Monte Carlo Simulations of Thermal Spreading Resistance in Ballistic-Diffusive Regime for GaN HEMTs including Phonon Dispersion

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Overview

Background

In GaN HEMTs, the heat transfer process is dominated by thermal spreading processes. Moreover, the phonon mean free paths (MFPs) of GaN are comparable with the channel layer thickness and the heat spot width, resulting in the invalidity of Fourier's heat conduction law.

Main content

Dr.Hua investigated the thermal spreading resistance of GaN HEMTs by phonon Monte Carlo (MC) methods under gray-media approximation, and developed a semiempirical thermal resistance model.

In this work, we took the phonon dispersion of GaN into considersion and compared the differences between the results of gray mc and dispersion mc. Also, the thermal resiatance model was further improved.

Outline

GaN HEMTs

GaN HEMTs hold a very small heat source area compared with the channel layer length and width.

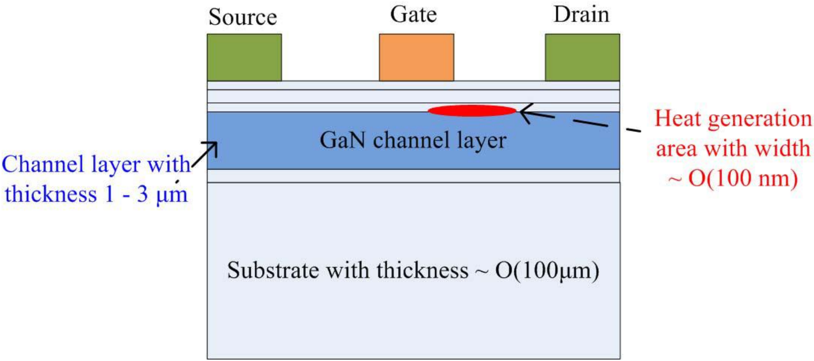


Figure 1: Typical structure of GaN HEMTs.

Thermal Spreading Resistance

When heat spreads from a small source to a much larger area, there is a significant thermal spreading resistance, that can dominate heat transfer processes.

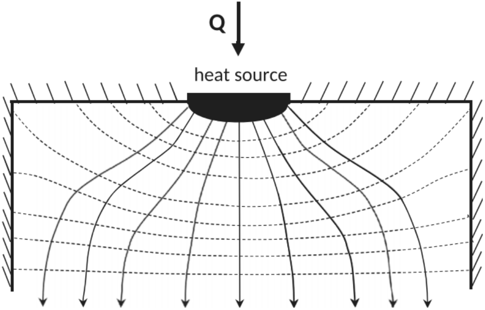


Figure 2: Arbitrary shape heat source on a flux channel.

$$R = R_{1D} + R_s = \frac{\bar{T}_s - T_{z\to\infty}}{Q}, R_{1D} = \frac{\bar{T}_{z=0} - T_{z\to\infty}}{Q}$$

GaN HEMTs

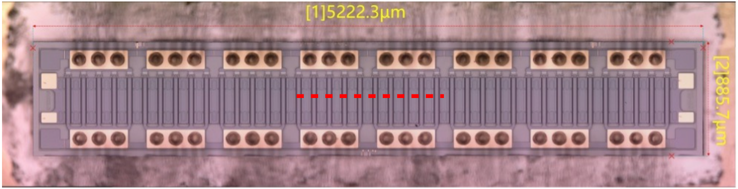


Figure 3: Real GaN HEMTs.

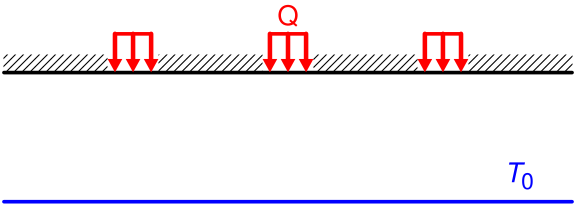


Figure 4: Schematic for the basic system with multiple periodically arrayed heat spots.

Simulation System

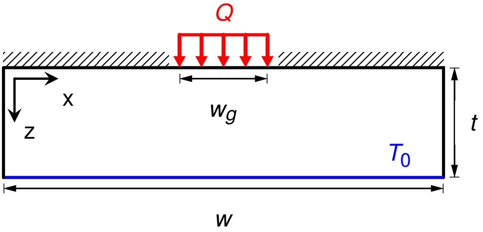


Figure 5: Schematic for the basic system in a single period.

