热电相移器仿真

2019.03.13 畅星兆

衡量热电调制器的几个参数

Table 1. Summary of recent thermo-optic waveguide phase shifter parameters where L is the total heater length, V_π and P_π are the applied voltage and power necessary to reach π radians of phase shift, respectively, and τ is the limiting rise or fall time constant. In results where τ is not reported, the single-pole approximation $\tau = \frac{0.35}{f_3 dB}$ is used to convert between metrics.

	Material	Cladding	L (μ m)	Loss (dB)	V_π (V)	P_π (mW)	τ (μs)	$P_\pi \cdot \tau$ (mW·μs)
Here	SOI	SiO_2	61.6	0.23 dB	4.36	24.77	2.69	66.9
[10]	Si	Air	>9.42	0.5 dB	11.93	12.7	2.4	30.5
[12]	TiN in SOI	Air	1000	0.3 dB	0.86	0.49	144	70.5
[11]	NiSi in SOI	Air	200	5 dB	1	20	2.8	56
[17]	Cr-Au in SOI	SiO_2	700	32 dB	1.66	46	3.5	160
[14]	Ti in SOI	Air	100	8 dB	13.3	10.6	34.9	370
[16]	Metal in SOI	SiO_2	2500	< 12 dB	-	235	60	14100

需要关注的参数: material, length, loss, V_π, P_π, τ, $P_\pi \cdot \tau$

Harris, Nicholas C et al., Efficient, compact and low loss thermo-optic phase shifter in silicon, Optics express, 2014.

对流换热系数

- 单位温差时的单位面积上的热通量, 单位: $W/(m^2 \cdot K)$

影响因素:

1.对流运动成因和流动状态

2.流体的物理性质(随种类、温度和压力而变化)

3.传热表面的形状, 尺寸和相对位置

4.流体有无相变(如气态与液态之间的转化)

对流换热系数的大致量级:

空气自然对流: 5 – 25	气体强制对流 20 ~ 300	水的自然对流 200 ~1000
水的强制对流 1000 ~ 15000	油类的强制对流 50 ~ 1500	水蒸气的冷凝 5000 ~ 15000
有机蒸汽的冷凝 500 ~ 2000	水的沸腾 2500 ~ 25000	

3类边界条件

1. 第一类边界条件 规定了边界上的温度值

$$\text{当}\tau > 0\text{时}, \mathrm{t}_w = f_1(\tau)$$

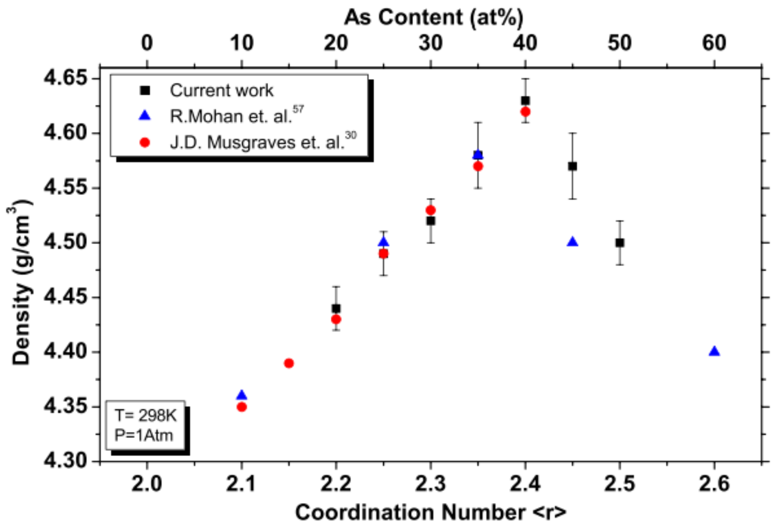
2. 第二类边界条件 规定了边界上的热流密度值

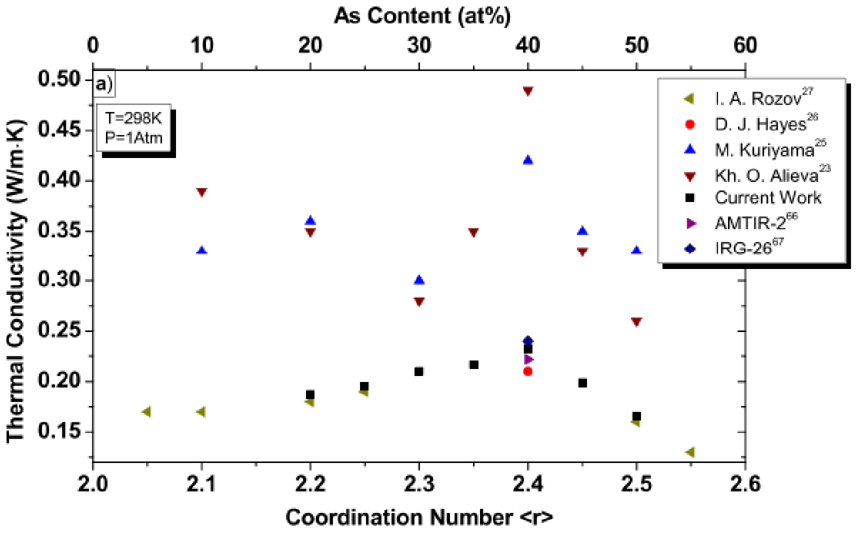
$$\text{当}\tau > 0\text{时}, -\lambda\left(\frac{\partial \mathrm{t}}{\partial x}\right)_w = f_2(\tau)$$

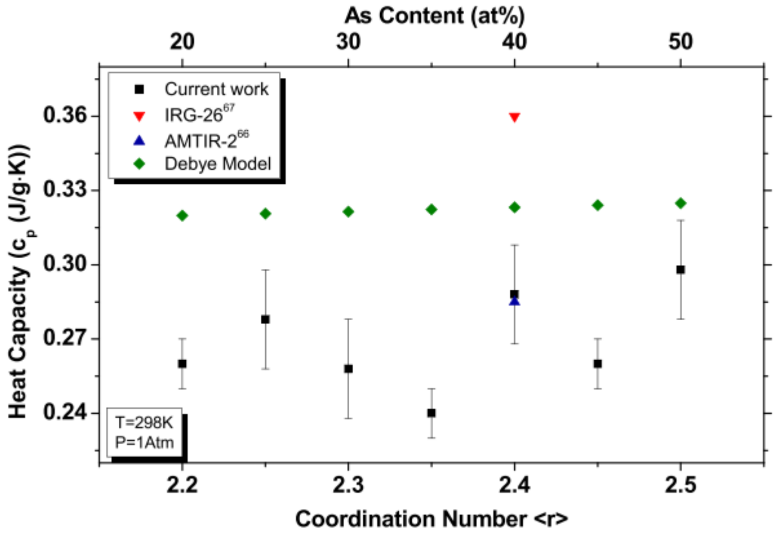
3. 第三类边界条件 规定了边界条件上表面传热系数以及外界温度

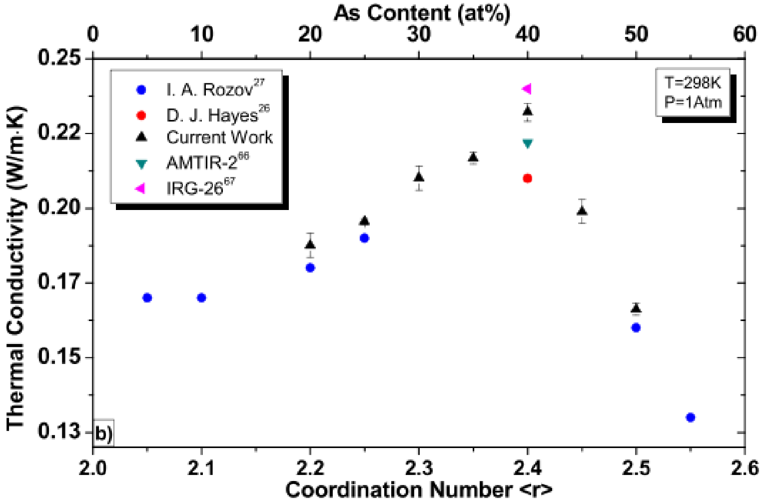
$$\text{当}\tau > 0\text{时}, -\lambda\left(\frac{\partial \mathrm{t}}{\partial x}\right)_w = h\left(\mathrm{t}_w - \mathrm{t}_f\right)$$

硫系玻璃(chalcogenide glasses)的热学属性









硫系玻璃总结:

密度(density):

$\sim 4500\ kg/m^3$

比热容(heat capacity):

$\sim 300\ J/kg \cdot K$

导热系数(thermal conductivity):

$\sim 0.3\ \mathrm{W}/m \cdot K$

Jason Lonergan et al., Thermophysical properties and conduction mechanisms in AsxSe1−x chalcogenide glasses ranging from x = 0.2 to 0.5, Journal of Applied Physics, 2016

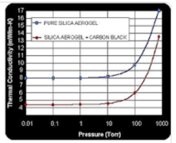
气凝胶(silica aerogel)的热学属性

丸子
对外贸易

导热系数极低。国外阿斯彭气凝胶常温下可以做到0.013。国内气凝胶常温下的导热系数最好可以做到0.017。气凝胶是目前已知的固体材料中，在两百度内保温效果最好的产品。普通隔热材料，例如高温玻璃棉，常温下的导热系数在0.045左右。这意味着1cm厚的气凝胶的保温效果相当于3cm厚的玻璃棉。

使用温度：-200C~650C. 能够满足绝大多数保温温度的需求。

A typical silica aerogel has a total thermal conductivity of ~0.017 W/mK (~R10/inch). A major portion of this energy transport results from the gases contained within the aerogel.



Thermal Properties of Silica Aerogels | The Norris Research ...
https://pamelanorris.wordpress.com › resources › thermal-properties

AEROGEL THERMAL CONDUCTIVITY RESULTS

The aerogel blanket displayed a thermal conductivity reading of 0.024 W/mK at 20˚C.

According to the manufacturer, the known thermal conductivity of this aerogel blanket is 0.023 W/mK at 100˚C. As can be seen, by these results, a close correlation exists between the stated manufactured thermal conductivity and the

Aerogels Products

Supplier	Product	Thermal conductivity [W / m K]	Density [g / cc]	Min. Temp. [°C]	Max. Temp. [°C]	Material
Aspen Aerogels	Cryogel Spaceloft Pyrogel	0.0135 0.0125 – 0.0135 0.0145 – 0.0155	0.13 0.17 0.12 – 0.17	-200 -200 -200	40 200 650	Foam-like Hydrophobic Tensile strenght 88kPa
Separex	-	0.005 – 0.02 0.0015 – 0.0085 0.0175 – 0.012	0.1 0.209 0.26	-	-	PU (monolith)
MarkeTech International Inc	-	0.004 (vac.) 0.016 (air)	0.1 (0.01 – 0.3)	-	-	Silica (monolith) Tensile strenght 16kPa
Airglass	Airglass	0.021 (20°C) 0.2 (300°C)	0.05 – 0.2	-	-	Silica (monolith) 60 x 60 x 2 cm³
Cabot Corporation	translucent IR opac. beds Fine particle Aerogel beds	0.018	0.090 – 0.100 0.090 – 0.100 0.040 – 0.100 0.090 – 0.100	-	-	Silica (beads / particles) Hydrophobic
NanoPore	HP-150 HT-170	0.0034 – 0.020 0.0038 – 0.021	0.015 – 0.016 0.0165 – 0.017	-273 -273	150 600	VIP

气凝胶总结:

密度(density):

$\sim 130\ kg/m^3$

比热容(heat capacity):

$1900\ J/kg\cdot K \sim 2300\ J/kg\cdot K$

导热系数(thermal conductivity):

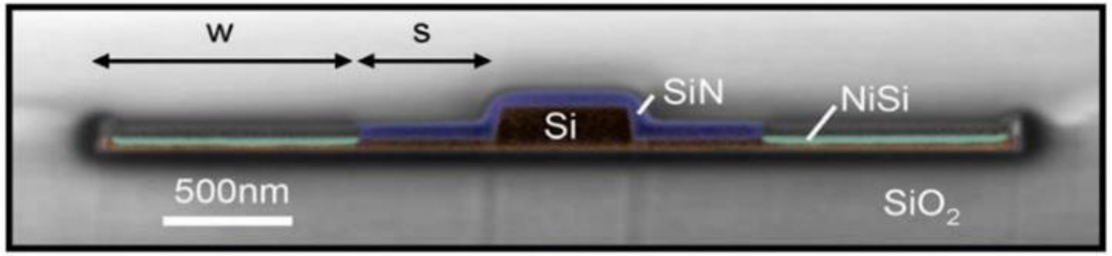
$0.013\ W/m\cdot K \sim 0.024\ W/m\cdot K$

气凝胶的导热系数比空气略低.

http://esther.ist.utl.pt/pages/yurisnight2011/ActiveSpaceTech.pdf

论文

1.



