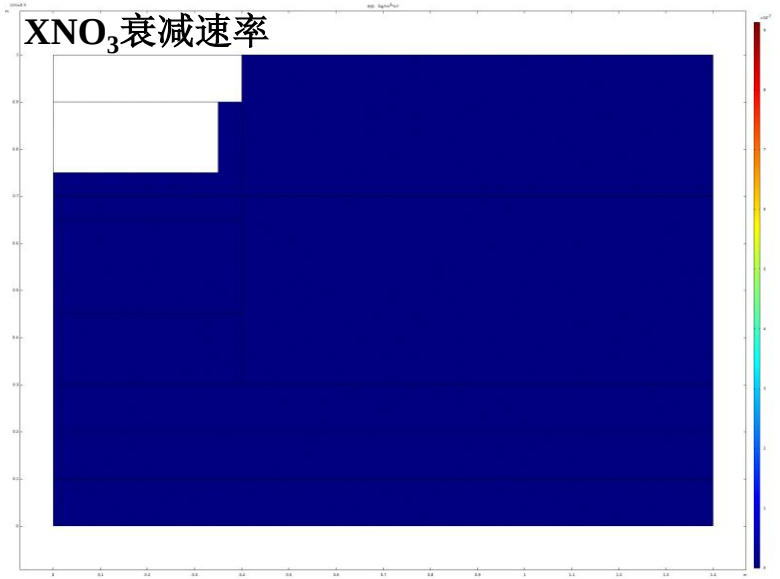
$$\frac{\partial X_i}{\partial t}=Y\left(1-\frac{X_i}{\rho_{X_i}(\varepsilon_0-\theta_r)}\right)V_iX_i\frac{C_{DOC}}{K_{DOC}+C_{DOC}}\frac{C_{SO42-}}{K_{SO42-}+C_{SO42-}}$$