The geometry of the system can be characterized by:

$$w_g/w \quad \text{and} \quad w/t$$

Ballistic Effect Characterization

Two Knudsen numbers, Kn_t and Kn_w, were defined to characterize the strength of ballistic effects,

$$Kn_t = l_0/t, \quad Kn_w = l_0/w_g$$

Average MFP:

$$l_0 = \frac{\int_0^{\omega_m} C_\omega v_{g_\omega} l_\omega \mathrm{d}\omega}{\int_0^{\omega_m} C_\omega v_{g_\omega} \mathrm{d}\omega} = 4.086 \times 10^{-7}\,\mathrm{m}$$

Characteristic Thermal Resistance

1-D thermal resistance for purely diffusive heat conduction:

$$R_{1D\_0} = \frac{t}{kw}$$

Characteristic and dimensionless temperature rise:

$$\Delta T_0 = QR_{1d\_0} = Qt/(k_b w), \; \theta = \frac{\Delta T}{\Delta T_0} = \frac{\Delta T}{QR_{1d\_0}} = \frac{R}{R_{1d\_0}}$$

1-D thermal resistance in ballistic-diffusive regime:

$$R_{1d} = \overline{\theta}_{z=0} R_{1d\_0}$$

Total thermal resistance:

$$R_t = \overline{\theta}_s R_{1d\_0}$$

Phonon Dispersion

- An isotropic sine-shaped phonon dispersion is used.
- Longitudinal and transverse branches are not differentiated.

$$\omega(k) = \omega_{\max} \sin\left(\pi k / 2k_m\right)$$

$$k_m = \left(\frac{6\pi^2 N}{V}\right)^{1/3}, \; a = \pi / k_m, \; \omega_m = 2v_{0g}/a$$

Table 1: Phonon dispersion parameters for GaN.

N/V (1×10^{28} m^{-3})	k_m (1×10^{10} m^{-1})	a (1×10^{-10} m)	ω (1×10^{13} rad/s)
2.16	1.09	2.89	3.5

Relaxation time

Matthiessen's rule:

$$\tau^{-1} = \tau_{impurity}^{-1} + \tau_U^{-1} = A\omega^4 + B\omega^2 T \exp(-C/T)$$

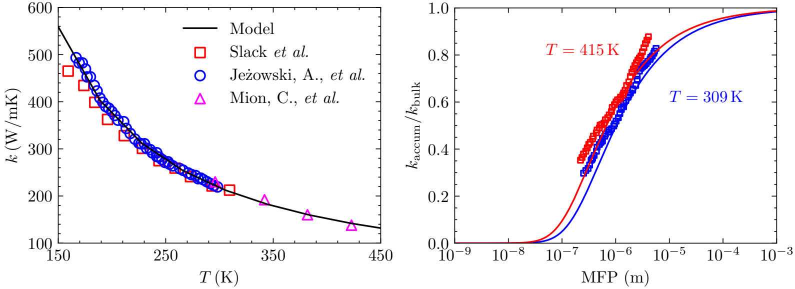
Thermal conductivity fitting:

$$\mathscr{L}(A, B, C) = \sum \left\| \frac{1}{3} \sum_p \int_0^{\omega_m} C_\omega v_\omega^2 \tau_\omega \mathrm{d}\omega - k_{exp} \right\|^2$$

$$C(\omega, p) = \hbar\omega D(\omega, p) \frac{\partial f^{BE}}{\partial T} = \hbar\omega \frac{\kappa^2}{2\pi^2 \left| v_g \right|} \frac{\hbar\omega e^{\frac{\hbar\omega}{T k_B}}}{T^2 k_B \left(e^{\frac{\hbar\omega}{T k_B}} - 1 \right)^2}$$

Phonon Dispersion and Relaxation time

$$A = 2.75 \times 10^{-45}\,\mathrm{s}^3,\ B = 0.90 \times 10^{-19}\,\mathrm{s/K},\ C = 113.10\,\mathrm{K}$$



(a) Temperature dependent thermal conductivity of GaN.

(b) Thermal conductivity accumulation function.

Figure 6: Model validation.

Energy-based Variance-reduced Monte Carlo

When considering phonon dispersion, the main difference is that phonon bundles emitted from phonon baths will have different properties, and their properties will be redetermined after phonon–phonon scattering.