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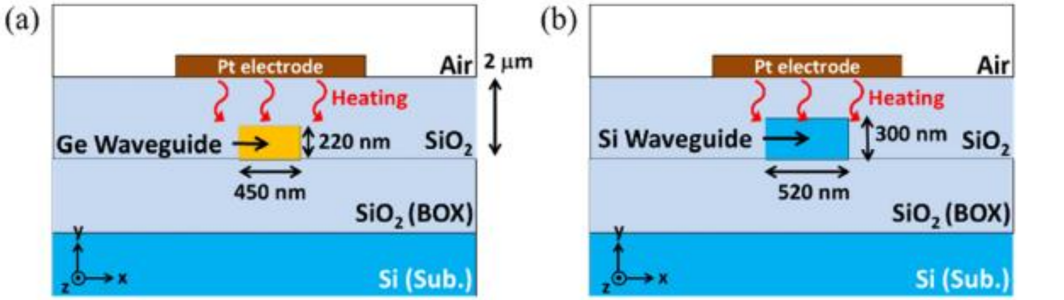
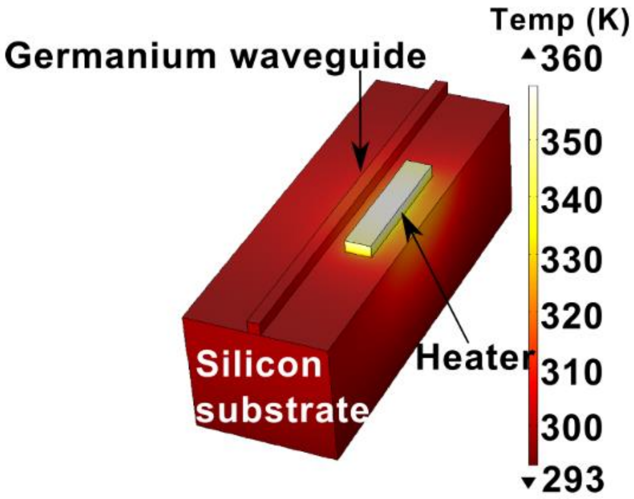


Fig. 1. Cross-sectional schematics of (a) Ge and (b) Si TO phase shifters operating at a wavelength of 1.95 µm.

2.

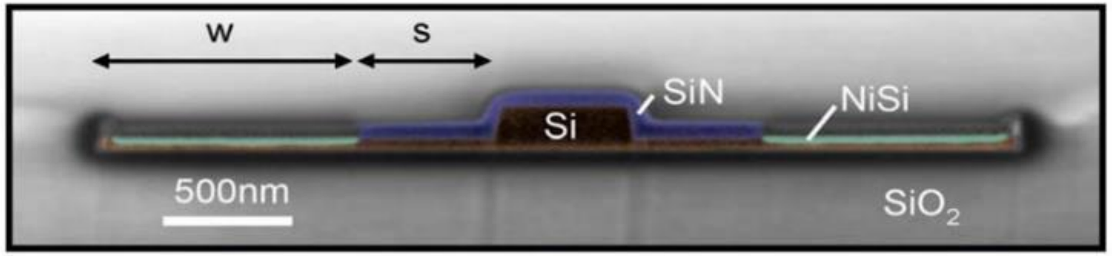


1. Joris Van Campenhout et al., Integrated NiSi waveguide heaters for CMOS-compatible silicon thermo-optic devices, Optics Letters, 2010.

2. Aditya Malik et al., Ge-on-Si and Ge-on-SOI thermo-optic phase shifters for the mid-infrared, Optics Express, 2014

3. Takumi Fujigaki et al., High-efficiency Ge thermo-optic phase shifter on Ge-on-insulator platform, Optics Express, 2019

论文1



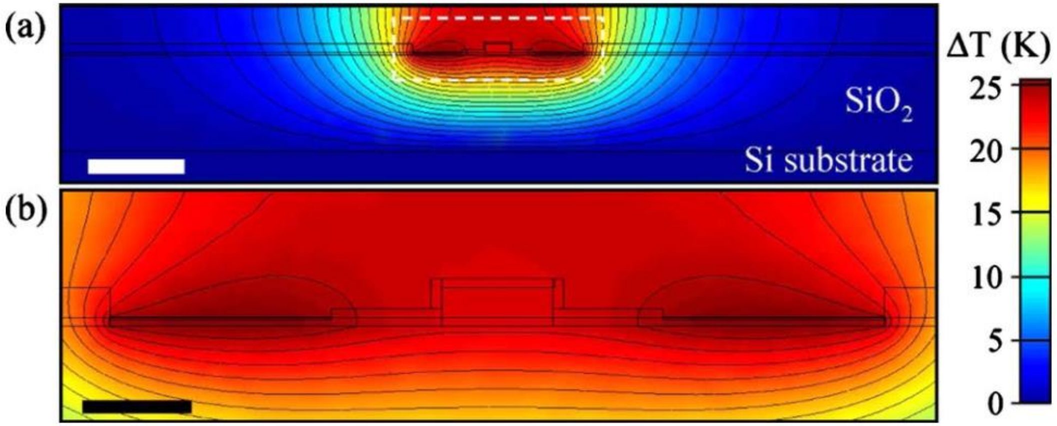


Fig. 4. (Color online) (a) Simulated 2-D distribution of the expected temperature increase (in kelvin) for 0.1 mW/μm power dissipation. The scale bar is 2 μm long. (b) Magnification of (a), showing a temperature increase in the waveguide core of 23 K. The scale bar is 500 nm long.

steady-state 2-D thermal simulation, 设定热源, 边界条件, 初始值, 求稳态解. (只有热学仿真)

热源: 面热源(2D图中为两条线)

$$0.1mW/\mu m \rightarrow 10^8 W/m^2$$

变量: w = 1 um, s = 0.5 um

结果: dt(waveguide) ~ 23K

Joris Van Campenhout et al., Integrated NiSi waveguide heaters for CMOS-compatible silicon thermo-optic devices, Optics Letters, 2010.

问题

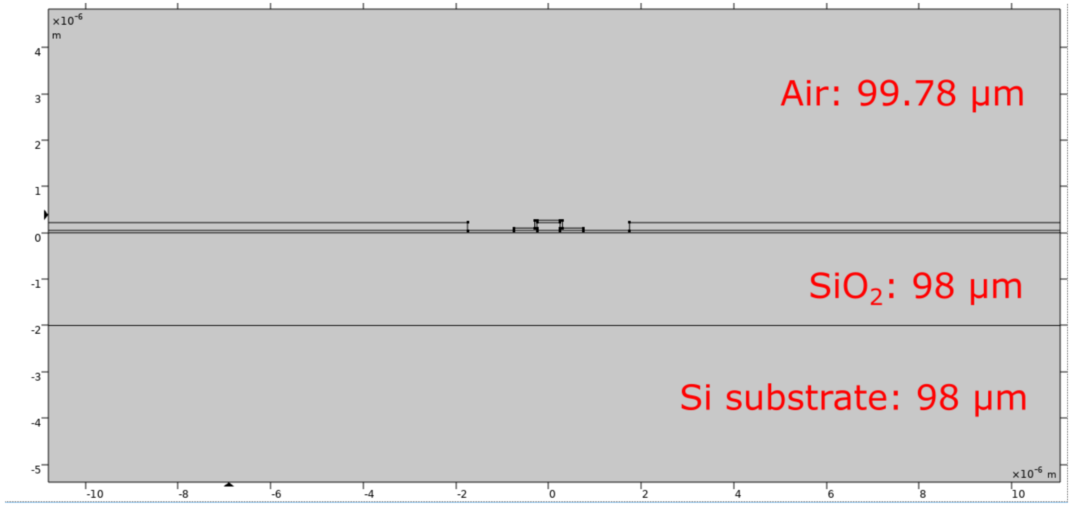
1. 功率的转换

$$0.1mW/\mu m \ \rightarrow \ 5 \times 10^{7} W/m^{2}$$

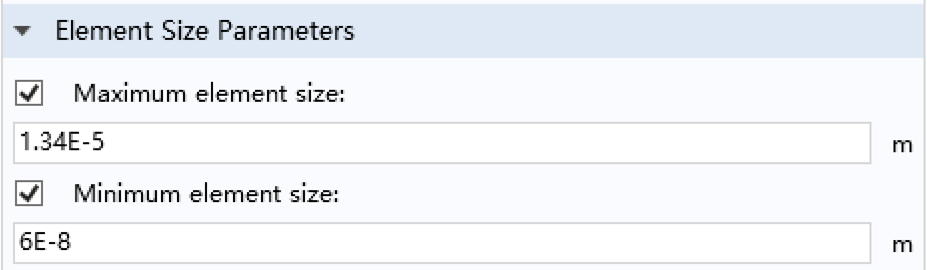
2. 网格密度的确定
3. 边界条件的确定
4. 结构不确定
   - 空气层厚度
   - 仿真区域大小
   - 尝试去掉两边的Si薄板

网格密度的影响

初始结构



网格大小



标签: mesh\initial-right-geo.mph

结果:

所有边界: T = 293.15 K

温度(波导中心): 309.01 K, d = 15.86 K

中间区域:

所有边界: T = 293.15 K
温度(波导中心): 309.01 K, d = 15.86 K

☑ Maximum element size:
1e-6 m
☑ Minimum element size:
60e-9 m

中间区域:

所有边界: T = 293.15 K
温度(波导中心): 309.01 K, d = 15.86 K

☑ Maximum element size:
100e-9 m
☑ Minimum element size:
20e-9 m

外部区域: (之前 1 μm)

所有边界: T = 293.15 K
温度(波导中心): 309.01 K, d = 15.86 K

☑ Maximum element size:
500e-9 m
☑ Minimum element size:
4E-9 m

中间区域:

所有边界: T = 293.15 K
温度(波导中心): 309.02 K, d = 15.87 K

Maximum element size:
50e-9 m
Minimum element size:
10e-9 m

所有边界: T = 293.15 K
温度(波导中心): 309.02 K, d = 15.87 K
标签: mesh\initial-right-geo-mesh-
extr

Maximum element size:
1e-6 m
Minimum element size:
60e-9 m

Maximum element size:
50e-9 m
Minimum element size:
10e-9 m

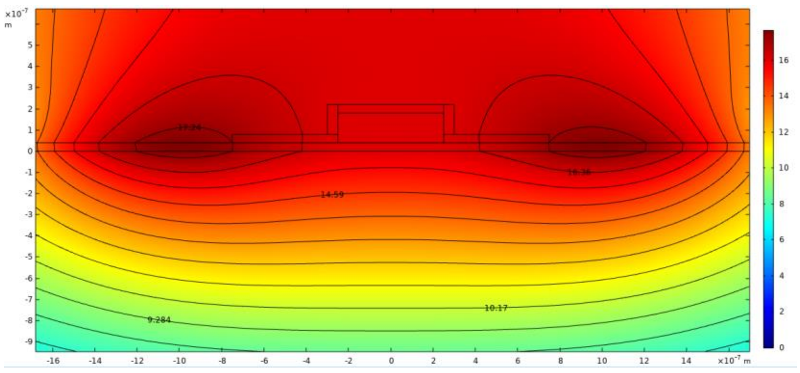
Maximum element size:
250e-9 m
Minimum element size:
4E-9 m

结论:

在该区间内加密网格对结果基本没有影响.

