2021 Asia and Pacific Mathematical Contest in Modeling

Problem B

Optimal Design of Thermal Emitter in Thermophotovoltaic Technology

In recent years, the world's major powers have turned their eyes one after another to "the sea of stars", formulating various plans of space exploration. In 2020, China's "Tianwen-1" was launched and navigated through space to Mars; then in 2021, the rover "Zhurong" completed its projected mission, and staying on Mars, it is still working for more findings of the vast universe. To ensure that the various instruments and devices carried by the rover could operate well without sun exposure, and to provide necessary technical support for its long-time work, scientists explored and developed thermophotovoltaic technology. This picture below shows a test prototype of a thermophotovoltaic device.

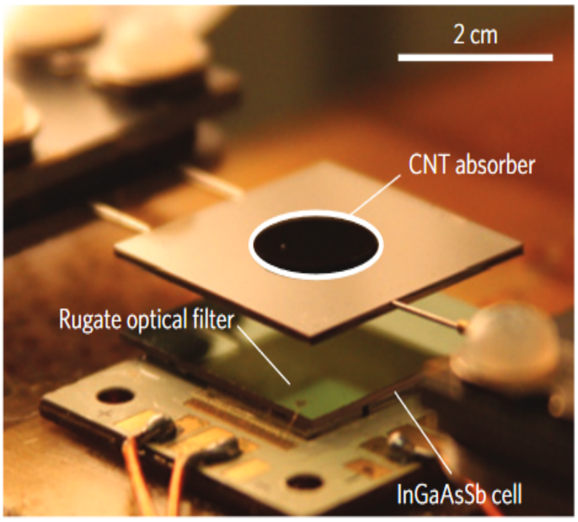

Figure 1: The test prototype of the thermophotovoltaic device

The thermophotovoltaic technology is a technology that uses various heat sources to heat a thermal emitter (absorber), and then converts the infrared radiation of the thermal emitter into electricity through photovoltaic cells. There are many types of heat sources, including chemical energy, solar energy, nuclear energy, etc. The thermal emitter in the system mainly utilizes different material structures to regulate the emission of the heat absorbed, so that most of the emitted photons are below the band-gap wavelength of the photovoltaic cell. The photovoltaic cell mainly converts the high-energy photons that are below a particular band-gap wavelength. It possesses a certain band-gap energy, and therefore a corresponding band-gap wavelength. For example, a silicon solar cell with a band-gap wavelength of 1100 nanometers can only absorb the high-energy photons below the wavelength aforementioned and convert them into electrical energy, while low-energy photons above the wavelength absorbed by the cell cannot be converted into electrical energy through the photoelectric effect. Instead, they can only be transformed into thermal energy, and the photoelectric conversion efficiency of the cell is thus reduced. Therefore, to improve the thermoelectric conversion efficiency of the thermophotovoltaic system, it is essential to regulate the emission spectrum of the thermal emitter. Calculation methods of the emission spectrum mainly include the Transfer Matrix Method (TMM) [1-2], the Finite Difference Time Domain Method (FDTD), and the Rigorous Coupled Wave Analysis Method (RCWA). And chief factors affecting the emission spectrum of the thermal emitter are the optical properties (refractive index or dielectric constant) and structural properties (thickness) of the material. Wang et al. [3] have developed a sub-micron-thick multilayer selective solar absorber, which is composed of tungsten, silicon dioxide and silicon nitride, and has an absorption rate up to 0.95 in the solar waveband. In 2014, the Evelyn Wang team of the Massachusetts Institute of Technology designed a photon-controlled solar thermophotovoltaic device that operated well in experiments. In their work, the thermal emitter is a multilayer film structure composed of silicon and silicon dioxide. The thickness of each layer is optimized so that its emission spectrum corresponds to the band gap of indium gallium arsenide antimonide (InGaAsSb) batteries. The refractive index or dielectric constant of different materials can be found by searching documents or referring to the optical property database of materials [5], which provides the refractive index of common materials. Please solve the following problems according to the above introduction.

(1) Please express the relationship between the emission spectrum of the single-layer structure and the material properties (refractive index, thickness), and calculate the emission spectrum of a 50-nanometer-thick tungsten (as shown in the picture below) within 0.3-5 microns.