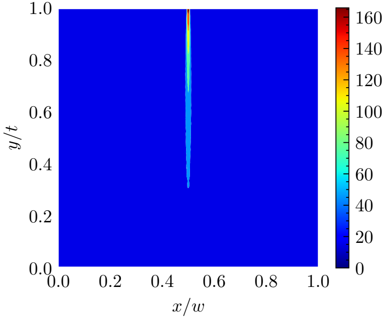
Emitting Sampling

$$W_{\mathrm{ph-bnd}} = \frac{C_{p,\omega} v_{p,\omega}}{\sum_p \int_\omega C_{p,\omega} v_{p,\omega} \mathrm{d}\omega} \mathrm{d}\omega$$

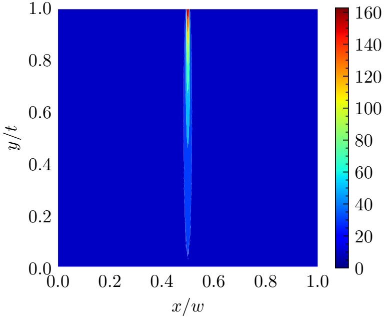
Scattering Sampling

$$W_{\mathrm{ph-ph}} = \frac{C_{p,\omega} v_{p,\omega} / l_{p,\omega}}{\sum_p \int_\omega \left(C_{p,\omega} v_{p,\omega} / l_{p,\omega} \right) \mathrm{d}\omega} \mathrm{d}\omega$$

Dimensionless Temperature Distributions



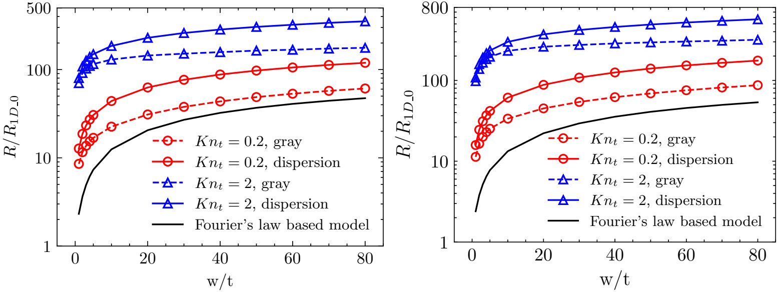
(a) Gray mc.



(b) Dispersion mc.

Figure 7: Dimensionless temperature distributions with $w/t = 40$ and $w_g/w = 0.01$, $Kn_t = 2$.

Total Thermal Resistance



(a) $w_g/w = 0.01$ (b) $w_g/w = 0.005$

Figure 8: Dimensionless total thermal resistance as a function of w/t.

Model for Thermal Resistance

$$\frac{R_t}{R_{1d\_0}} = \frac{R_F}{R_{1d\_0}} \cdot \frac{R_{1d}}{R_{1d\_0}} \cdot \left[\frac{R_t}{R_{1d}} \left(\frac{R_F}{R_{1d\_0}} \right)^{-1} \right]$$

$\frac{R_F}{R_{1d\_0}}$: Thermal spreading effect

$\frac{R_{1d}}{R_{1d\_0}}$: Cross-plane ballistic effect

$r_w = \left[\frac{R_t}{R_{1d}} \left(\frac{R_F}{R_{1d\_0}} \right)^{-1} \right]$: Ballistic effect with w_g comparable with MFP

Thermal Spreading Part

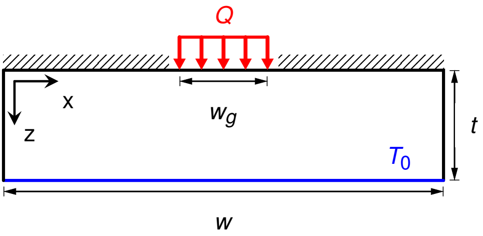


Figure 9: Schematic for the basic system.

$$R_F/R_{1D\_0} = 1 + \sum_{n=1}^{\infty} \frac{8\sin^2\left(\frac{w_g n\pi}{2w}\right)\cos^2(\frac{n\pi}{2})}{w_g^2 t(\frac{n\pi}{w})^3\coth(\frac{tn\pi}{w})}$$

$$= 1 + (\frac{w}{w_g})^2(\frac{w}{t})\sum_{n=1}^{\infty} \frac{8\sin^2\left(\frac{w_g n\pi}{2w}\right) * \cos^2(\frac{n\pi}{2})}{(n\pi)^3\coth(\frac{tn\pi}{w})}$$