微生物繁殖衰减速率

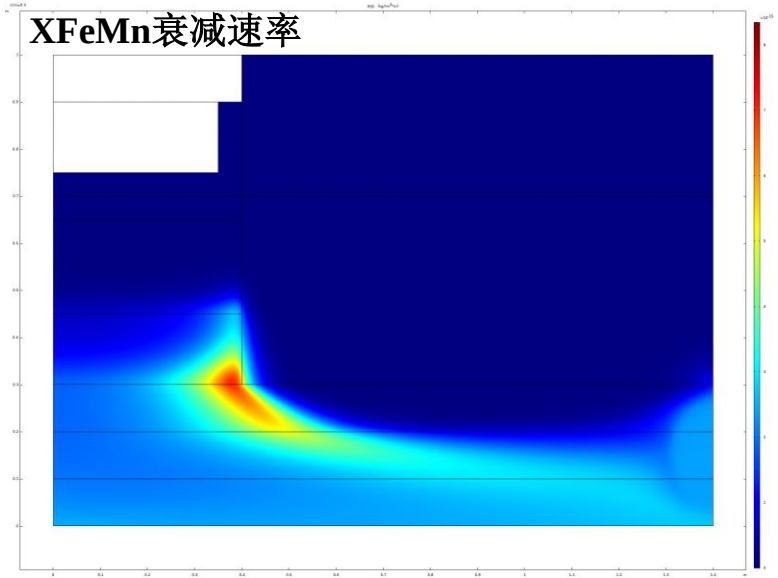
XO_2衰减速率



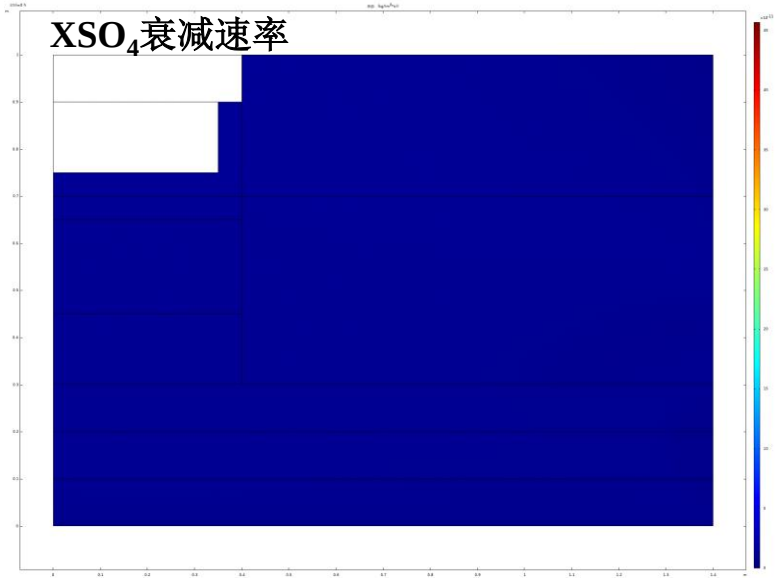
XNO_3衰减速率



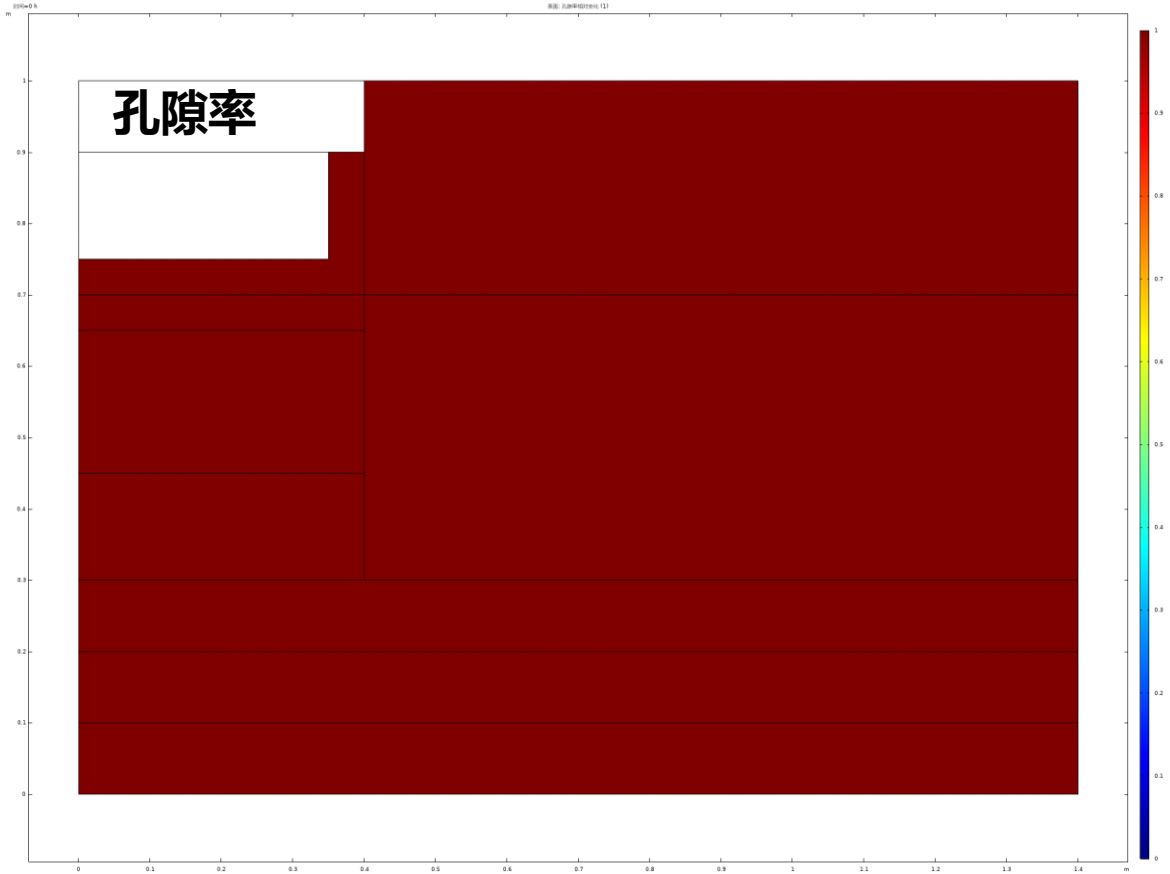
XFeMn衰减速率

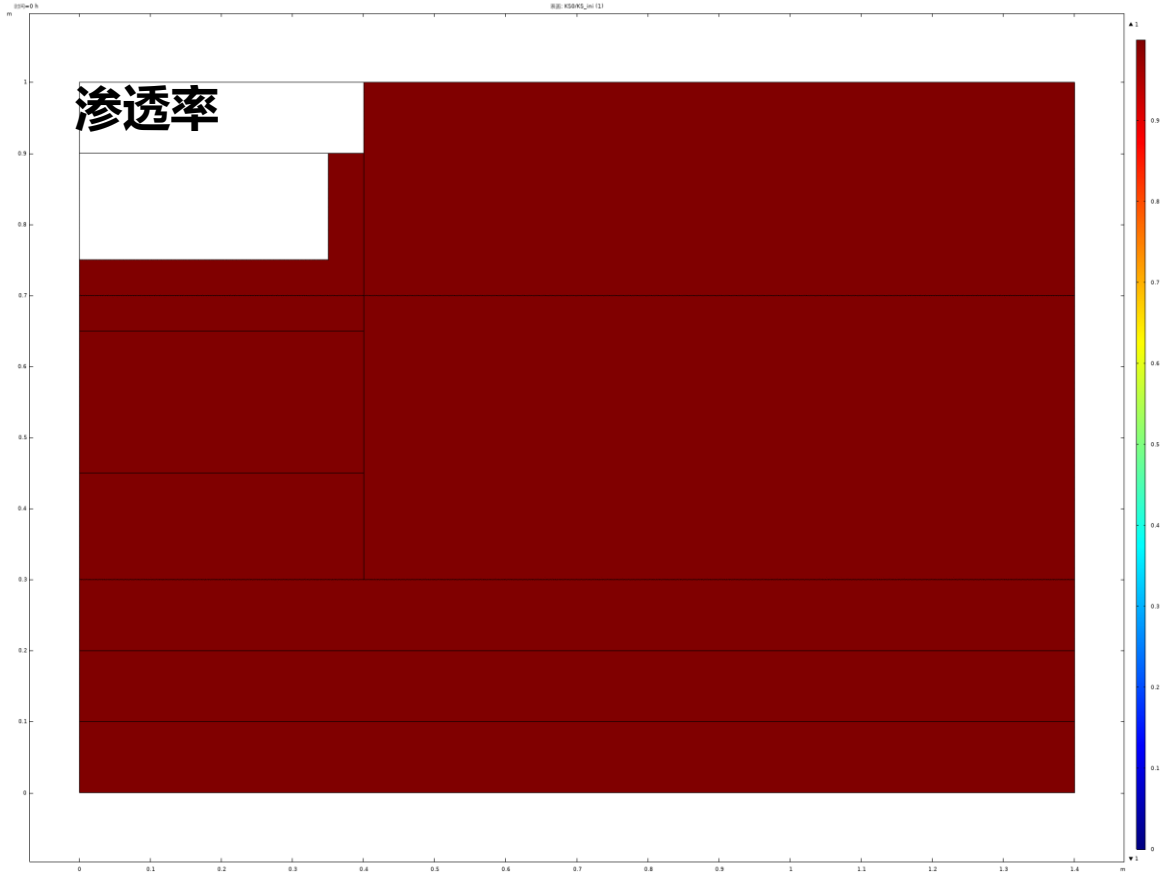


XSO_4衰减速率



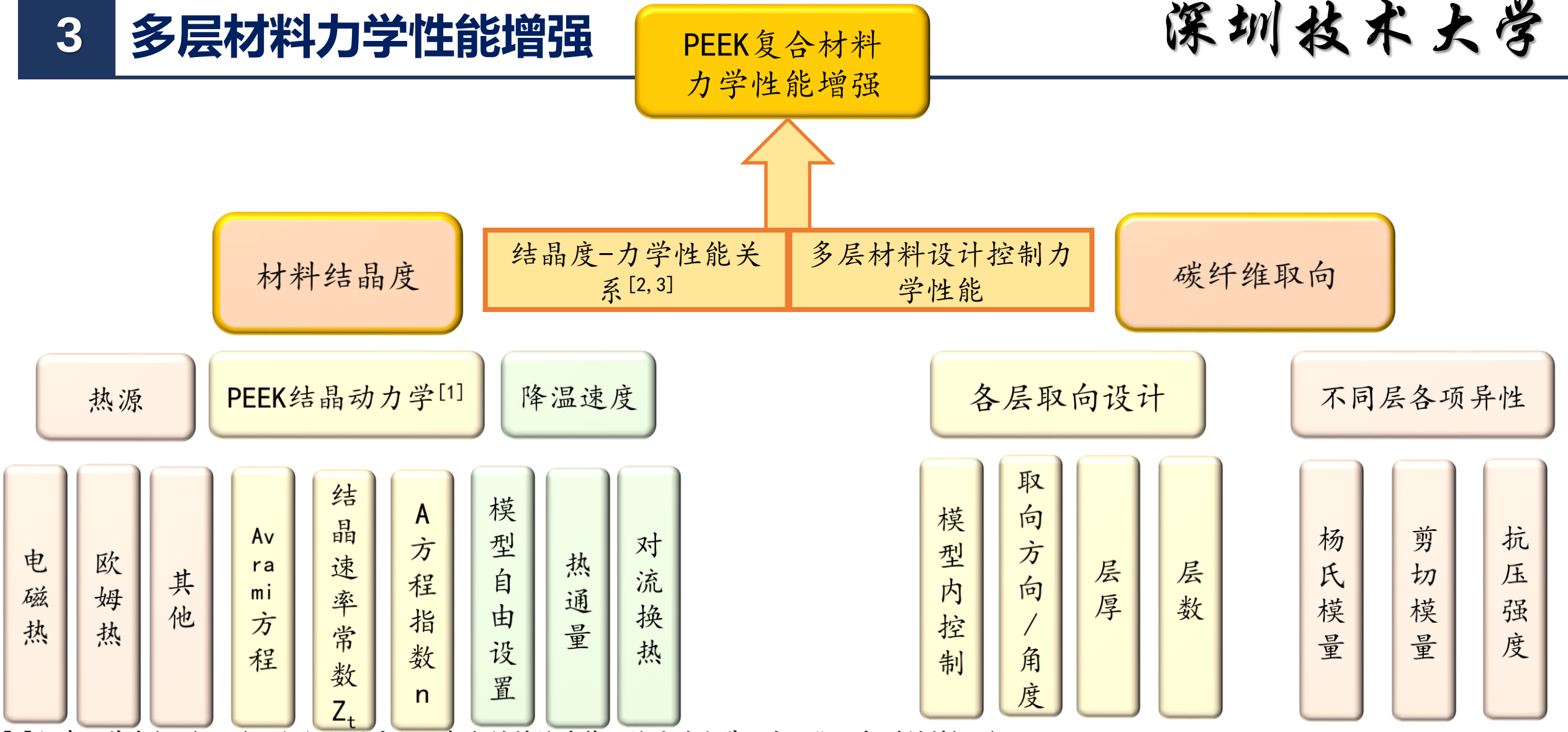
微生物淤积导致孔隙率（左）和渗透率（右）相对变化





3 多层材料力学性能增强

深圳技术大学



[1]倪卓，莫少妮（2022）. 短纤维填充peek复合材料的非等温结晶动力学研究. *化工新型材料*(002)，050.

[2]Dong Yang, Yi Cao, Effects of crystallinity control on mechanical properties of 3D-printed short-carbon-fiber-reinforced polyether ether ketone composites,Polymer Testing,Volume 97,2021,107149

[3] Satheesh B ,et al.Peel strength characterisation on ply/ply interface using wedge and T-peel/pull-type tests[J].Polymers and Polymer Composites, 2018, 26(8-9):096739111880920.DOI:10.1177/0967391118809205.