网格密度(max-size: 1e-6m, min-size: 60e-9m)足够.

边界条件的确定



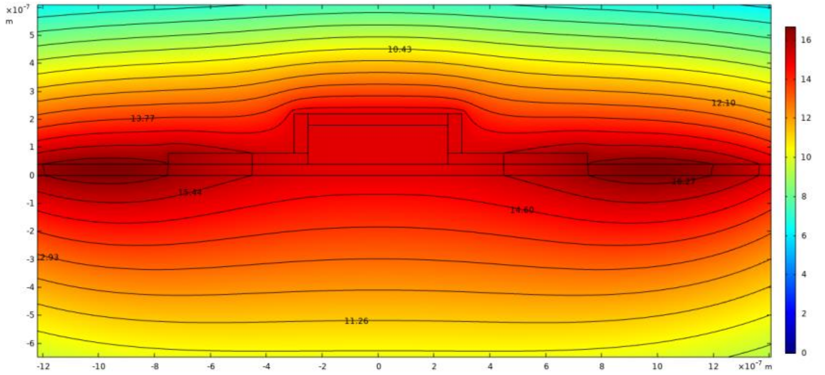
左右下边界: T = 293.15 K

上边界: heat flux 热交换,

T = 293.15 K, $h = 25\ W/(m^2 \cdot K)$

温度(波导中心): 309.21 K,

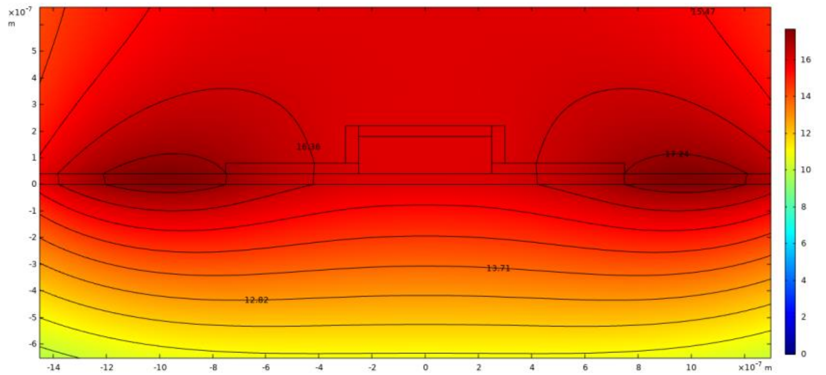
d = 16.06 K



所有边界: T = 293.15 K

温度(波导中心): 308.23 K,

d = 15.08 K



左右下边界: T = 293.15 K

上边界: heat flux 热交换,

T = 293.15 K, $h = 5\ W/(m^2 \cdot K)$

温度(波导中心): 309.21 K,

d = 16.06 K

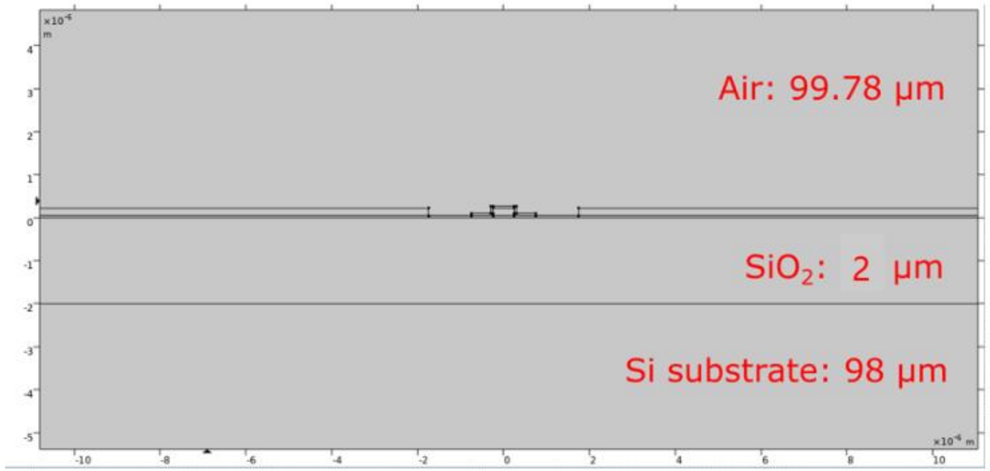
结论:

1. 排除四个边界均为恒温的情况
2. 边界条件应为: 左右下边界恒温, 上边界恒定热流密度. (实际情况的理想化) 同时, 这一情况也与文中的温度分布更相符.

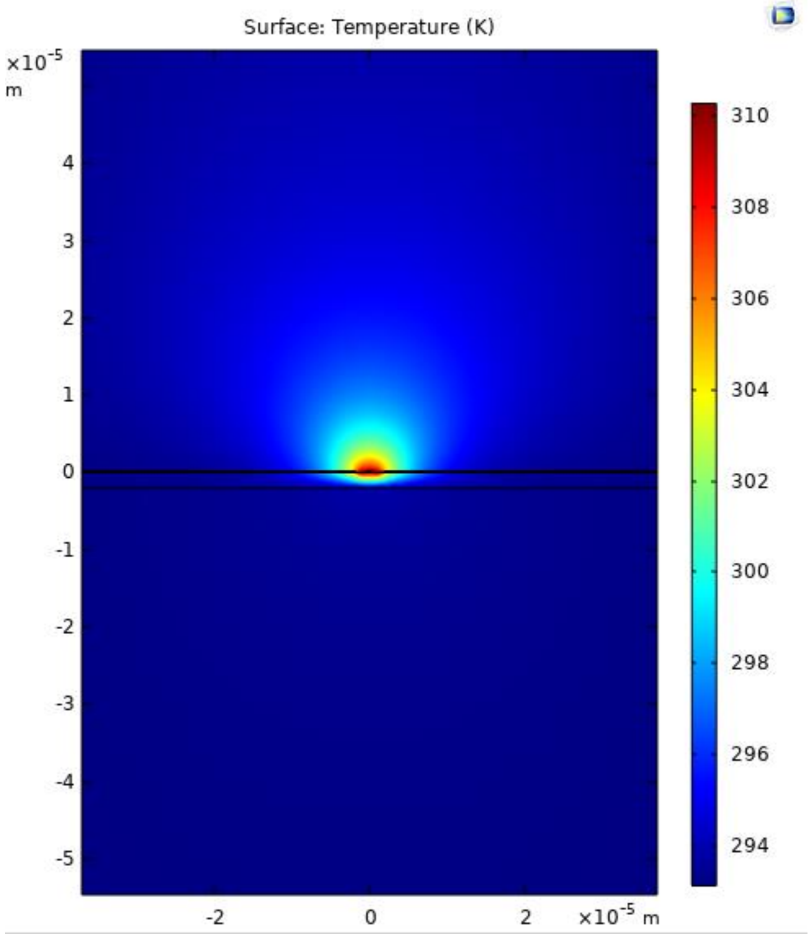
增大仿真区域

改变结构

1. 仿真区域: [μm] 100 x 200 (w, h)

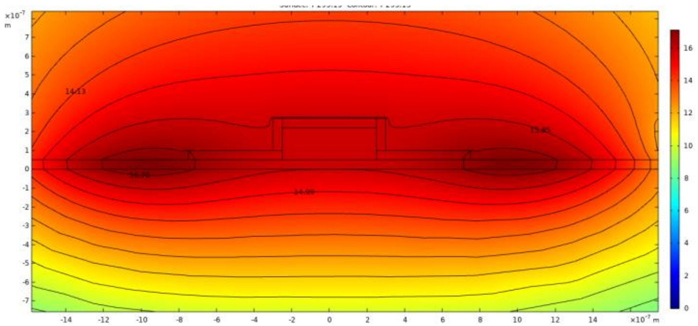


仿真区域大小



整个区域温度分布

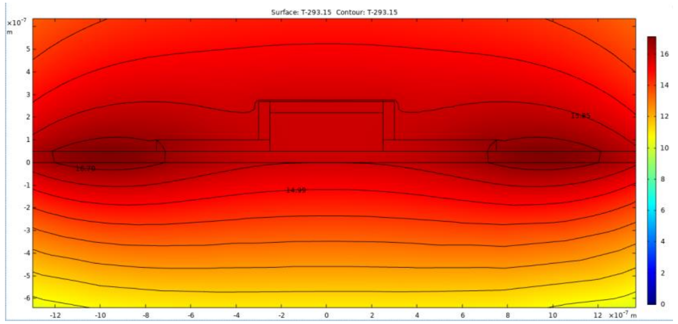
增大仿真区域



左右下边界: T = 293.15 K

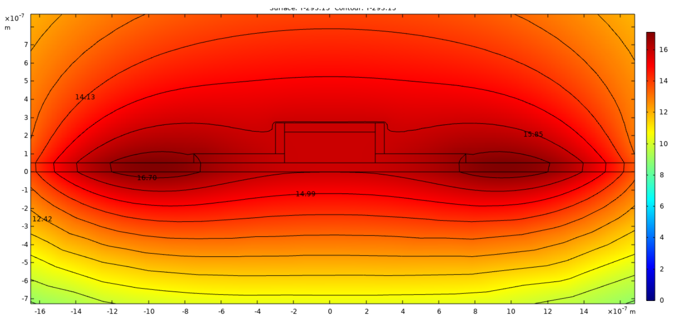
上边界: heat flux 热交换, T = 293.15 K, $h = 25\, W/(m^2 \cdot K)$

温度(波导中心): 309.01 K, d = 15.86 K



所有边界: T = 293.15 K

温度(波导中心): 309.01 K, d = 15.86 K



左右下边界: T = 293.15 K

上边界: heat flux 热交换, T = 293.15 K, $h = 5\, W/(m^2 \cdot K)$

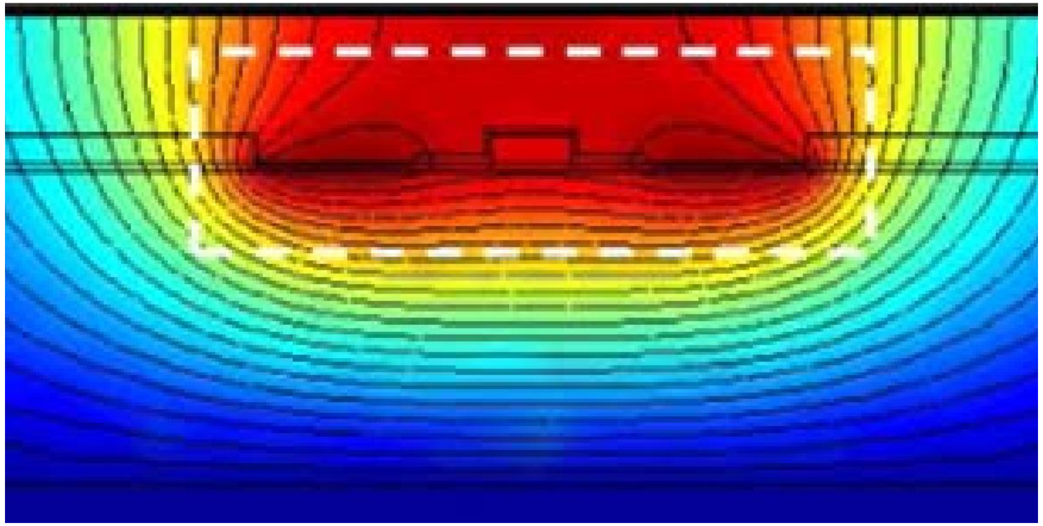
温度(波导中心): 309.01 K, d = 15.86 K

结论:

