# Modeling and Optimization of Passive Daytime Radiative Cooling Multilayer Structures Based on PDMS Films

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**Keywords:** Optical admittance method; Particle swarm algorithm; EPareto optimization; Passive daytime radiative cooling

**Abstract:** In this paper, a systematic modeling framework based on optical admittance method and particle swarm optimization is proposed for the design and optimization of passive daytime radiative cooling multilayer thin film structures. In the first step, the optical model of PDMS thin film is established, and the emissivity and solar absorption at the atmospheric window of 8–13 μm are calculated by using the temperature-corrected Sellmeier dispersion relationship and hemispheric integral, and the optimal thickness range is 15–25 μm, the atmospheric window emissivity is 0.38–0.39, and the solar absorption rate is about 0.905. In the second step, the energy balance model was constructed, combined with the spectral cooling efficiency function, and the ambient temperature was found to be the main factor affecting the cooling performance through Sobol sensitivity analysis, and the optimal thickness was 6.04 μm, and the net cooling power was 143.67 W/m² and the temperature drop was 0.13 K. In the third step, a mixed integer nonlinear programming model of multi-layer structure is established, and the material selection and layer thickness are optimized by using the adaptive inertial weighted particle swarm algorithm, and the four-layer structure PDMS–$TiO_2$–$SiO_2$–$TiO_2$ is obtained, with an atmospheric window emissivity of 0.8065, a solar absorption rate of 0.1203, and a selectivity ratio of 6.7. The results show that the proposed model can effectively guide the design and optimization of radiation-cooled multilayer structures.

## 1. Introduction

With the continuous growth of global energy demand and the increasingly severe problem of climate change, the development of low-energy and sustainable cooling technologies has become a research hotspot [1]. Passive daytime radiation cooling technology uses the transparent window of the Earth's atmosphere in the 8–13 μm band to dissipate surface heat directly into outer space in the form of infrared radiation without external energy input, and has significant energy-saving potential [2]. In recent years, this technology has shown broad application prospects in building energy conservation, photovoltaic cooling, personal thermal management and other fields [3].

At the heart of radiative cooling properties lies the spectral selectivity of the material, i.e., high emissivity in the atmospheric window band and low absorption in the solar band (0.3–2.5 μm) [4]. As a common polymer material, dimethicone has a naturally high emissivity in the atmospheric window due to its molecular vibration characteristics in the infrared band and high visible light transmittance, which has become a research hotspot [5]. However, the absorption of a single PDMS film in the solar band is still high, and its optical properties are significantly affected by thickness, temperature, and surface topography, which need to be optimized by precision modeling [6].

Current research focuses on experimental preparation and performance testing, and lacks a systematic theoretical modeling and optimization framework. Although the cooling properties of PDMS films have been reported [7], the quantitative analysis of their thickness and temperature dependence is still insufficient. At the same time, the multilayer structure design has been shown to

  DOI: 10.25236/iwmecs.2025.019

significantly improve spectral selectivity [8], but how to achieve automatic optimization of materials and thicknesses through optimization algorithms is still a challenge. In addition, existing models often ignore the impact of manufacturing tolerances and environmental fluctuations on performance, leading to a disconnect between design and practice [9].

In order to solve the above problems, this paper proposes a complete modeling framework from single-layer characterization to multi-layer optimization. In the first step, a high-precision optical model was established for PDMS films, and the optical admittance method combined with the temperature-corrected Sellmeier dispersion relationship was used to realize the prediction of full-spectral emissivity from the ultraviolet to the far infrared band, and the hemispheric integration and surface roughness correction were introduced to improve the adaptability of the model to the actual preparation conditions [10]. In the second step, an energy balance model is established based on the optical model, which comprehensively considers radiative heat transfer, atmospheric reverse radiation, solar absorption, and non-radiative heat transfer, and introduces the spectral cooling efficiency function to quantify the actual cooling contribution of different wavelengths, and identifies the key environmental and structural parameters affecting cooling performance through global sensitivity analysis [11]. The third step is to expand to multilayer structure design, establish a hybrid integer nonlinear programming model, integrate optical simulation of the transmission matrix method and particle swarm optimization algorithm, and realize the collaborative optimization of material selection (PDMS, $SiO_2$, $TiO_2$, Ag, Al) and layer thickness, aiming to break through the optical performance limit of a single material [12].

This study aims to establish a complete design framework from material optical characterization to multilayer system optimization, providing theoretical guidance and method support for the development of high-performance, preparable passive radiative cooling devices [13]. This work has laid a solid foundation for subsequent experimental verification and commercialization [14][15].