失效准则

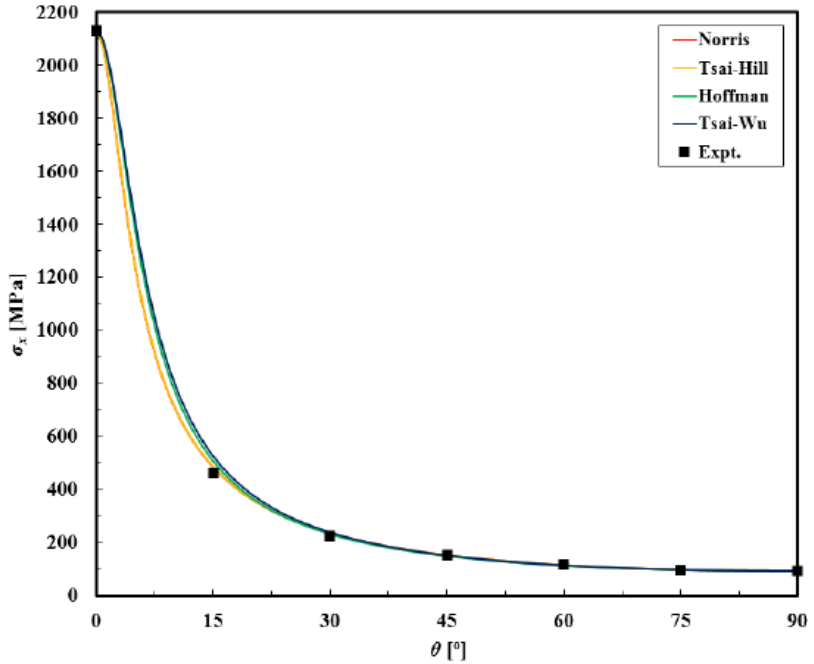


图1 AS4/PEEK单向板偏轴拉伸强度
理论预测曲线与试验数据对比[1]

表1 国际常用失效准则[1]

max stress [20]	$\left(\left\|\frac{\sigma_x}{X}\right\|,\left\|\frac{\sigma_y}{Y}\right\|,\left\|\frac{\tau_{xy}}{S}\right\|\right)=1$	(1)
Tsai-Hill [21]	$\left(\frac{\sigma_x}{X}\right)^2-\frac{\sigma_x\sigma_y}{X^2}+\left(\frac{\sigma_y}{Y}\right)^2+\left(\frac{\tau_{xy}}{S}\right)^2=1$	(2)
Hoffman [22]	$\frac{\sigma_x^2}{X_tX_c}+\frac{\sigma_y^2}{Y_tY_c}+\frac{\tau_{xy}^2}{S^2}-\frac{\sigma_x\sigma_y}{X_tX_c}+\frac{\sigma_x}{X_tX_c}+\frac{\sigma_y}{Y_tY_c}=1$	(3)
Hashin [22]	$\left(\frac{\sigma_x}{X_t}\right)^2+\left(\frac{\tau_{xy}}{S}\right)^2=1,\sigma_x>0;-\frac{\sigma_x}{X_c}=1,\sigma_x<0$ $\left(\frac{\sigma_y}{Y_t}\right)^2+\left(\frac{\tau_{xy}}{S}\right)^2=1,\sigma_y>0$ $\left(\frac{\sigma_y}{2S}\right)^2+\left(\frac{\tau_{xy}}{S}\right)^2+\left[\left(\frac{Y_c}{2S}\right)^2-1\right]\frac{\sigma_y}{Y_c}=1,\sigma_y<0$	(4)
Tsai-Wu [23]	$\left(\frac{1}{X_t}-\frac{1}{X_c}\right)\sigma_x+\left(\frac{1}{Y_t}-\frac{1}{Y_c}\right)\sigma_y+\frac{1}{X_tX_c}\sigma_x^2+\frac{1}{Y_tY_c}\sigma_y^2+2a_{xy}\sqrt{\left(\frac{1}{X_tX_c}\frac{1}{Y_tY_c}\sigma_x\sigma_y\right)}+\frac{1}{S^2}\tau_{xy}^2=1$	(5)
Puck [24,25]	$\left\|\frac{\sigma_x}{X_t}\right\|=1,\sigma_x>0;\left\|\frac{\sigma_x}{X_c}\right\|=1,\sigma_x<0$ $\sqrt{\left(\frac{\tau_{xy}}{R_{\perp\parallel}}\right)^2+\left(1-p_{\perp\parallel}^{(+)}\frac{R_\perp^{(+)}}{R_{\perp\parallel}}\right)^2\left(\frac{\sigma_y}{R_\perp^{(+)}}\right)^2}+p_{\perp\parallel}^{(+)}\frac{\sigma_y}{R_{\perp\parallel}}=1,\sigma_y\geq0$ $\frac{1}{R_{\perp\parallel}}\left(\sqrt{\tau_{xy}^2+\left(p_{\parallel\perp}^{(-)}\sigma_y\right)^2}+p_{\parallel\perp}^{(-)}\sigma_y\right)=1,\sigma_y<0,\left\|\frac{\sigma_y}{\tau_{xy}}\right\|\leq\frac{R_{\perp\perp}^A}{\left\|\tau_{xyc}\right\|}$ $\left[\left(\frac{\tau_{xy}}{2\left(1+p_{\perp\perp}^{(-)}\right)R_{\perp\parallel}}\right)^2+\left(\frac{\sigma_y}{R_\perp^{(-)}}\right)^2\right]\frac{R_\perp^{(-)}}{-\sigma_y}=1,\sigma_y<0,\left\|\frac{\sigma_y}{\tau_{xy}}\right\|\geq\frac{R_{\perp\perp}^A}{\left\|\tau_{xyc}\right\|}$	(6)