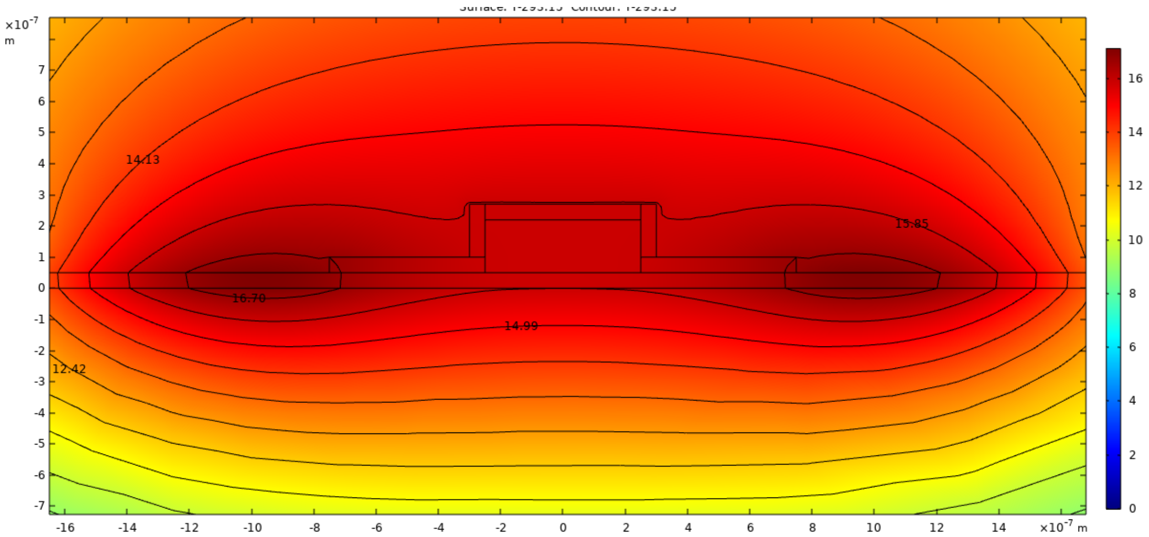
1. 增大仿真区域基本不改变中心区域温度分布
2. 影响成二次方衰减 (中心区域周围的材料对于温度分布的影响更为关键)

去掉两边的Si薄板

原因: 仿真论文中的等温线十分平滑



论文中的



我的

去掉两边的Si薄板

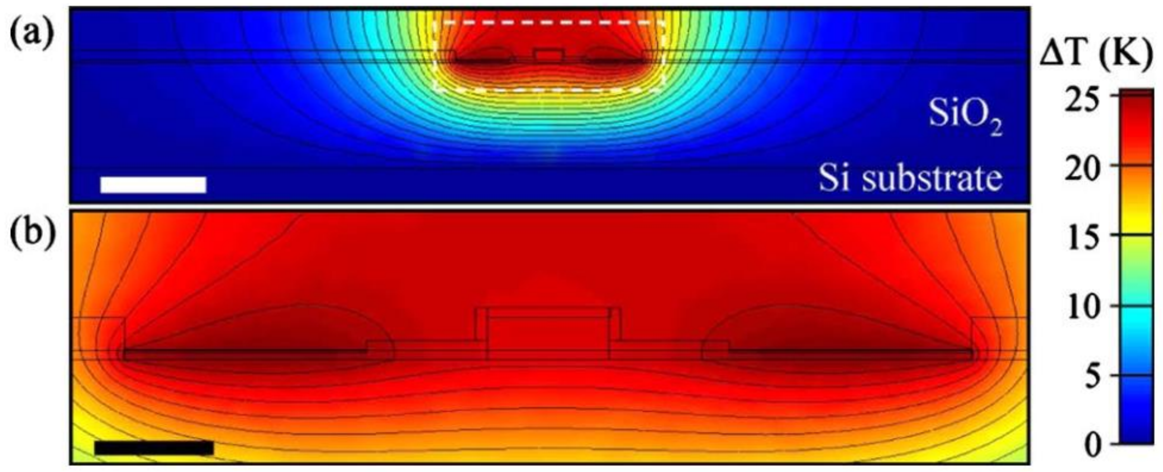
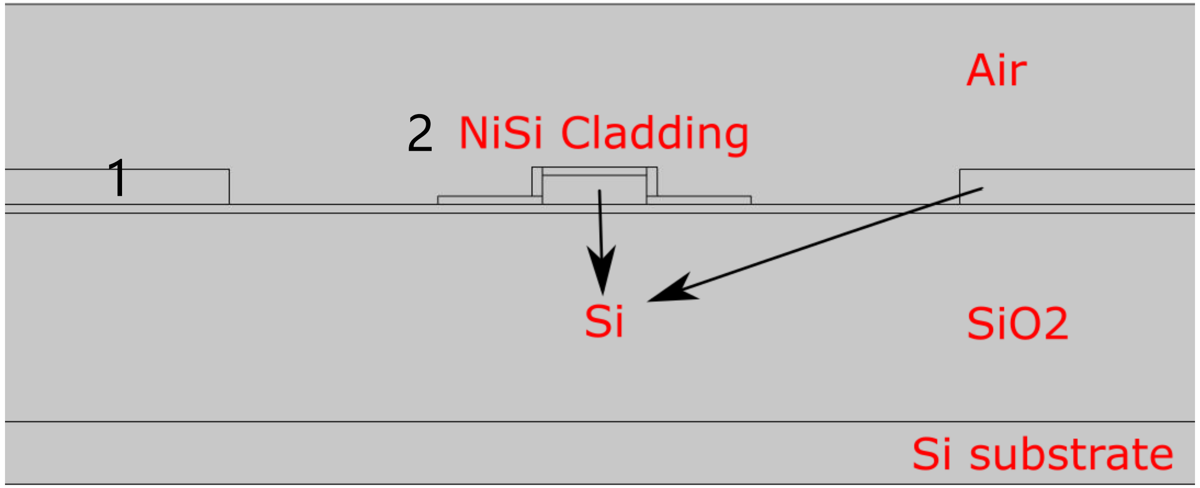


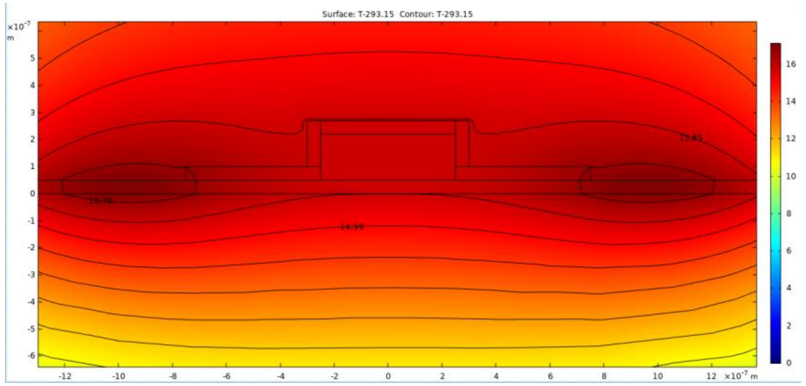
Fig. 4. (Color online) (a) Simulated 2-D distribution of the expected temperature increase (in kelvin) for 0.1 mW/μm power dissipation. The scale bar is 2 μm long. (b) Magnification of (a), showing a temperature increase in the waveguide core of 23 K. The scale bar is 500 nm long.

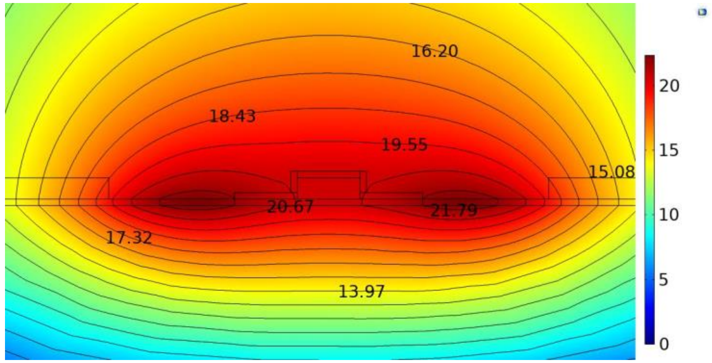


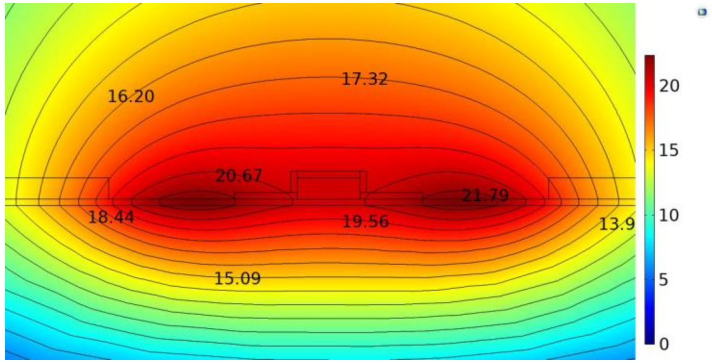
task:

1. 只去掉周围Si平板
2. NiSi也同时去掉

去掉两边的Si薄板







原始

温度(波导中心): 309.01 K,
d = 15.86 K

只去掉周围Si平板

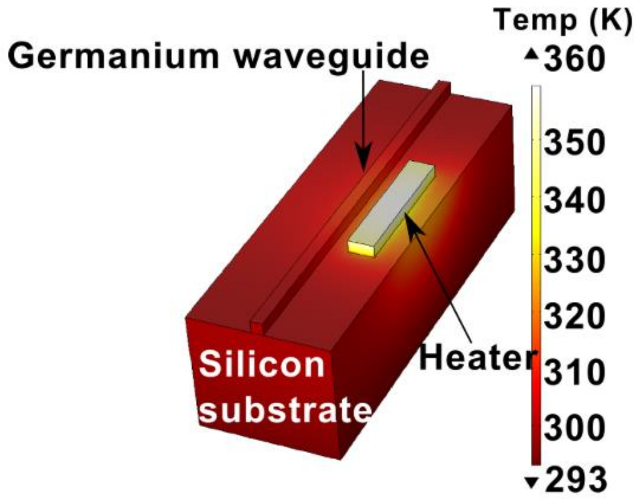
dT = 20.60 K

Si3N4也同时去掉

dT = 20.57 K

结论：温度变化对于周围结构（的导热系数） 很敏感。

论文2



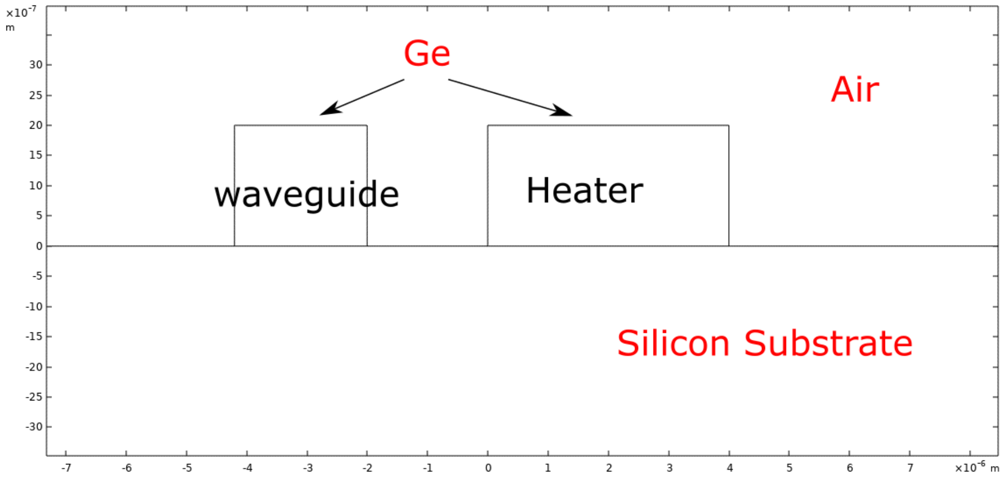
二维以及三维结构

单边加热

波导:[μm] 2.2 x 2 x 1100

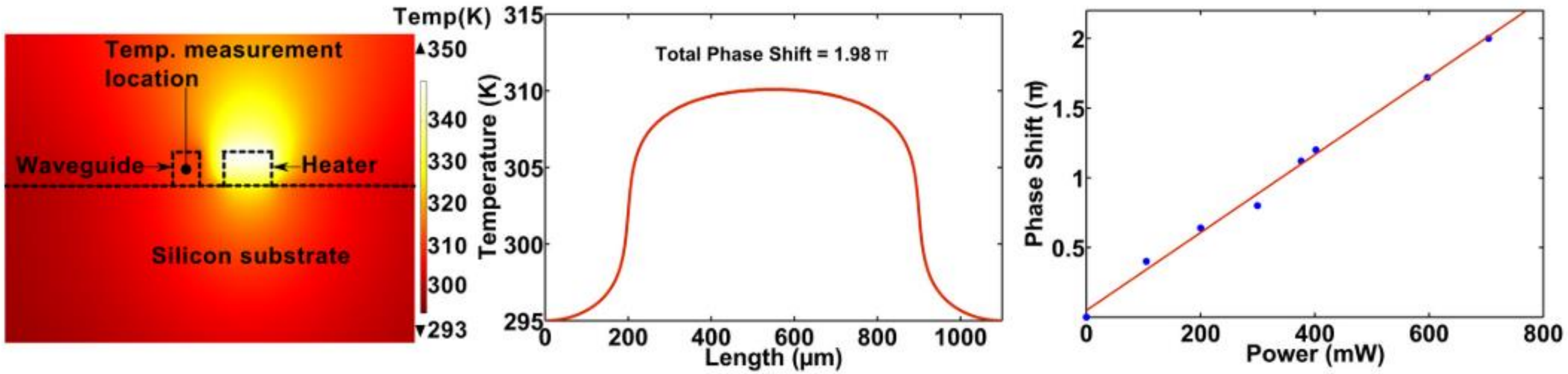
heater: :[μm] 4 x 2 x 700

功率: 700 mW



Aditya Malik et al., Ge-on-Si and Ge-on-SOI thermo-optic phase shifters for the mid-infrared, Optics Express, 2014

