

Establishing a curve equation model based on Fourier transform

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Abstract: We established a curve equation model based on Fourier transform. By establishing the equation and combining with the neural network model, we calculated that the number of layers, material and thickness of each layer and emission spectrum of GaSb battery design multilayer heat emitter under the highest thermoelectric conversion efficiency were 4 layers, and the four layers were GaSb, GA, GA, and Sb, with a thickness of 94.732.

Keywords: genetic algorithm, equation, GaSb

1. Background

In recent years, world powers have set their sights on the "star sea" and formulated various space exploration plans. In 2020, China's "tianwen-1" was launched into Mars; Well, in 2021, the "zhurong" Mars rover completed its scheduled mission, continued to stay on Mars and continued to work for more discoveries in the vast universe. In order to ensure that various instruments and equipment carried by the rover can operate normally without sunlight, and provide necessary technical support for its long-term work, scientists have explored and developed thermal photovoltaic technology.

Thermal photovoltaic technology is a technology that uses various heat sources to heat objects. The heat emitter (absorber) then converts the infrared radiation of the heat emitter into power generation through photovoltaic cells. There are many types of heat sources, including chemical heat sources, solar energy, nuclear energy, etc. The thermal radiator in the system mainly uses different material structures to adjust the emission of absorbed heat, so that most of the emitted photons are lower than the band gap wavelength of photovoltaic cells. Photovoltaic cells mainly convert high-energy photons lower than a specific band gap wavelength. It has a certain band gap energy, so it has a corresponding band gap wavelength. For example, silicon solar cells with a band gap wavelength of 1100 nm can only absorb high-energy photons lower than the above wavelength and convert them into electrical energy, while low-energy photons higher than the cell absorption wavelength cannot be converted into electrical energy through photoelectric effect.

On the contrary, they can only be converted into heat energy, so the photoelectric conversion efficiency of the battery is reduced. Therefore, in order to improve the thermoelectric conversion efficiency of thermal photovoltaic system, the thermal emission spectrum transmitter must be adjusted. The calculation methods of emission spectrum mainly include transfer matrix method (TMM), finite difference time domain method (FDTD) and rigorous coupled wave analysis method (RCWA). And the main factors affecting the emission spectrum are the optical properties (refractive index or dielectric constant) of the thermal emitter and the structural properties (thickness) of the material. Wang et al. A submicron thick multilayer selective solar absorber is developed, which is composed of tungsten, silicon dioxide and silicon nitride. The absorption rate in the solar band is as high as 0.95. In 2014, Evelyn Wang's team at MIT designed a thermal photovoltaic device with photon controlled solar energy that works well in the experiment. In their work, the heat emitter is a multilayer structure composed of silicon and silicon dioxide. The thickness of each layer is optimized so that its emission spectrum corresponds to the band gap antimony arsenide (InGaAsSb) battery of indium gallium. Materials with different refractive index or dielectric constant can find the material database by searching documents or referring to optical properties to provide the refractive index of common materials.

2. Introduction

The topic requires us to select reasonable materials, design multilayer heat emitters for GaSb batteries to achieve as high thermoelectric conversion efficiency as possible and give the design parameters of multilayer structure (including number of layers, material and thickness of each layer), as well as its emission spectrum. We established a curve equation model based on Fourier transform. By establishing the equation and combining with the neural network model, we calculated that under the highest thermoelectric conversion efficiency, the number of layers, material and thickness of each layer and emission spectrum of GaSb battery design multilayer heat emitter were 4 layers, and the four layers were GaSb, GA, GA and Sb, with a thickness of 94.732.

3. Symbol and Assumptions

3.1 Symbol Description

Table 1: Symbolic meaning

Symbol	Symbolic meaning
y	Observable random variable
ε_i	random error
β	Coefficient of regression equation
α	Significance level
p	freedom
y'	Thermoelectric conversion efficiency
f	Nonlinear relation
ω	The weights of connecting neurons in the network
E	Connecting the threshold of each neuron
M	training sample
Z	Comprehensive thermoelectric conversion efficiency
y_{ij}	Actual output value

3.2 Fundamental assumptions

- (1) It is assumed that it strictly abides by the laws of light propagation and reflection.
- (2) There is no gap between composite materials.
- (3) Relativistic effects are not considered.
- (4) The influence of any other force majeure factors shall not be considered.

4. Problem restatement

Gallium antimonide (GaSb) batteries are more advanced at present. The band gap wavelength is assumed to be 1.71 microns. The emission spectrum of the idealized heat emitter is roughly represented by the red dotted line in the figure below. The blue dotted line represents the external quantum efficiency (EQE), and its influence can be properly considered. Please select reasonable materials, design multilayer heat emitter for GaSb battery to achieve as high thermoelectric conversion efficiency as possible and give the design parameters of multilayer structure (including number of layers, material, and thickness of each layer), as well as its emission spectrum.

5. Establishment and solution of model

Based on the above analysis of the problem, the following will start to establish the mathematical model and explain the establishment process, and then use the mathematical model to solve the problem.