当前模型用的是Tasi-Hill准则：
在各向同性 von-Mises准则基础上，引入各向异性强度参数，将其推广到正交各向异性材料中[3]。

[1]蔡登安. 纤维增强复合材料的力学行为与多轴疲劳性能研究[D]. 南京航空航天大学, 2018.

[2] Merhar M .Application of Failure Criteria on Plywood under Bending[J].Polymers, 2021, 13.DOI:10.3390/polym13244449.

[3]谈炳东, 郑健, 许进升, 等. 短纤维增强三元乙丙薄膜拉伸破坏率相关Tsai-Hill强度准则[J]. 复合材料学报, 2018, 35(6):6.

结晶度　热源位置升温快，因此热源位置降温速度也更快，结晶程度更高

时间=540 s　表面: 降温/升温速率 (K/s)

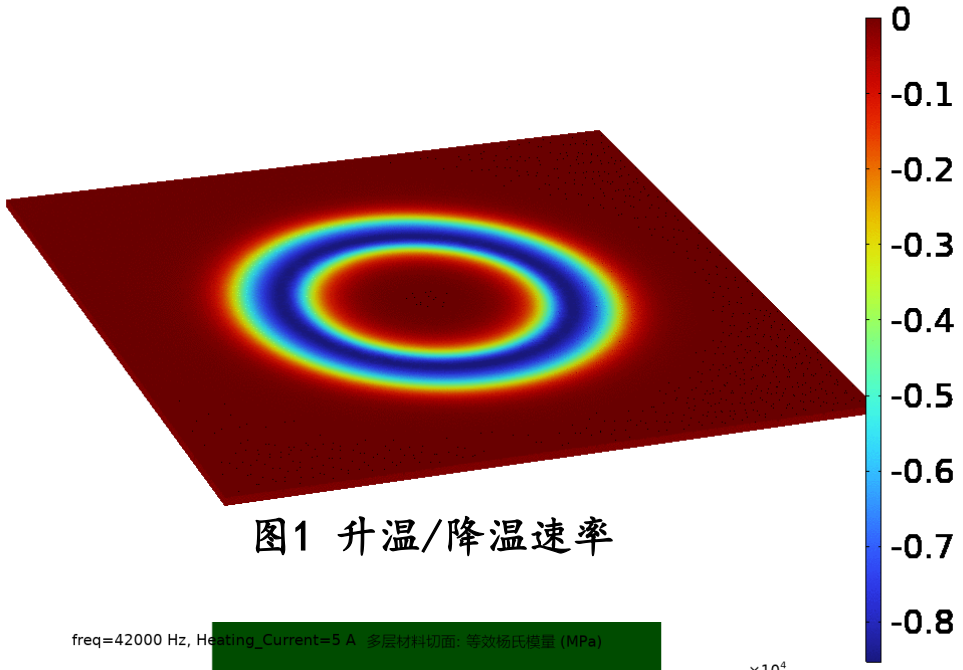
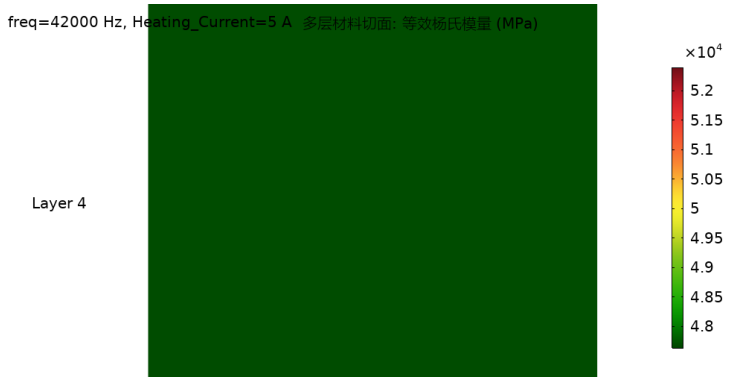