论文中的仿真



(a) (b) (c)

1. 三维仿真
2. 波导中心直线上温度分布
3. 由2求得相位变化

问题

1. 复现结果
2. 网格密度的确定
3. 边界条件的确定
4. 结构的确定

Initial

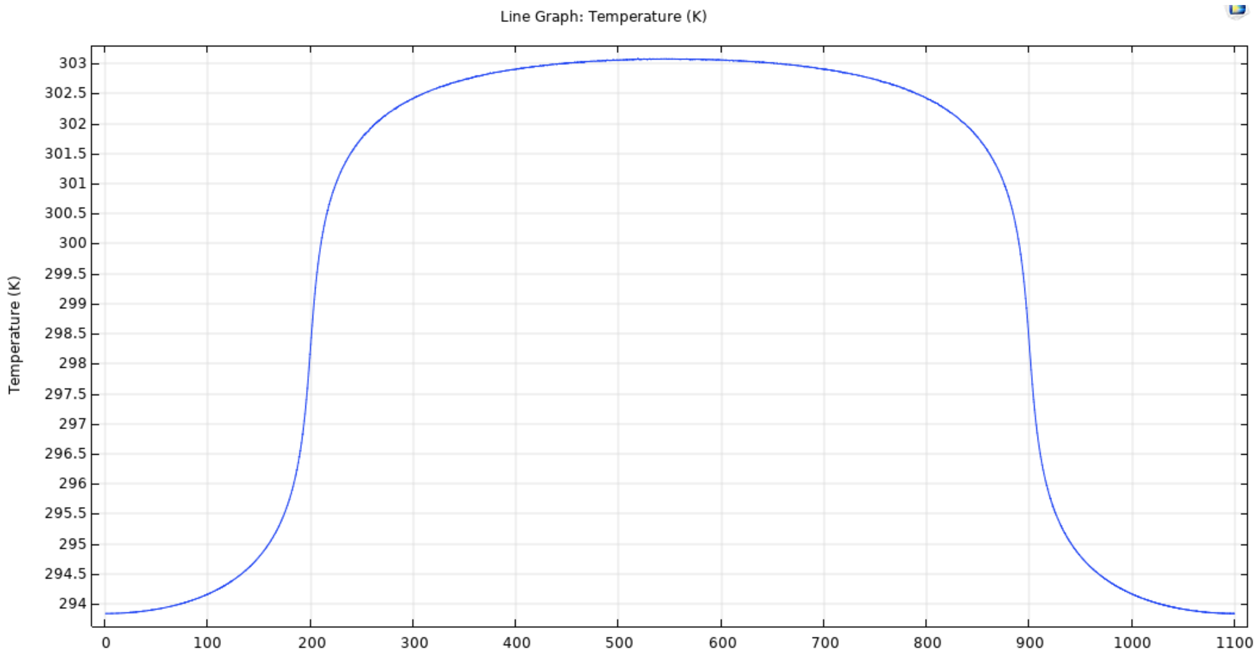
Material Property

	Thermal Conductivity (W/m*K)	Density (kg/m3)	Heat capacity (J/kg*K)
silicon	130	2330	711
air	built-in material		
germanium	58	5323	310

Boundary Condition

	Boundary Condition
上	Convective heat flux, h=10 W/(m2*K)
下	fixed temperature, T=initial value
波导方向	Convective heat flux, h=10 W/(m2*K)
其余两个方向	Convective heat flux, h=10 W/(m2*K)

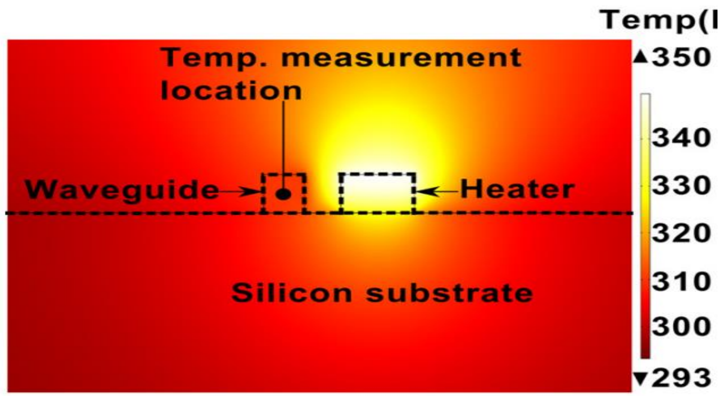
Results

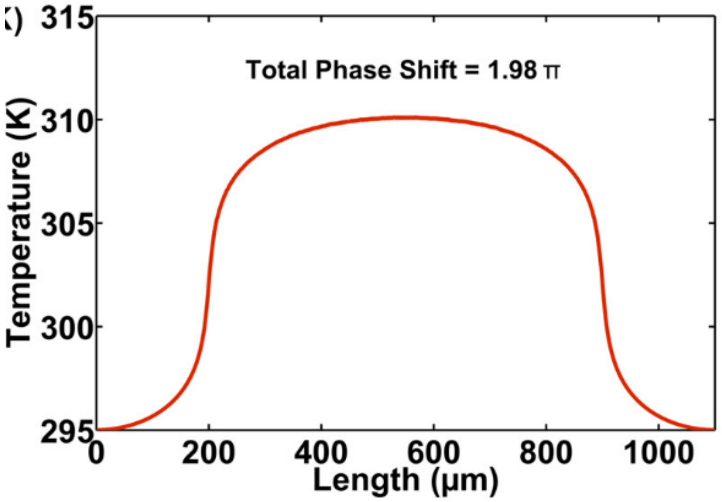


ref

最高温度在303K左右

论文中和initial的结果

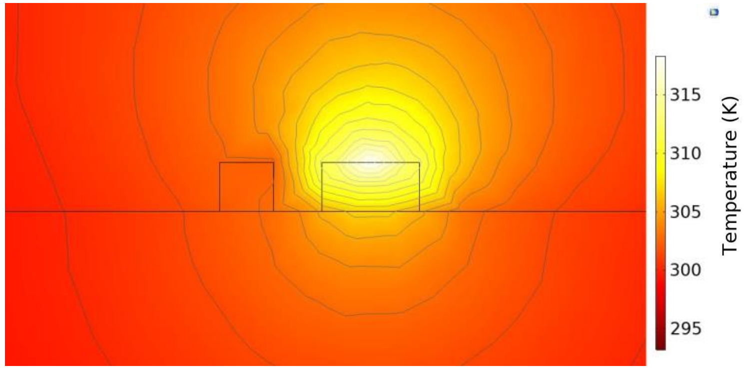


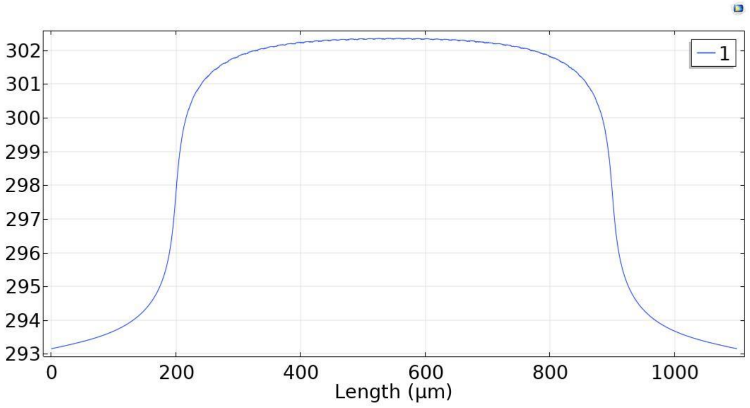


论文中的

Tmax = ~ 310 K

光程差: 1.98π





initial

Tmax = ~ 302.36 K

光程差: 1.08π

内部, 外部网格大小,单位: m, 后同

Maximum element size:	Maximum element size:
2.2E-5	2.2E-5
Minimum element size:	Minimum element size:
2.2E-7	2.2E-7

Aditya Malik et al., Ge-on-Si and Ge-on-SOI thermo-optic phase shifters for the mid-infrared, Optics Express, 2014

论文中结果不匹配

原因分析:

1. 可能论文中使用的是线状热源

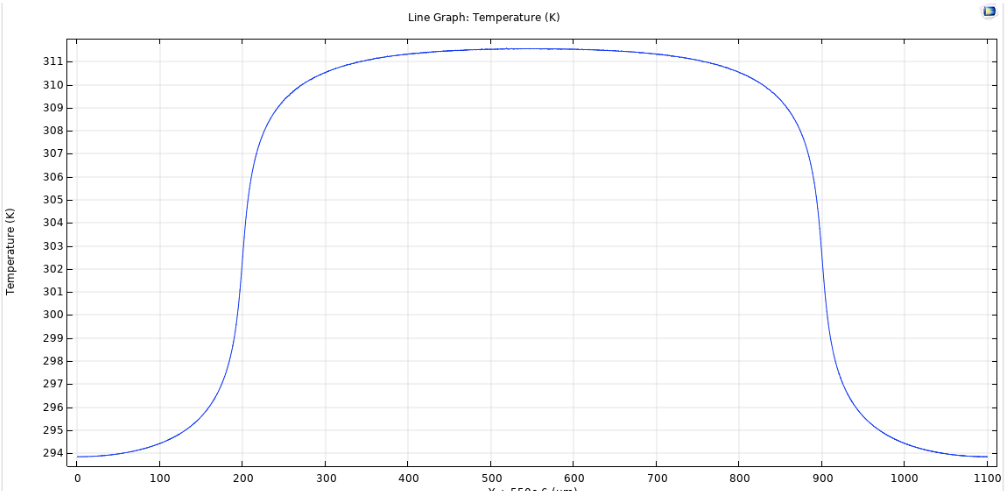
    两图等温线形状无法匹配(圆 椭圆)