The training process of BP neural network is the process of adjusting the connection weight and

threshold between neurons according to the sample set. The training process of neural network based on particle swarm optimization is the same. Firstly, all connection weights and thresholds between neurons are encoded into real vectors to represent individuals in the population; Randomly generate the groups of these vectors, and then iterate according to the original steps of the algorithm: the newly generated individual vectors in the iteration are restored to the weights and thresholds of the neural network. Calculate the mean square deviation index (fitness) generated by all samples through neural network. If the mean square deviation is less than the error accuracy specified by the system. Then the training process stops, otherwise the iteration continues until the maximum number of iterations is reached. The specific process of training BP neural network with PSO algorithm is as follows:

Step1: first initialize the network structure. Set the number of neurons in the input layer, hidden layer and output layer of the network.

Step 2: initial population size N , inertia weight ω , acceleration factors c_1 and c_2 , maximum speed V_{\max} , maximum number of iterations n_{\max} , accuracy requirements ε ;

Initial speed V_{id} , initial position X_{id} .

Step 3: calculate the fitness value of each particle according to the fitness function (i.e., the output mean square error MES of the neural network)

(1) Each sample in the training set has an output value. The output value of each sample is calculated according to the structure, weight, and threshold of the current network.

(2) Through the formula:

$$MES = \frac{1}{2N} \sum_{i=1}^N \sum_{j=1}^m (Y_{ij} - y_{ij})^2$$

Where $i=1, 2, \dots, N$, N is the total number of samples in the training set, and $j=1, 2, \dots, m$ and m are the number of neurons in the output layer. Y_{ij} is the desired output value; y_{ij} is the actual output value.

Step4: for each particle, compare its fitness value with the fitness value of the individual extreme value pbest. If it is better, replace pbest: for each particle, compare its fitness value with the fitness value of the global extreme value gbest. If it is better, replace gbest;

Step 5: check the particle fitness and the current maximum number of iterations. If $MES > \varepsilon$ or the maximum number of cycles n_{\max} is not reached, enter the next step: otherwise, exit.

Step 6: update the speed and position of particles according to formulas L and 2 to generate the next generation of particles.

Step 7: the number of iterations is increased by 1, and the inertia weight is adjusted at the same time ω ; Go back to step 3.

Step 8: output a group of globally optimal particles and map them to the weights and thresholds of the neural network.

Step 9: end of training.

It is assumed that the comprehensive thermoelectric conversion efficiency has the following nonlinear relationship with the design parameters of multi-layer structure: $Z = g(x, y, h)$ (26)

Where x, y, h represents geographical location, temperature and time respectively. Next, the neural network is used for simulation training. The neural network model can be divided into the following four steps:

Step 1: input layer data and select temperature and time as independent variables.

Step 2: use the processed data to train the network, as follows:

- A. The model is established and trained by trainlm function
- B. The specified learning rate is 0.065
- C. The maximum training cycle is 5000 times
- D. Set the standard error to 0.025
- E. Start training the network

Step 3: use the trained BP network to simulate the original data.

Step 4: compare the simulation results with the original data. If the error is less than 0.025, the training is completed

According to the above steps, we use MATLAB software to call the neural network toolbox for programming (see the program in the appendix) and get the following results:

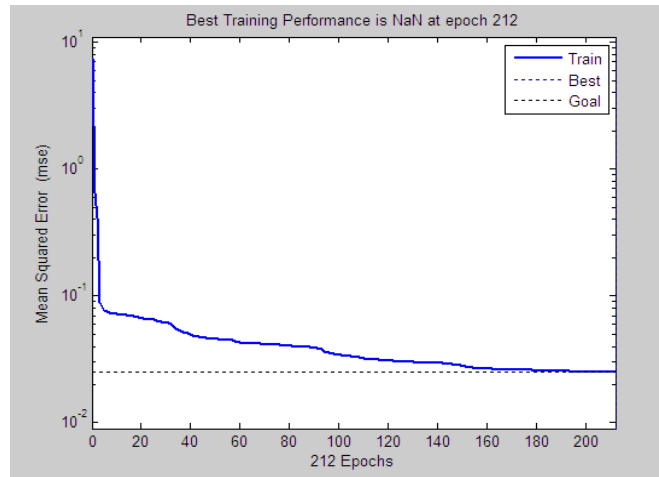


Figure 1: Schematic diagram of error reduction

5.1 Curve equation model based on Fourier transform

We know that gallium antimonide (GaSb) batteries are more advanced at present. The band gap wavelength is assumed to be 1.71 microns. The emission spectrum of the idealized heat emitter is roughly represented by the red dotted line in the figure below. The blue dotted line represents the external quantum efficiency (EQE). We want to make GaSb battery design multilayer heat emitter to achieve as high thermoelectric conversion efficiency as possible and give the design parameters of multilayer structure (including number of layers, material and thickness of each layer), as well as its emission spectrum.