图1 升温/降温速率



时间=0 s　表面: Dependent variable crystal (1)

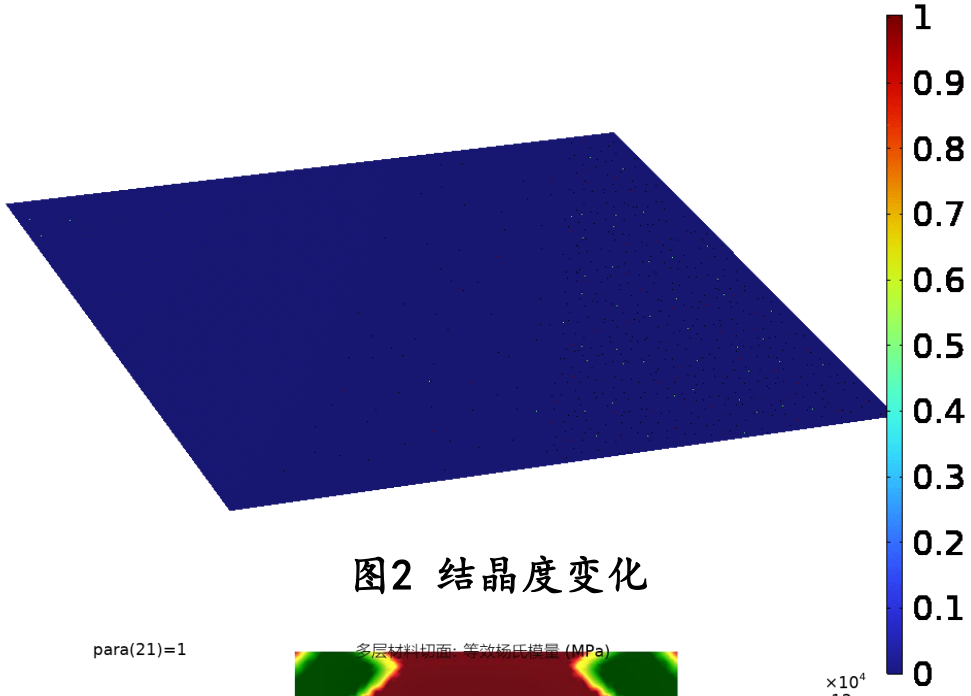
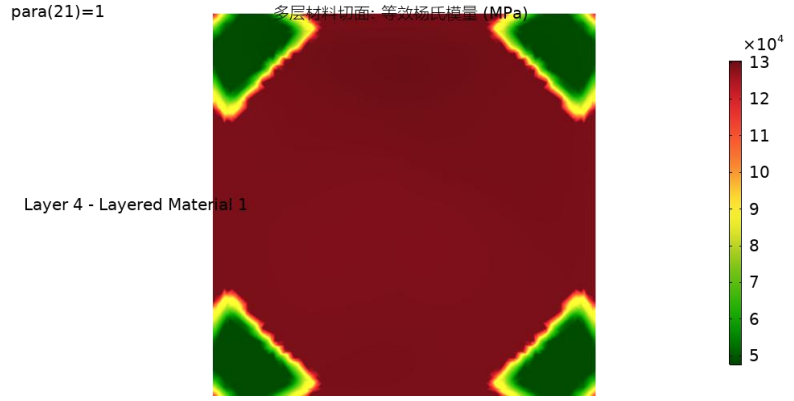
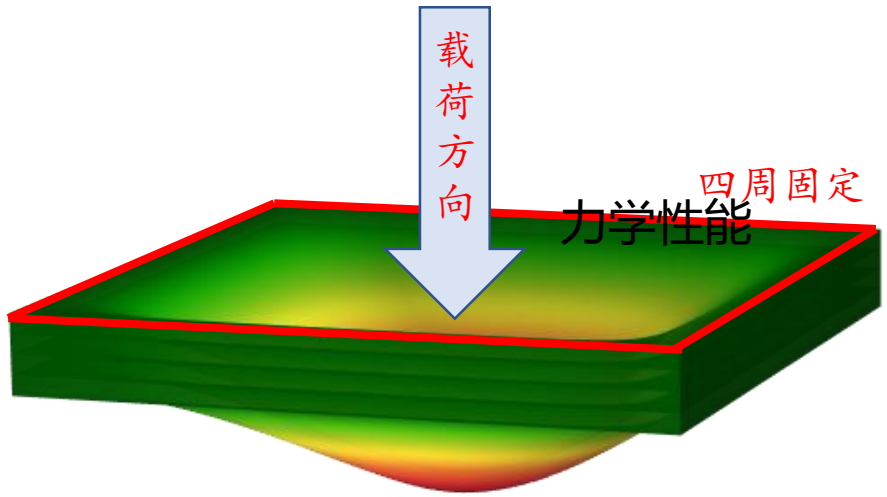