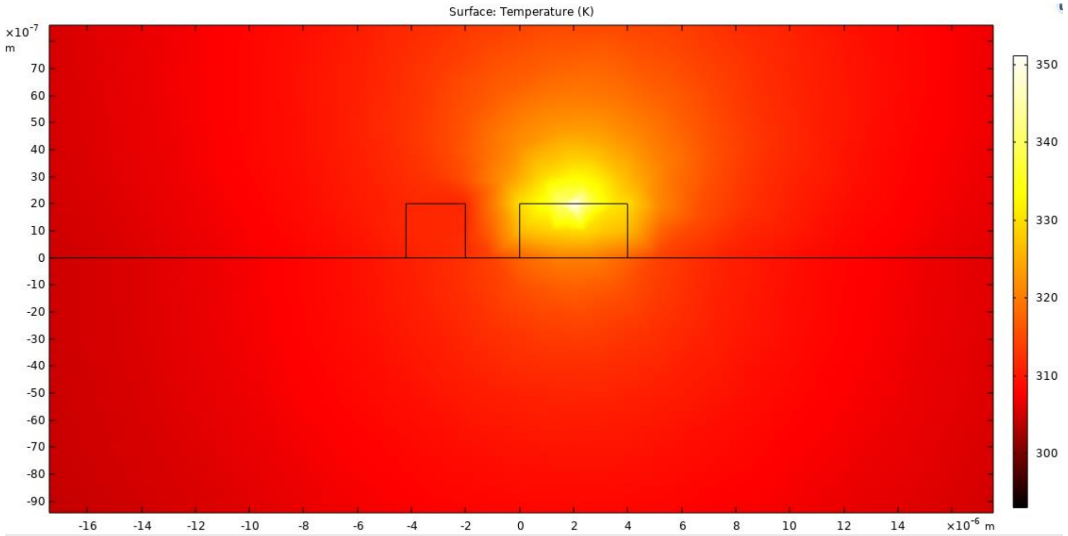
2. 边界条件错误

3. 有无可能是线段不够密集

    等温线不圆 为可见的折线段

变为线状热源





Tmax = 311.59 K

光程差 = 6.8427 = 2.178 pi

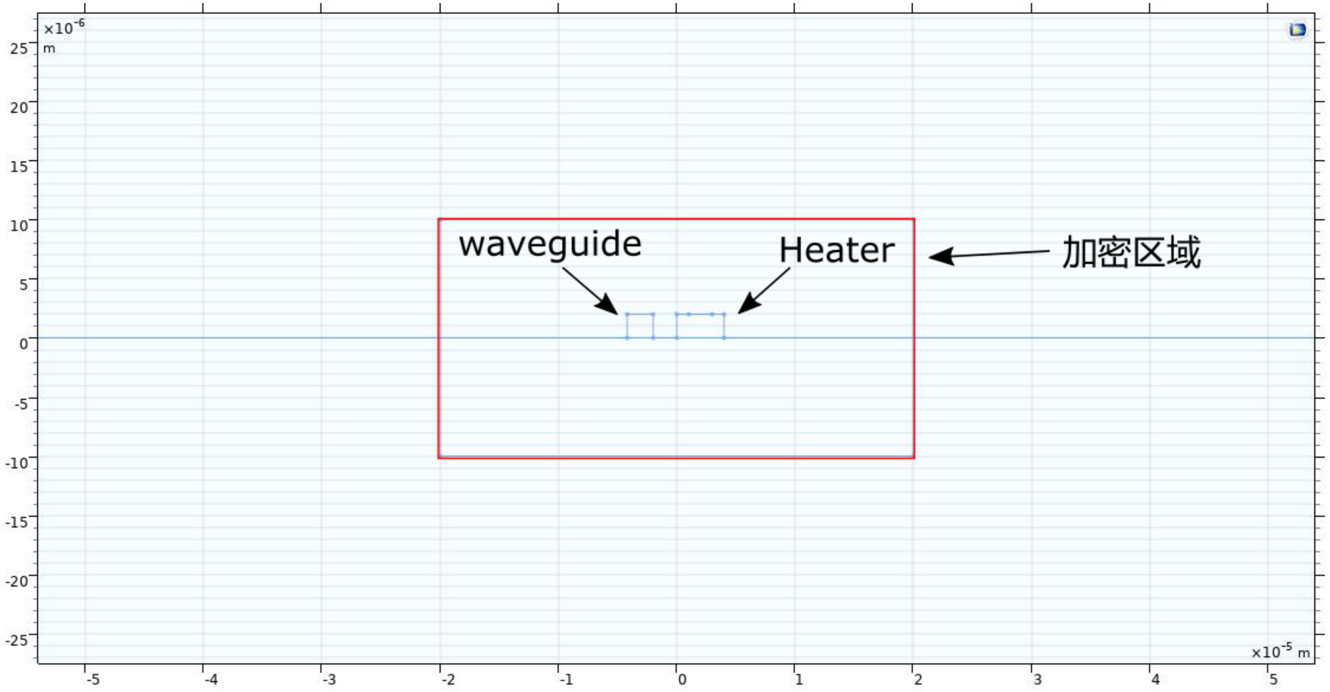
论文中:

光程差 = 1.98 pi

ref

网格密度的确定

Initial

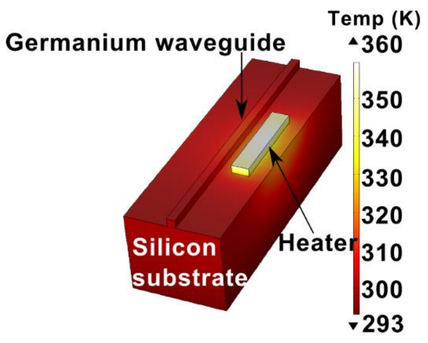


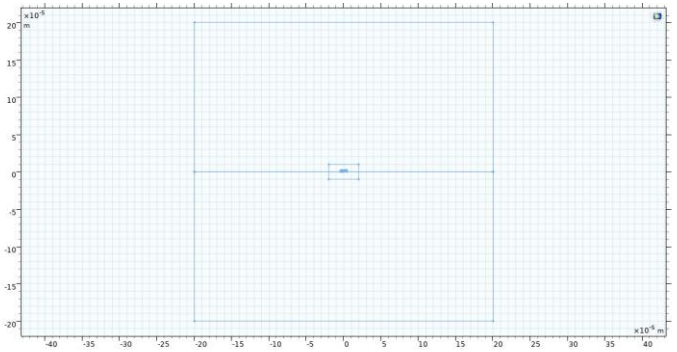
热源: 带状热源

边界条件: 固定温度, T = 293.15 K

加密:

区域: 40 μm x 20 μm x 1100 μm





网格大小:

区域内:

☑ Maximum element size:

2.2E-5 m

☑ Minimum element size:

2.2E-7 m

区域外:

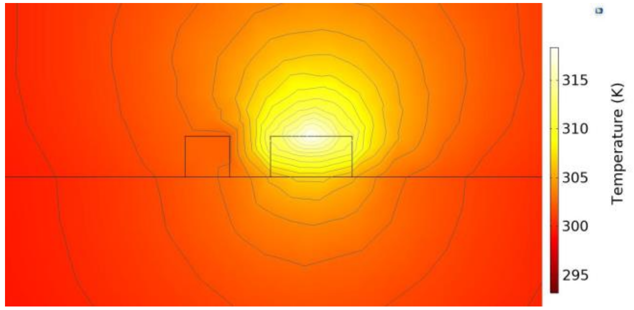
☑ Maximum element size:

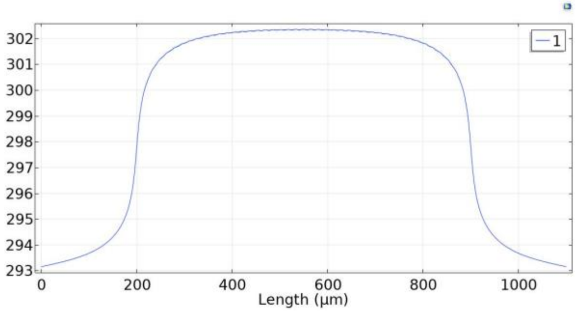
1.1E-4 m

☑ Minimum element size:

1.98E-5 m

网格密度的确定

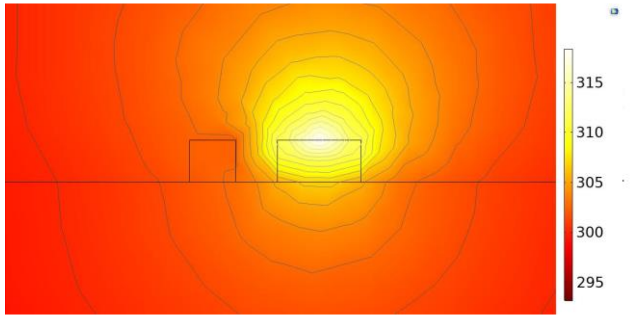


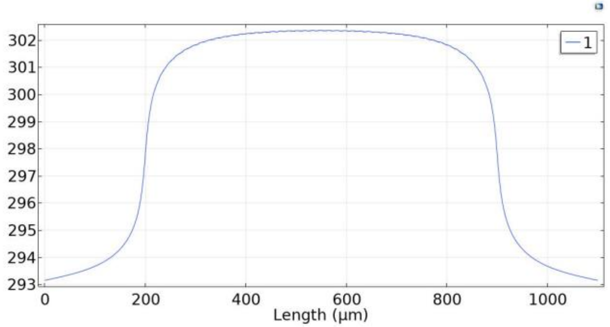


Tmax = ~ 302.36 K 光程差: 1.08π

☑ Maximum element size:	☑ Maximum element size:
10e-6	2.2E-5
☑ Minimum element size:	☑ Minimum element size:
100e-9	2.2E-7

Complete mesh consists of 740090 domain elements, 57029 boundary elements, and 6922 edge elements.
Number of degrees of freedom solved for: 998085 (plus 238240 internal DOFs).
Solution time (Study 1): 123 s. (2 minutes, 3 seconds)

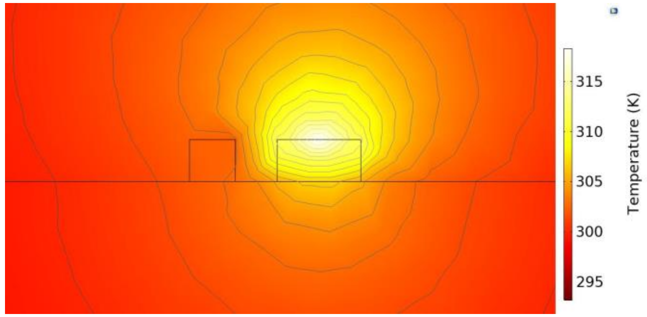


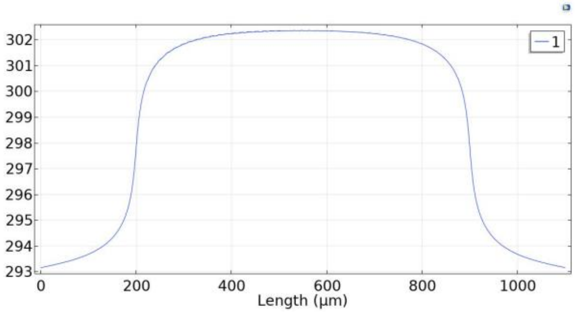


Tmax = ~ 302.36 K 光程差: 1.08π

☑ Maximum element size:	☑ Maximum element size:
10e-6	10e-6
☑ Minimum element size:	☑ Minimum element size:
100e-9	100e-9

Complete mesh consists of 3428284 domain elements, 103505 boundary elements, and 7492 edge elements.
Number of degrees of freedom solved for: 4616425 (plus 349376 internal DOFs).
Solution time (Study 1): 622 s. (10 minutes, 22 seconds)