Cross-Plane Ballistic Part

BTE + temperature jump boundary conditions,

$$Q = -k_b w \frac{\partial T}{\partial z}$$

$$T\Big|_{z=0} - T_0 = -\frac{2}{3}\frac{\int_0^{\omega_m} C_\omega \tau_\omega v_{g_\omega}^2 \mathrm{d}\omega}{\int_0^{\omega_m} C_\omega v_{g_\omega} \mathrm{d}\omega}\frac{\partial T}{\partial z}$$

$$-\frac{\partial T}{\partial z} = \left(T\Big|_{z=0} - T_0\right)/t$$

which yields,

$$R_{1d}/R_{1d\_0} = 1 + \frac{2}{3}\frac{\int_0^{\omega_m} C_\omega v_{g_\omega} l_\omega \mathrm{d}\omega}{\int_0^{\omega_m} C_\omega v_{g_\omega} t \mathrm{d}\omega} = 1 + \frac{2}{3} Kn_t$$

1D Thermal Resiatance

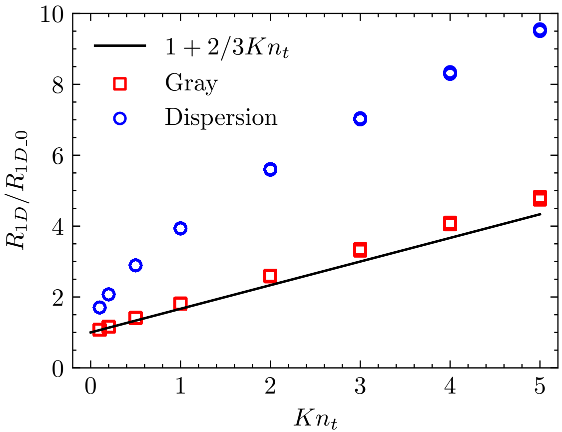
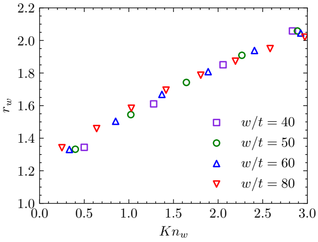
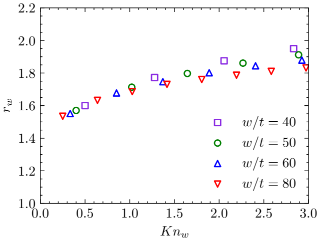


Figure 10: Dimensionless 1D thermal resiatance.

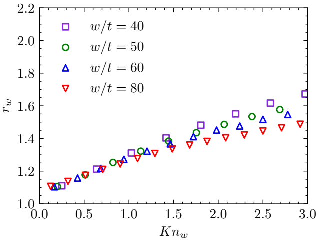
Narrow Heat Source Ballistic Part ($r_w = \left[\frac{R_t}{R_{1d}}\left(\frac{R_F}{R_{1d\_0}}\right)^{-1}\right]$)



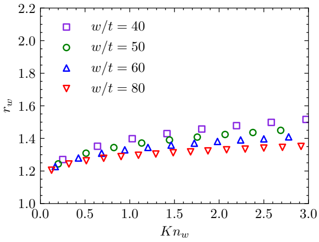
(a) $w_g/w = 0.005$, Gray



(b) $w_g/w = 0.005$, Dispersion



(c) $w_g/w = 0.01$, Gray



(d) $w_g/w = 0.01$, Dispersion

Unfinished and Expected Work

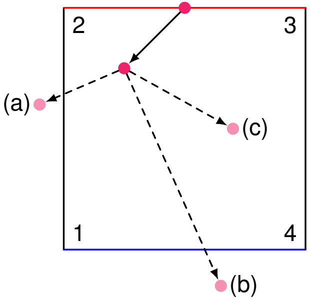
- Analyze the differences between gray mc and dispersion mc more detailedly.
- Investigate the effective thermal conductivity.
- Improve the thermal resistance model with the results of dispersion mc.

shengmc

- A Python based framework for 2d phonon monte carlo simulations.
- shengmc is based primarily on numpy, numba and mpi4py.

Basic Picture

- Every boundary is saved as an object.
- At every step, the emitted phonon is judged whether it's still in the simulation region using ray casting algorithm.
- If not, collision detection is conducted by a linear search.



(a): phonon-boundary scatter

(b): absorption

(c): phonon-phonon scatter

Figure 11: The basic physical picture of phonon monte carlo simulations conducted in shengmc.