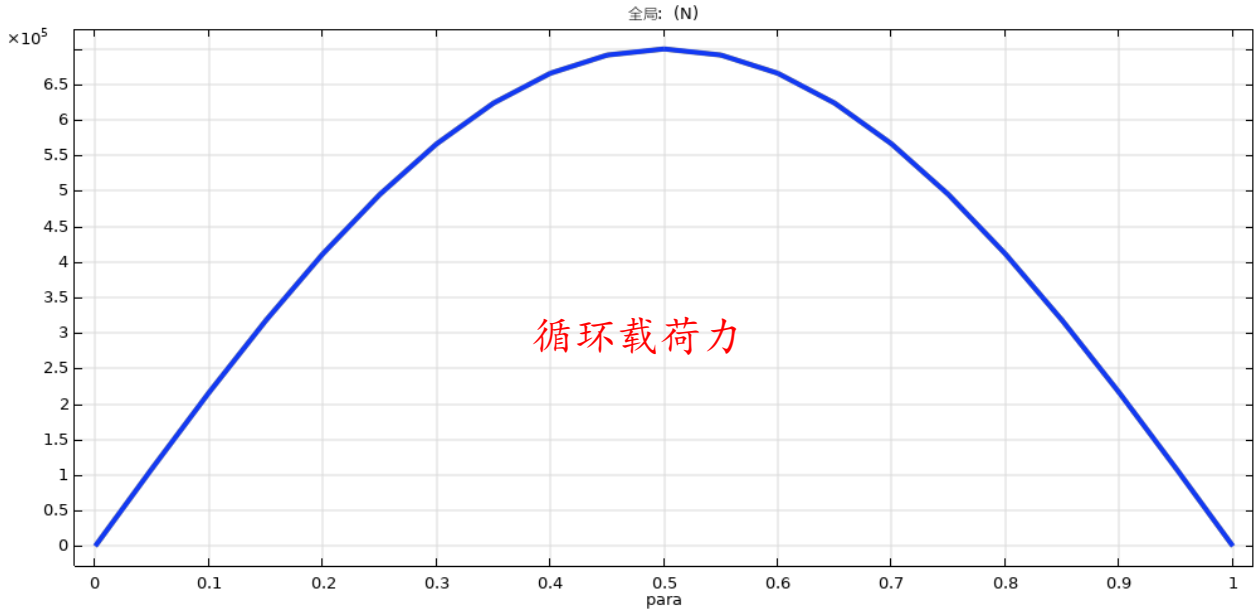


图2 结晶度变化



力学性能


载荷方向
四周固定
力学性能


全局: (N)
×10^5
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
para
循环载荷力

感谢各位同仁聆听，

希望和各位同仁多多探讨、交流。

手机号：17366236063
微信号：ZZZker1112