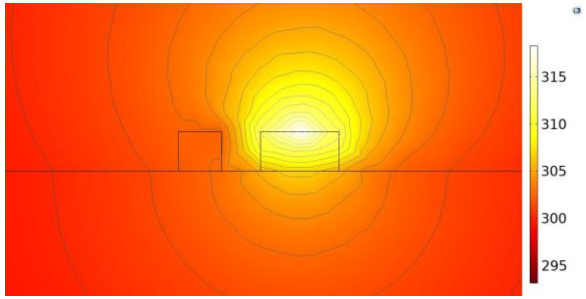


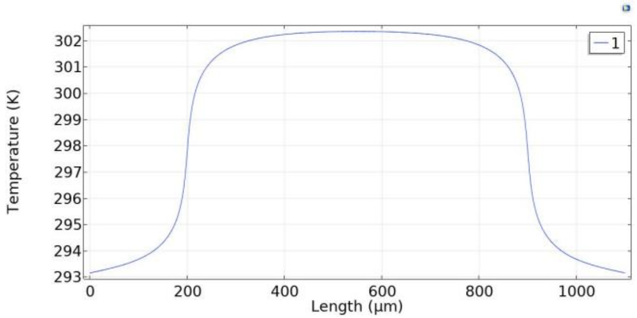
Tmax = ~ 302.37 K 光程差: 1.08π

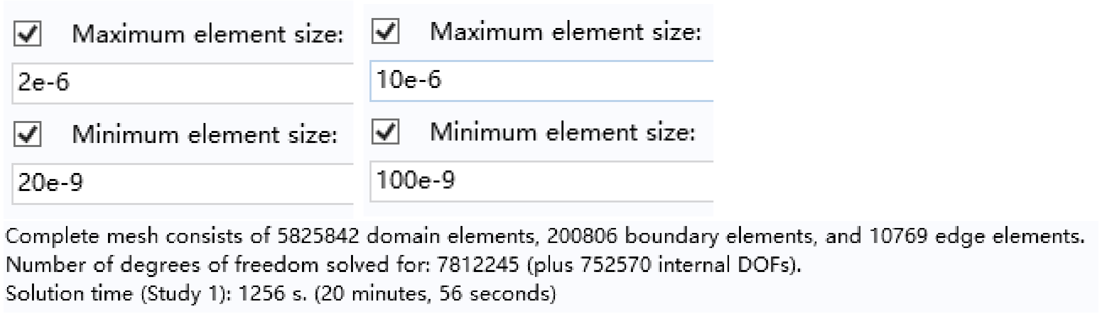
☑ Maximum element size:	☑ Maximum element size:
5e-6	10e-6
☑ Minimum element size:	☑ Minimum element size:
50e-9	100e-9

Complete mesh consists of 3515229 domain elements, 110367 boundary elements, and 7955 edge elements.
Number of degrees of freedom solved for: 4731839 (plus 379256 internal DOFs).
Solution time (Study 1): 680 s. (11 minutes, 20 seconds)

Tmax = ~ 302.36 K　光程差: 1.08π







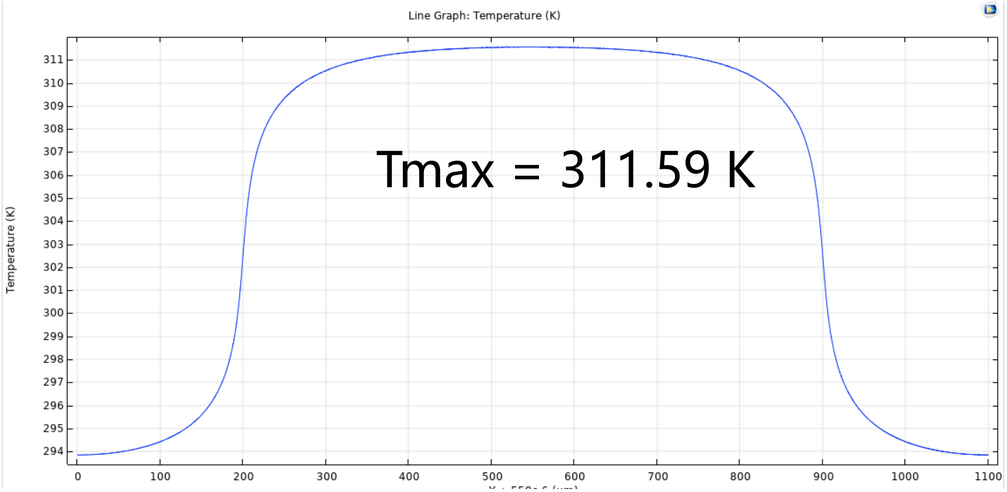
算到这里, mesh的时间已经非常长.(相比其他人)

猜想原因

- 可能是网格疏密没有设置好
- 模型较大 (1100 μm 400 μm 400 μm)
- 加密区域z方向较长 (1100 μm/ 2 μm)

但已经足够证明: 网格不是仿真结果不准确的原因…

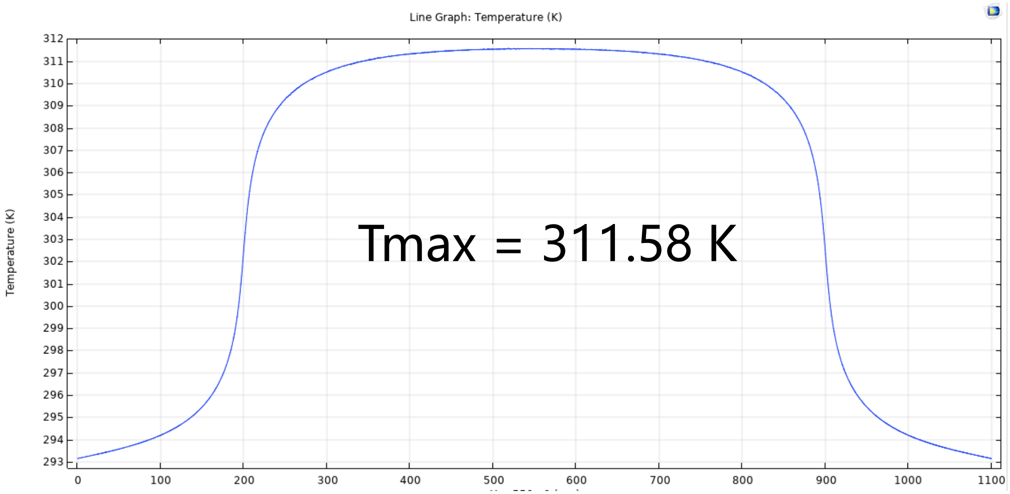
边界条件的确定



上下左右边界: T = 293.15 K

波导方向边界: heat flux, T = 293.15 K, $h = 10\ W/(m^2 \cdot K)$

光程差 = 2.17 pi



所有边界: T = 293.15 K

光程差 = 2.15 pi

论文3

Structure

area:

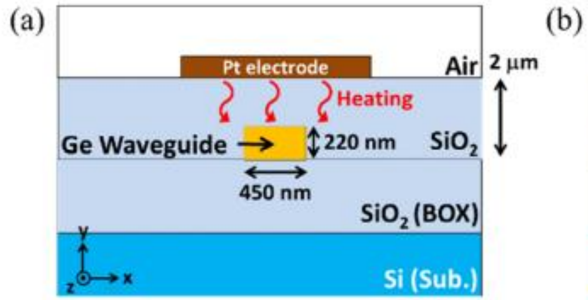


Fig. 1. Cross-sectional schematics of (a) Ge and (b) Si TO phase shifters operating at a wavelength of 1.95 μm.

Simulation

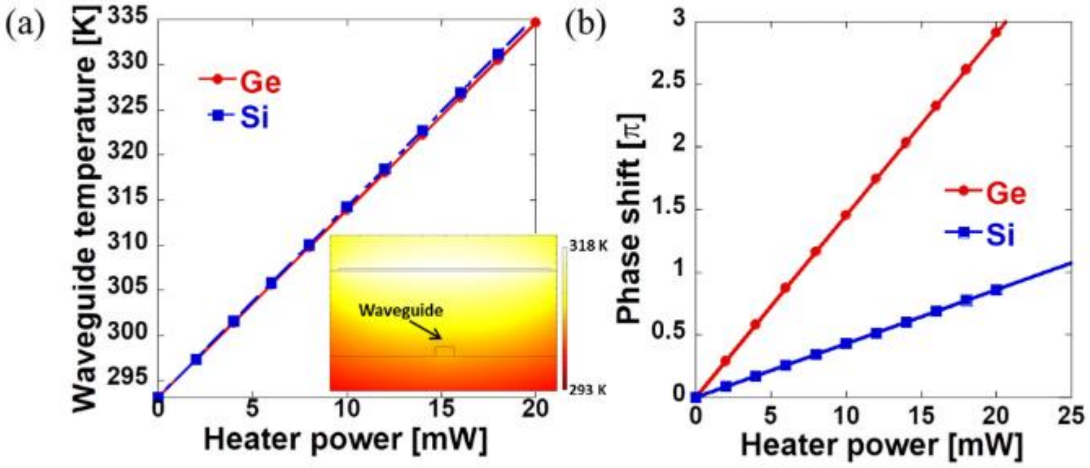
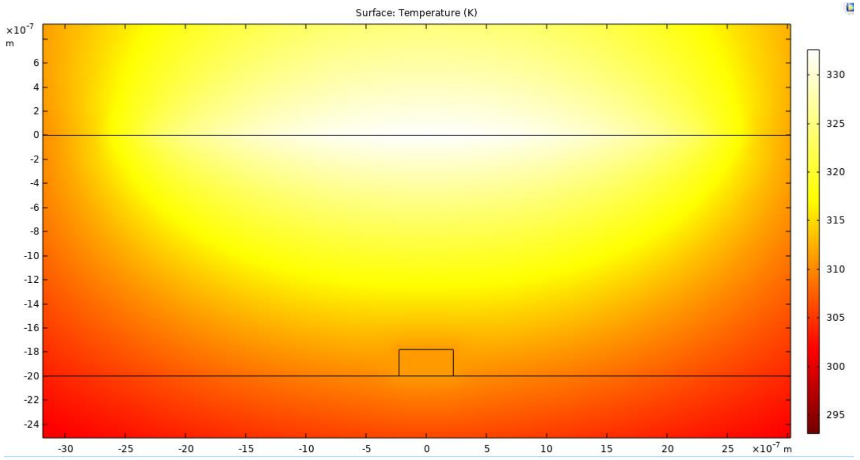


Fig. 2. Simulation results of (a) waveguide temperature and (b) phase shift in Ge and Si TO phase shifters as a function of heater power.

Takumi Fujigaki et al., High-efficiency Ge thermo-optic phase shifter on Ge-on-insulator platform, Optics Express, 2019

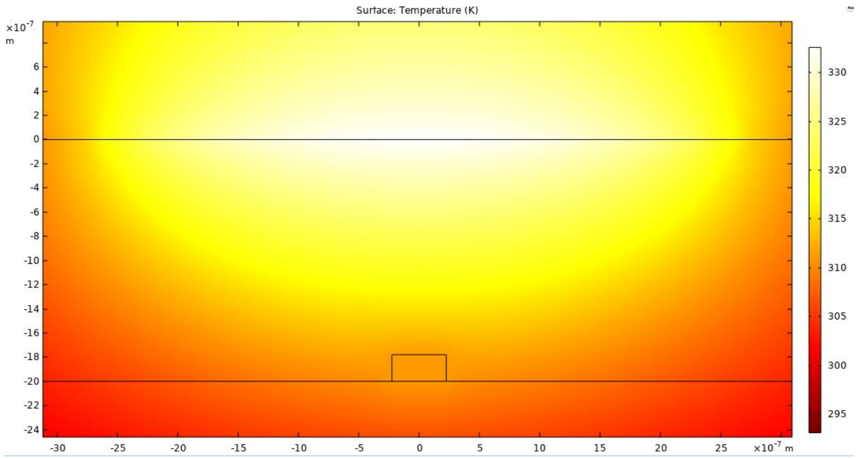
波导中心处温度: [K]

文献中: ~ 314



311.11

initial



311.11

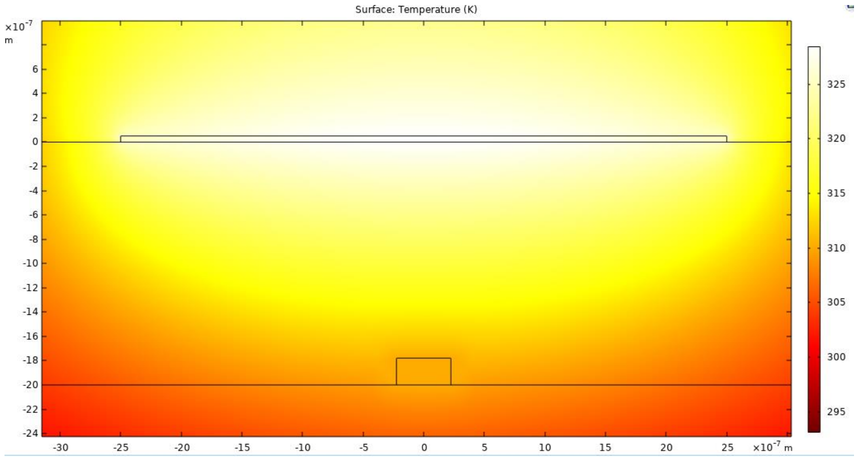
initial-air-fluid

将air设置为流体

结果: 结果完全相同(exactly the same)