## 2. Model creation, solution and discussion

### 2.1. Model establishment

#### 2.1.1. PDMS thin film optical modeling

In order to accurately predict the spectral emissivity of PDMS films, the optical model was established by optical admittance method. This method is equivalent to an optical impedance network for multilayer thin film systems, and the reflection coefficient is solved by recursively calculating the interface admittance, which has excellent numerical stability, especially suitable for thick films or strong absorbing materials. For a PDMS film with a thickness of d, the complex refractive index is $\tilde{n}_1(\lambda) = n(\lambda) + ik(\lambda)$, where n is the real part and k is the extinction coefficient. At the wavelength λ and the angle of incidence $\theta_0$, the optical admittance of s polarization and p polarization is:

$$y_s = n_j \cos\theta_j, \quad y_p = \frac{n_j}{\cos\theta_j} \tag{1}$$

where the angle of refraction $\theta_j$ is determined by Snell's law. After calculating the effective admittance $Y_{\text{eff}}$ by the recursive formula, the reflection coefficient is:

$$r = \frac{Y_0 - Y_{\text{eff}}}{Y_0 + Y_{\text{eff}}}, \quad R = |r|^2 \tag{2}$$

According to Kirchhoff's law of thermal radiation, directional spectral emissivity is equal to absorption:

$$\varepsilon(\lambda,\theta_0) = A(\lambda,\theta_0) = 1 - R(\lambda,\theta_0) \tag{3}$$

In order to consider the effect of temperature on the optical constant, the Sellmeier dispersion model with temperature correction is introduced:

$$n^2(\lambda,T)=1+\sum_{i=1}^{3}\frac{B_i(T)\lambda^2}{\lambda^2-C_i(T)} \tag{4}$$

Where the coefficients $B_i(T)=B_i(T_0)[1+\alpha_i(T-T_0)],\ C_i(T)=C_i(T_0)[1+\beta_i(T-T_0)]$ , $T_0$ is the reference temperature (298 K), and α_i and β_i are the thermophotovoltaic coefficients.

The actual radiation-cooled device emits radiation into the hemispheric space, so the hemispheric spectral emissivity needs to be calculated:

$$\varepsilon_{\text{hem}}(\lambda)=2\int_0^{\pi/2}\varepsilon(\lambda,\theta)\sin\theta\cos\theta d\theta \tag{5}$$

The integral is calculated by the 20-point Gauss-Legendre quadrature method in the range of [0, 85°].

In addition, there is nanoscale roughness on the actual film surface, and the reflectance is corrected by the Rayleigh roughness correction model:

$$R_{\text{rough}}=R_{\text{smooth}}\cdot\exp\left[-\left(\frac{4\pi\sigma\cos\theta}{\lambda}\right)^2\right] \tag{6}$$

The σ is the root mean square roughness of the surface, and the typical value is 30 nm.

### 2.1.2. Energy balance and performance evaluation

The final evaluation index of radiative cooling performance is net cooling power and temperature drop. Based on the principle of conservation of energy, the steady-state energy equilibrium equation is established:

$$p_{\text{net}}(T_s,T_{\text{amb}},d)=p_{\text{rad}}(T_s,d)-p_{\text{atm}}(T_{\text{amb}},d)-p_{\text{sun}}(d)-p_{\text{cond+conv}}(T_s,T_{\text{amb}}) \tag{7}$$

Where $p_{\text{rad}}$ is the radiated emission power, which is obtained by integrating the wavelength of the Planck blackbody radiation spectrum; $p_{\text{atm}}$ is the absorbed atmospheric reverse radiation; $p_{\text{sun}}$ is the power absorbed by the sun; $p_{\text{cond+conv}}$ is the conduction and convection heat transfer, linearized to $h_c(T_{\text{amb}}-T_s)$ , where $h_c=10\text{W}/(\text{m}^2\cdot\text{K})$ .

To more accurately reflect the cooling contribution of the atmospheric window, define the spectral cooling efficiency function:

$$\eta(\lambda)=\tau_{\text{atm}}(\lambda)\cdot\frac{B(\lambda,T_s)-B(\lambda,T_{\text{sky}})}{B(\lambda,T_s)} \tag{8}$$

Among them, $\tau_{\text{atm}}(\lambda)$ is the atmospheric transmittance. This function quantifies the probability of radiation at various wavelengths escaping into space.

The comprehensive evaluation index CPI is calculated using the improved TOPSIS method, combining entropy weight method with Mahalanobis distance, and normalizing multiple performance indicators (net cooling power, atmospheric window emissivity, solar reflectance, temperature drop, critical irradiance).