Thermal Spreading Resistance

```python
import numpy as np

wg, w = 0.01, 40
heat_length = wg * w
boundary_points = np.array(
    [
        [0, 0] # 1,
        [0, 1] # 2,
        [w / 2 - heat_length / 2, 1] # 3,
        [w / 2 + heat_length / 2, 1] # 4,
        [w, 1] # 5,
        [w, 0] # 6,
    ]
)
boundary_conditions = np.array([2, 3, 4, 3, 2, 1])
x_grids = np.arange(0, w + heat_length/10, heat_length/5)
y_grids = np.linspace(0, 1, 101)
```

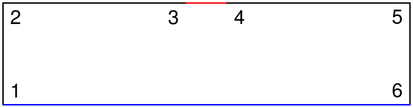


Figure 12: Schematic of boundary settings.

Run Under Gray-Medium Approximation

```
shengmc.run.hello_run(
        boundary_points,
        boundary_conditions,
        x_grids,
        y_grids,
        gray=True,
        number_of_phonons=1e6,
        characteristic_length=1e-08,
        gray_MFP=4.09e-07,
        phonon_distribution_save_name='phonon.npy',
        boundary_distribution_save_name='boundary.npy'
)
```

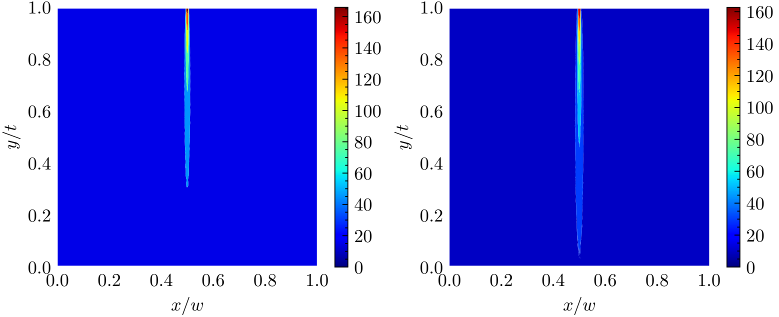
Phonon Dispersion

```
dispersion_model = shengmc.dispersion.Sine(
    omega_m=3.5e13, k_m=10.94e9
)
relaxation_model = shengmc.dispersion.RelaxationBulk(
    A=2.75e-45, B=9.01e-20, C=113.10, T=300
)
GaN_model = shengmc.dispersion.Dispersion(
    dispersion_model, relaxation_model
)
mcinfo = GaN_model.cal_mcinfo()
```

Run with Phonon Pispersion

```
shengmc.run.hello_run(
    boundary_points,
    boundary_conditions,
    x_grids,
    y_grids,
    gray=False,
    number_of_phonons=1e6,
    characteristic_length=1e-08,
    probability_phonon_phonon_distribution=mc_info[0][0],
    probability_phonon_boundary_distribution=mc_info[0][1],
    MFP_phonon_phonon_distribution=mc_info[1][0],
    MFP_phonon_boundary_distribution=mc_info[1][1],
    phonon_distribution_save_name='phonon.npy'
    ,
    boundary_distribution_save_name='boundary.npy'
    ),
)
```

Results of GaN



(a) Gray mc.

(b) Dispersion mc.

Figure 13: Dimensionless temperature distributions with $w/t = 40$ and $w_g/w = 0.01$, $Kn_t = 2$.

Square Film

```python
import numpy as np

boundary_points = np.array([[0, 0], [0, 1], [1, 1], [1, 0]])
boundary_conditions = np.array([3, 1, 3, 0])
x_grids = np.linspace(0, 1, 21)
y_grids = np.linspace(0, 1, 41)
```

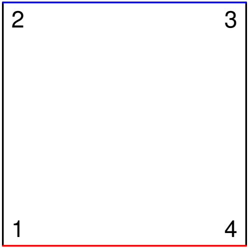
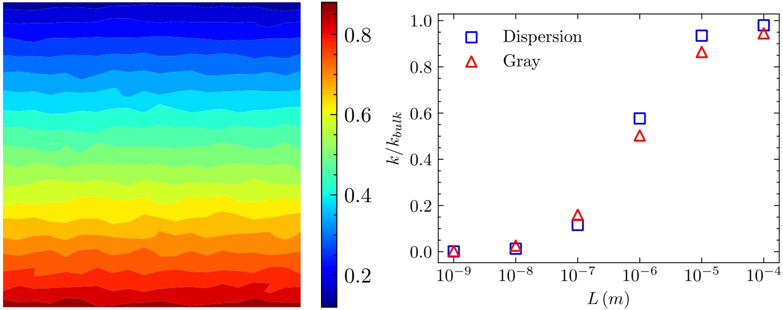


Figure 14: Schematic of boundary settings.