Figure 2: The schematic of 50-nanometer-thick tungsten

(2) Please express the relationship between the emission spectrum of the multilayer structure and the material properties (refractive index, thickness), and calculate the emission spectrum of the composite structure formed by tungsten (50 nm) and silica (50 nm) (as shown in the picture below) within 0.3-5 microns.

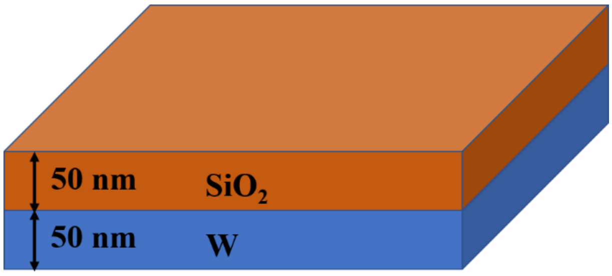

Figure 3: The schematic of multilayer structure formed by tungsten and silica

(3) In order to improve the spectral-control ability of the radiator, sometimes the thermal emitter is designed to emit in a narrow-band form, that is, the emission is concentrated within a very small band, thereby improving the thermoelectric conversion efficiency of the thermophotovoltaic device, such as the multilayer narrow-band emitter designed by Sakurai et al. [6] with silicon, silicon dioxide and germanium. Please select reasonable materials, design a multiplayer thermal emitter to make its emission as narrow-band and high as possible, and give the design parameters of the multilayer structure (including the number of layers, the material and thickness of each layer), as well as its emission spectrum. Note that the idea thermal emitter in this question has the sharp and high thermal emission at 1.5 microns, and the calculated wavelength range is 0.3-5 microns.

(4) The gallium antimonide (GaSb) battery is currently more advanced among others. Assume that its band-gap wavelength is 1.71 microns. The emission spectrum of its idealized thermal emitter is roughly shown by the red-dotted line in the picture below. The blue-dotted line represents the External Quantum Efficiency (EQE), and its influence can be considered properly. Please select reasonable materials, design a multilayer thermal emitter for the GaSb battery to achieve the highest possible thermoelectric conversion efficiency, and give the design parameters of the multilayer structure (including the number of layers, the material and thickness of each layer), as well as its emission spectrum.

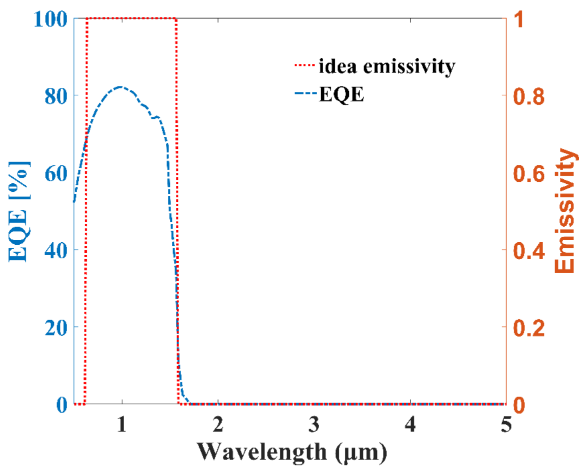

Figure 4: The EQE and ideal emission spectrum of GaSb for thermophotovoltaic

Note: The emission spectra here are all of vertical emission.

Explanation of professional terms:

Thermophotovoltaic: a device that includes heat sources, thermal emitters, photovoltaic cells, and heat-dissipation systems etc. for converting thermal energy into electrical energy.

Thermal emitter: a component that emits thermal radiation when heated.

References:

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[4] Lenert A, Bierman D M, Nam Y, et al. A nanophotonic solar thermophotovoltaic device[J]. Nature nanotechnology, 2014, 9(2): 126-130.

[5] https://refractiveindex.info/ (Refractive index database)

[6] Sakurai A, Yada K, Simomura T, et al. Ultranarrow-band wavelength-selective thermal emission with aperiodic multilayered metamaterials designed by Bayesian optimization[J]. ACS central science, 2019, 5(2): 319-326.