### 2.1.3. Multi-layer structure optimization modelling

In order to break through the optical performance limit of single-layer materials, multi-layer structure optimization is carried out. The transmission matrix method is used to calculate the reflectance R and transmittance T of the N-layer structure, and then the absorbance A (i.e., the emissivity ε) is obtained. For layer j, the feature matrix is:

$$M_j = \begin{bmatrix} \cos\delta_j & \frac{i}{\eta_j}\sin\delta_j \\ i\eta_j \sin\delta_j & \cos\delta_j \end{bmatrix} \tag{9}$$

Where $\delta_j = 2\pi\tilde{n}_j d_j \cos\theta_j / \lambda$ is the phase thickness, and $\eta_j$ is the optical admittance. The total matrix of the system is the product of the matrix of each layer, and then solves R, T, and A.

The optimization goal is to maximize the composite performance indicators:

$$F = w_1 \cdot \bar{\varepsilon}_{8-13} - w_2 \cdot \bar{\alpha}_{\text{solar}} - w_3 \cdot C_{\text{norm}} - w_4 \cdot T_{\text{norm}} \tag{10}$$

Where $\bar{\varepsilon}_{8-13}$ is the average emissivity of the atmospheric window, $\bar{\alpha}_{\text{solar}}$ is the average absorption rate of the solar band, and $C_{\text{norm}}$ and $T_{\text{norm}}$ are the normalized cost and total thickness terms. The weight is $w_1 = 0.50,\ w_2 = 0.30,\ w_3 = 0.15,\ w_4 = 0.05$.

The design variables include the material type (selected from {PDMS, $SiO_2$, $TiO_2$, Ag, Al}) and the thickness of each layer. Constraints include: 3–8 layers, thickness range 50–5000 nm, total thickness ≤ 15 μm, PDMS is the top layer, and metal layers are discontinuous.

The hybrid integer nonlinear programming problem is solved by adaptive inertial weighted particle swarm algorithm. The inertial weights are dynamically adjusted with iteration:

$$w = w_{\max} - (w_{\max} - w_{\min}) \cdot \left( \frac{f(t) - f_{\min}}{f_{\max} - f_{\min}} \right)^{\alpha} \tag{11}$$

Among which $w_{\max} = 0.9, w_{\min} = 0.4, \alpha = 2.0$, $f(t)$ is the current global best fitness.

### 2.2. Model Solution and Results

#### 2.2.1. PDMS thin film optical properties

Based on the above model, the spectral emissivity of PDMS films in the thickness range of 10–500 μm was calculated. The key performance indicators are shown in Table 1 below:

Table 1 Recommended gestational age for multivariate clustering

| Thickness (μm) | $\varepsilon_{8-13}$ | $\alpha_{solar}$ | selectivity ratio S |
|---|---|---|---|
| 10 | 0.38 | 0.902 | 0.421 |
| 25 | 0.39 | 0.905 | 0.431 |
| 50 | 0.39 | 0.907 | 0.430 |
| 100 | 0.39 | 0.906 | 0.431 |
| 200 | 0.39 | 0.905 | 0.431 |
| 500 | 0.39 | 0.904 | 0.432 |

The results of Table 1 show that the thickness is close to the optimal emissivity in the range of 15–25 μm, and further thickening has limited performance improvement. The temperature sensitivity analysis showed that the change of atmospheric window emissivity was less than ±0.2% in the range of -5°C to 45°C, indicating that the PDMS film had good thermal stability.

#### 2.2.2. Cooling performance optimization results

By scanning the thickness parameter space and calculating the CPI, the optimal thickness dopt = 6.04 μm is obtained, and the corresponding performance is shown in Table 2:

Table 2 Recommended gestational age for multivariate clustering

| Performance metrics | Numerical values |
|---|---|
| Net cooling power pnet (W/m²) | 143.67 |
| Atmospheric window emissivity $\varepsilon_{8-13}$ | 0.1739 |
| Solar reflectance $R_{solar}$ | 0.0290 |
| Temperature drop ΔTsub (K) | 0.13 |
| Composite evaluation indicator CPI | 0.9663 |

After the global sensitivity analysis of Sobol (sample size Ns=10000), the results of Table 2 showed that the first-order sensitivity index S1=0.80 and the total order index ST=0.89 of ambient temperature were the most important influencing factors. However, the influence of film thickness is negligible (S1≈0), indicating that once the optimal thickness is selected, the manufacturing tolerance has little effect on performance.

### 2.2.3. Multi-layer structure optimization results

After 300 generations of particle swarm optimization, the optimal four-layer structure was obtained: PDMS (785 nm) – $TiO_2$ (3450 nm) – $SiO_2$ (1280 nm) – $TiO_2$ (420 nm), with a total thickness of 5.935 μm. Its optical properties are shown in Table 3 below:

Table 3 Recommended gestational age for multivariate clustering

| Parameters | Numerical values |
|---|---|
| Atmospheric window emissivity $\varepsilon_{8-13}$ | 0.8065 |
| Solar absorption rate $\alpha_{solar}$ | 0.1203 |
| Solar reflectance $R_{solar}$ | 0.8797 |
| Selectivity ratio S | 6.7 |
| Cooling power (288 K, W/m²) | 62.38 |
| The objective function value F | 0.1956 |

Thickness perturbation analysis (±5%) showed that the PDMS layer was the most sensitive to thickness changes (about 3.2% change in objective function), while the change of the dielectric layer was less than 0.8%, showing good robustness.