结论: 使用流体应设置压强 流速等

不适用与本情况



310.14

initial-pt-added

添加了薄pt层

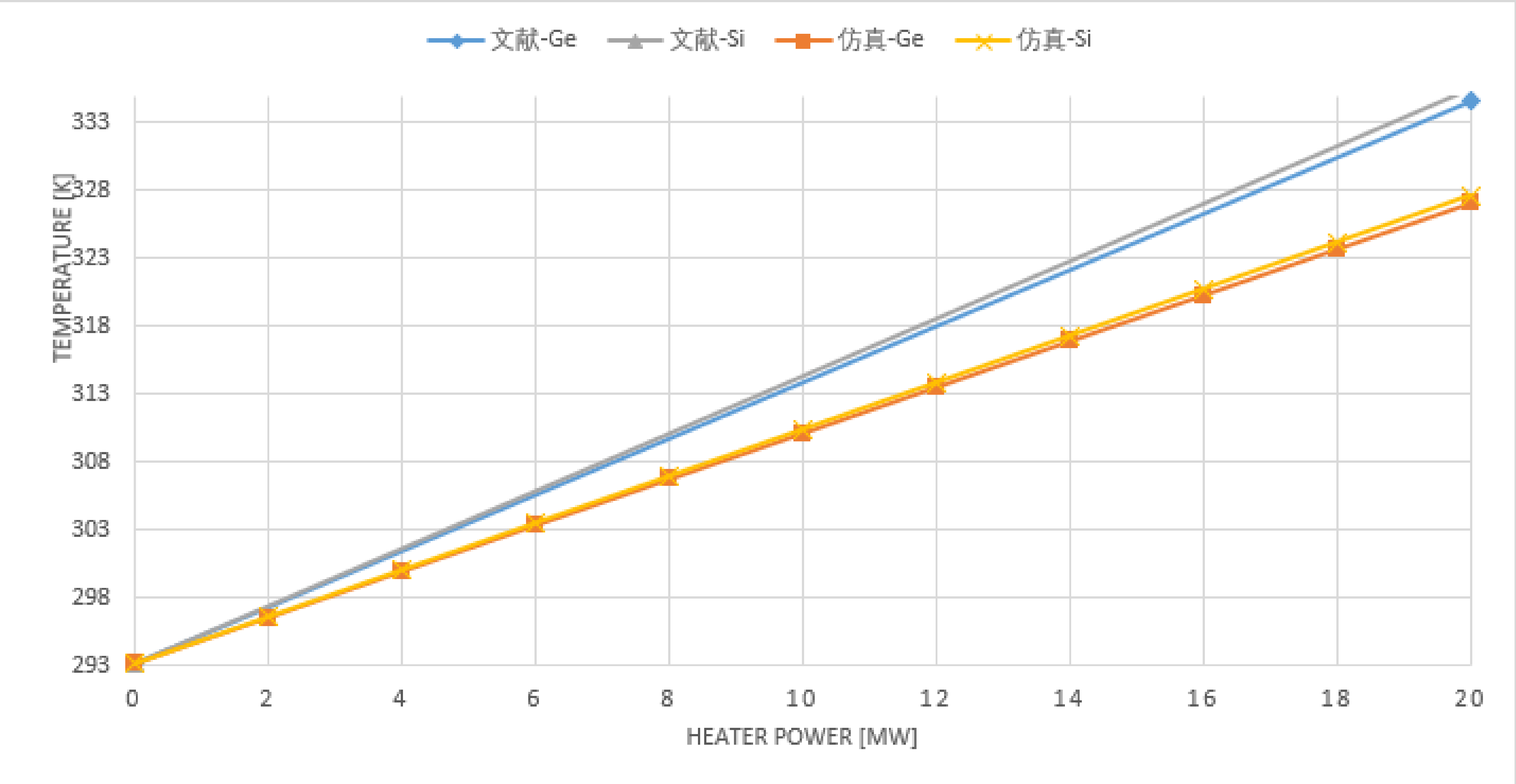
结果: 轻微变化 (slightly different)

Observation:

1. steady-state 与电学联系
    1. 形成平衡需要热源(source)和热井(sink), 热井可以是边界条件确定的 – 可以类比为高电势和低电势
    2. 热的传导: 热源和各个热井之间的材料形成热阻, 类比电阻
    3. 稳态解温度分布由热阻分布决定 – 电势分布由电阻决定
2. 稳态解的分布只与物体的导热系数(thermal conductivity)有关, 而与物体的比热容(specific heat)和密度(density)无关.

-- 解释上页中添加Pt层后温度变化

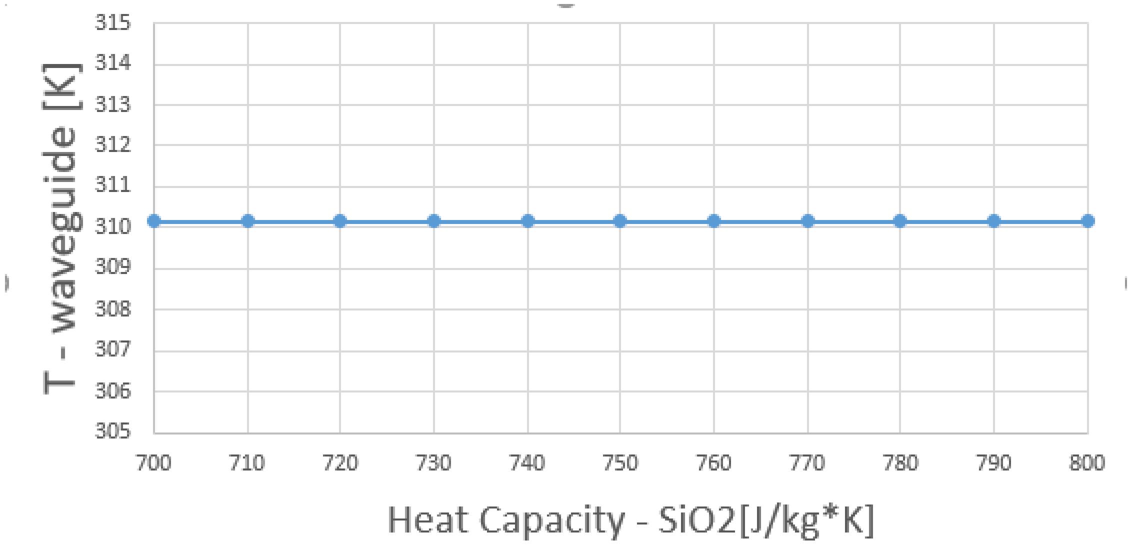
仿真结果

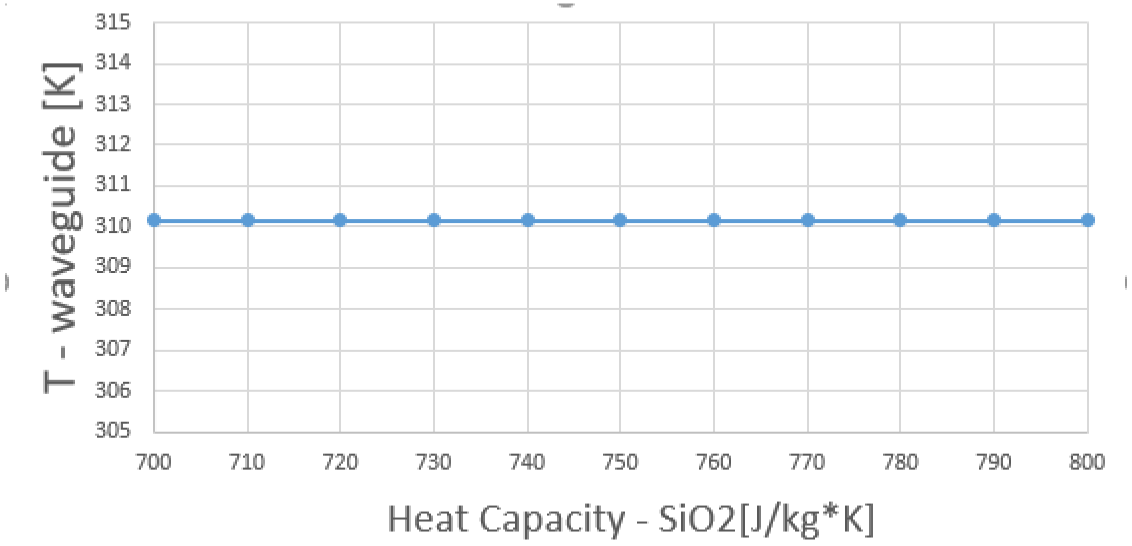


文献-Ge
文献-Si
仿真-Ge
仿真-Si
TEMPERATURE [K]
333
328
323
318
313
308
303
298
293
0
2
4
6
8
10
12
14
16
18
20
HEATER POWER [MW]

ref

验证: 材料的heat capacity, density不影响steady-state仿真结果

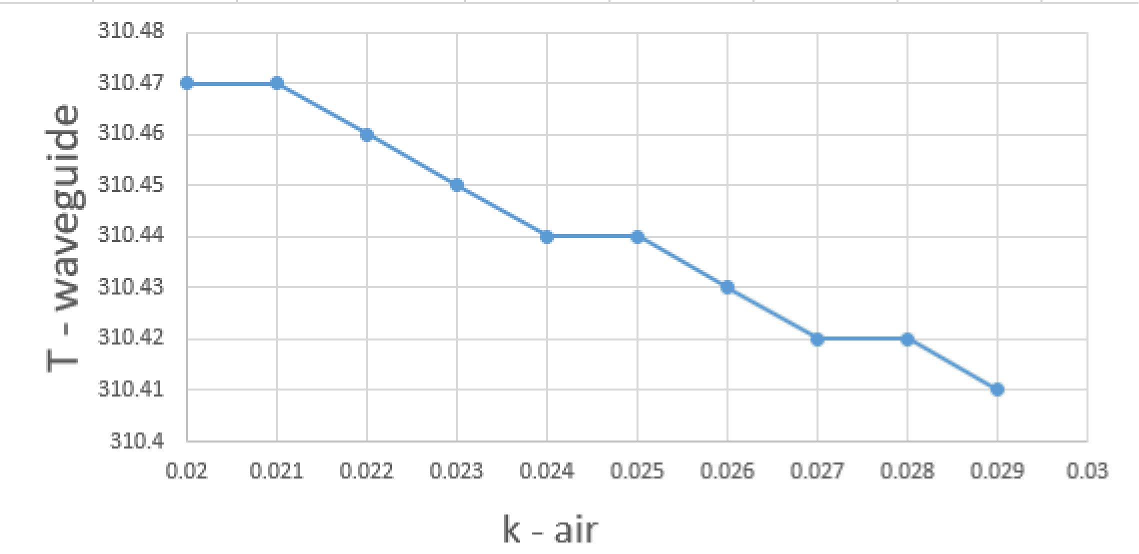




ref

改变空气导热系数的影响

猜想: K 上升, 空气侧热阻减小, 热源产生的热更多的从空气侧流失, 下侧温度降低.



结论: 与猜想相同, 但改变幅度 < 1 K

ref

网格密度的确定

数据对比: 波导中心处温度随功率的变化

Heater power [mW]	extremly fine	custom
0	293.15	293.15
2	296.55	296.55
4	299.95	299.95
6	303.35	303.35
8	306.75	306.75
10	310.14	310.15
12	313.54	313.55
14	316.94	316.94
16	320.33	320.34
18	323.73	323.73
20	327.12	327.13

结论: “custom”和“extremely fine”网格已经足够密

仿真方向

1. 新结构
2. 材料的应用
3. 性能优化 – 占地面积小
4. ？