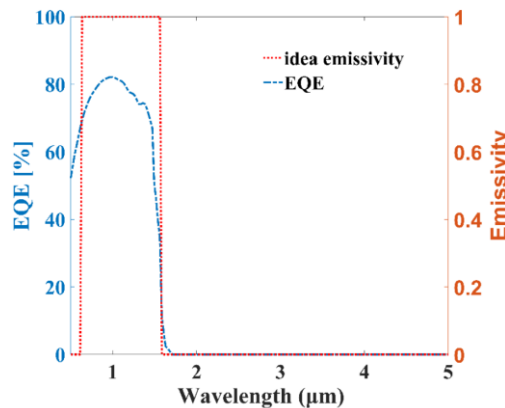


Figure 2: The EQE and ideal emission spectrum of GaSb for thermophotovoltaic

Based on the third question, we use neural network model combined with curve equation to solve this problem.

At point (x_0, y_0, z_0) , the thermoelectric conversion efficiency $u = u(x, y, z, t)$ is a function of x, y, z, t , which satisfies the Cauchy problem:

$$\begin{cases} \frac{\partial u}{\partial t} = a^2 \frac{\partial^2 u}{\partial x^2} + b^2 \frac{\partial^2 u}{\partial y^2} + c^2 \frac{\partial^2 u}{\partial z^2} - k^2 u \\ u(x, y, z, 0) = M\delta(x - x_0)\delta(y - y_0)\delta(z - z_0) \end{cases}$$

Fourier transform it, and make

$$\hat{u}(t, \lambda) = F[u(x, y, z, t)] \quad \hat{u}(t, \lambda) = F[u(x, y, z, t)]$$

Because

$$\begin{cases} F\left[\frac{\partial^2 u}{\partial x^2}\right] = -\lambda_1^2 \hat{u} \\ F\left[\frac{\partial^2 u}{\partial y^2}\right] = -\lambda_2^2 \hat{u} \\ F\left[\frac{\partial^2 u}{\partial z^2}\right] = -\lambda_3^2 \hat{u} \end{cases}$$

$$F[u(x, y, z, 0)] = Me^{-i(\lambda_1 x_0 + \lambda_2 y_0 + \lambda_3 z_0)}$$

Therefore, the Cauchy problem of ordinary differential equation is obtained:

$$\begin{cases} \frac{d\hat{u}}{dt} + (a^2 \lambda_1^2 + b^2 \lambda_2^2 + c^2 \lambda_3^2 + k^2) \hat{u} = 0 \\ \hat{u}(0, \lambda) = Me^{-i(\lambda_1 x_0 + \lambda_2 y_0 + \lambda_3 z_0)} \end{cases}$$

a, b, c, k is the correlation coefficient.

Get the unique solution:

$$\hat{u}(t, \lambda) = Me^{-(a^2 \lambda_1^2 + b^2 \lambda_2^2 + c^2 \lambda_3^2 + k^2)t - i(\lambda_1 x_0 + \lambda_2 y_0 + \lambda_3 z_0)}$$

Find the inverse transformation of F^{-1} , because

$$F^{-1}\left[e^{-\frac{\lambda_1^2}{4a^2}}\right] = \frac{a}{\sqrt{\pi}} e^{-a^2 x^2}$$

$$F^{-1}\left[e^{-\frac{\lambda_1^2}{4a^2}} e^{-i\lambda_1 x_0}\right] = \frac{a}{\sqrt{\pi}} e^{-a^2 (x - x_0)^2}$$

Hence

$$\begin{aligned} u(x, y, z, t) &= F^{-1}(\hat{u}) \\ &= \frac{M}{(2\sqrt{\pi})^3 \sqrt{a^2 b^2 c^2}} \exp\left[-\frac{(x - x_0)^2}{4a^2 t} - \frac{(y - y_0)^2}{4b^2 t} - \frac{(z - z_0)^2}{4c^2 t} - k^2 t\right] \\ &= \frac{M}{8\pi abc \sqrt{\pi}} \exp\left[-\frac{(x - x_0)^2}{4a^2 t} - \frac{(y - y_0)^2}{4b^2 t} - \frac{(z - z_0)^2}{4c^2 t} - k^2 t\right] \end{aligned}$$

To sum up, the derived thermoelectric conversion efficiency equation of multilayer heat emitter. It is not difficult to find that we can directly solve it in combination with the third question and use computer software to solve it. It is found that the number of layers, material and thickness of each layer and emission spectrum are 4 layers respectively, and the four layers are GaSb, GA, GA, and Sb, with a thickness of 94.732. In this case, GaSb battery design multilayer heat emitter has relatively high thermoelectric conversion efficiency.

6. Strengths and Weakness

6.1 Strengths

Particle swarm optimization algorithm consists of a group of particles moving in the search space, which is affected by its own best past position pbest and the best past position gbest of the whole group or its nearest neighbor. For some improved algorithms, a random term will be added to the last term of the speed update formula to balance the convergence speed and avoid premature convergence. According to the characteristics of location update formula, particle swarm optimization algorithm is more suitable for solving continuous optimization problems.

6.2 Weakness

(1) For the neural network method, the method itself needs to be effectively trained with a large amount of data to determine the rationality of the weight of secondary factors, but it can provide sufficient data in more aspects, so it takes a long time and process to popularize and use the model.

(2) Particle swarm optimization algorithm is not good for discrete optimization problems, and it is easy to fall into local optimization.

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