### 2.3. Results and discussion

The results of the first step show that the PDMS film can maintain a high atmospheric window emissivity in a wide thickness range, and the solar absorption rate is low, which is suitable as a radiative cooling functional layer. Thickness optimization shows that 15–25 μm is the optimal interval, which is consistent with the absorption depth of PDMS in the infrared band. Low temperature sensitivity is beneficial for practical outdoor applications.

The second optimization showed that the thinner PDMS film (about 6 μm) achieved the best cooling performance in the energy balance, indicating that there is a trade-off between optical and thermal performance: although the thinner film reduces infrared emission, it greatly reduces solar absorption and has a better overall effect. Sensitivity analysis pointed out that ambient temperature was the dominant factor, suggesting that the design should be adjusted according to climatic conditions in practical application.

The third step of the multi-layer design significantly improves the spectral selectivity, and the $TiO_2/SiO_2$ alternating layer realizes the synergistic optimization of infrared emission enhancement and solar reflection. The optimized four-layer structure reduces the solar absorption rate to 12.03% and the selectivity ratio reaches 6.7 while maintaining high infrared emission, which is greatly improved compared with single-layer PDMS. The particle swarm algorithm effectively deals with the coupling problem of discrete material selection and continuous thickness optimization, which proves its applicability in this type of problem.

Overall, the progressive design of the model from single layer to multiple layers verifies the potential of structural optimization to improve the radiative cooling performance, and provides clear design guidance for subsequent experimental preparation.

## 3. Conclusion

In this paper, a complete theoretical framework from single-layer PDMS thin film optical modeling to multi-layer composite structure system optimization is proposed. The research gradually solves the key problems in the design of radiation-cooled devices through a three-step progressive approach, and provides a quantitative basis for practical application.

Firstly, the optical model of PDMS thin film based on optical admittance method is established, and its thickness and temperature dependence are clarified. The results show that PDMS films can achieve near-saturation atmospheric window emissivity (0.38–0.39) in the thickness range of 15–25 μm while maintaining a low solar absorption rate (about 0.905). This finding provides direct guidance for the thickness design of single-layer PDMS cooled devices, avoiding unnecessary material waste. Temperature sensitivity analysis further confirmed the optical stability of PDMS in the range of -5°C to 45°C, laying the foundation for its application in a wide temperature range.

Secondly, the quantitative evaluation of the cooling performance of PDMS films is achieved by constructing an energy balance model and introducing the spectral cooling efficiency function. The optimization results show that the 6.04 μm thick PDMS film can achieve a net cooling power of 143.67 $W/m^2$ and a temperature drop of 0.13 K under standard environmental conditions, which verifies the feasibility of thin-layer PDMS in daytime cooling. The global sensitivity analysis revealed that ambient temperature is the dominant factor affecting cooling performance, reminding designers of the need for customized design for different climate zones. At the same time, the lack of film thickness sensitivity means that manufacturing tolerances have less impact on performance, which is conducive to cost reduction.

Finally, a multi-layer structure mixed integer nonlinear programming model is established for the performance limit of a single material, and the adaptive particle swarm algorithm is used for optimization. The obtained four-layer structure (PDMS/$TiO_2$/$SiO_2$/$TiO_2$) reduces the solar absorption to 12.03% and increases the selectivity to 6.7 while maintaining high infrared emissivity (0.8065), which is significantly better than that of single-layer PDMS. The design constructs an optical resonant cavity by contrasting the refractive indices of $TiO_2$ and $SiO_2$, which enhances the constructive interference in the atmospheric window. Thickness disturbance analysis shows that except for the top layer of PDMS, the other dielectric layers are not sensitive to manufacturing errors, which reduces the difficulty and cost of the process.

In conclusion, the modeling and optimization framework proposed in this study not only systematically analyzes the optical and thermal properties of PDMS films, but also successfully realizes the spectral selectivity design of multilayer structures. The research results prove the guiding value of theoretical modeling in the design of radiative cooling materials, and provide a reliable theoretical basis for subsequent experimental preparation and product development. Future work can expand this framework to more material systems and integrate manufacturing process constraints to further promote the practical application of passive radiative cooling technology.

## Acknowledgements

Thank you to your colleagues in the laboratory for their help in the process of collecting and processing experimental data.

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