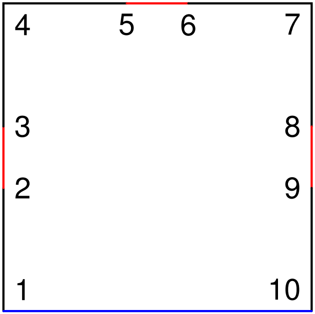
Results of Silicon



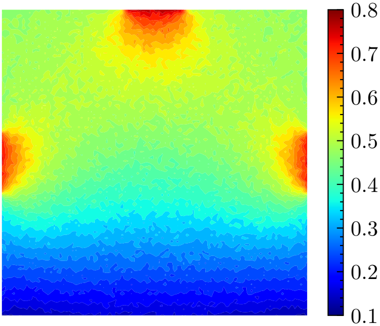
(a) $L = 1 \times 10^{-6}$ m (b) Effective thermal conductivity

Figure 15: Dimensionless temperature distribution and effective thermal conductivity.

Multiple Heat Sources - (1)



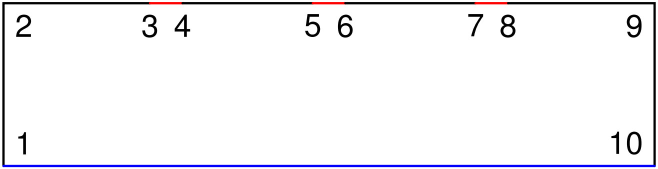
(a) Schematic of boundary settings.



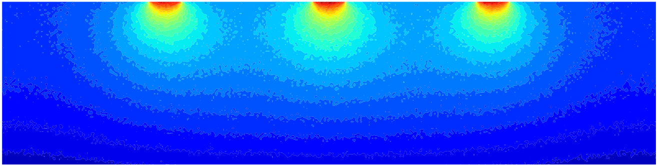
(b) Dimensionless temperature distribution when $Kn = 0.5$.

Figure 16: Boundary settings and dimensionless temperature distribution.

Multiple Heat Sources - (2)



(a) Schematic of boundary settings.



(b) Dimensionless temperature distribution when $Kn = 0.5$.

Figure 17: Boundary settings and dimensionless temperature distribution.

Executing Time

- 2.9 GHz Intel Core i5 (Macbook Pro 2016)

Table 2: Single-core computing time of $1e5$ phonons for square films with gray-medium approximation and phonon dispersion, respectively.

Lengthnm		17600	3520	1760	352	176	88	35.2	17.6
Effective Kn		0.01	0.05	0.1	0.5	1	2	5	10
Times	Gray	8.20	2.25	1.47	0.84	1.1	0.67	0.64	0.62
	Dispersion	149.89	30.98	15.89	3.87	3.94	1.63	1.17	0.98

Prospective Features

Short-Term Work

- Supplement more detailed documents
- Reorganize the project as a python library
- Support internal heat source

Long-Term Work

- Couple electron-phonon interaction
- Couple fourier's law
- Take interfaces into account

Github 🐱 🐱 🐱

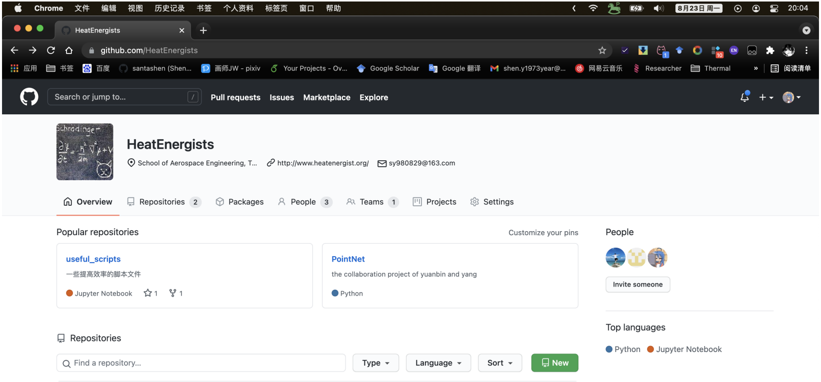


Figure 18: HeatEnergists Organization.

Thank You!