

**Studies on β -FeSi₂ Optical Thin Films
and Application to Thermal Radiation
Control**

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Chapter 1 Introduction

Abstract

Wavelength-selective radiation technology has shown great promise in improving energy efficiency in applications such as thermophotovoltaic (TPV) systems, gas sensing, and wavelength-selective infrared drying. These systems require bandpass filters (BPFs) that can selectively transmit infrared radiation at specific wavelengths corresponding to absorption bands of target materials or molecules. This study focuses on developing new β -FeSi₂-based BPFs that meet the requirements for high performance, large-area manufacturability, and low cost in wavelength-selective radiation applications. In addition, the potential of these BPFs for applied to wavelength-selective drying was explored at the laboratory scale.

In this chapter, introduction to the wavelength-selective radiation technology and the outline of this thesis are described.

1.1 Background

Thermal radiation refers to the phenomenon by which an object emits energy in the form of electromagnetic waves due to its intrinsic temperature. A typical example is the thermal radiation from the sun to the earth. Effective utilization of such thermal radiation is one of the key challenges in realizing a sustainable society in the future. The spectral distribution of radiation emitted by an idealized emitter, known as a blackbody, which absorbs all incident radiation, is quantitatively described by Planck's law. Specifically, Planck's law defines how the radiation intensity of a blackbody varies across different wavelengths at a given temperature:

$$E_{\lambda}(\lambda, T)d\lambda = \frac{2\pi hc^2}{\lambda^5} \frac{d\lambda}{e^{hc/\lambda k_b T} - 1} \quad (1.1)$$

where E_{λ} denotes the spectral radiance of a blackbody at wavelength λ and absolute temperature T ; h is Planck's constant; c is the speed of light in vacuum; k_b is the Boltzmann constant. According to Planck's law, the spectrum of blackbody radiation exhibits distinct characteristics: it features a clear radiation intensity peak at a particular wavelength, which is uniquely determined by the temperature. Additionally, the emitted radiation spans a wide range of wavelengths. Normal materials, however, differ significantly from an ideal blackbody. Their radiative properties are often characterized by emissivity, defined as the ratio of the radiation emitted by the real object to that emitted by a blackbody at the same temperature. The emissivity value ranges between 0 and 1. For materials that have not undergone specific surface treatments, emissivity is typically dependent upon both the intrinsic properties of the material itself and the condition of its surface. In recent years, technologies that control the radiation spectrum by designing nanostructures on material surfaces have attracted significant attention due to their potential to significantly enhance energy utilization efficiency.[1-4]

A representative application of this technology is the thermophotovoltaic (TPV) system, [5-9] as illustrated in Figure 1.1(a), which converts infrared (IR) radiation emitted from high-temperature heat sources, such as blast furnaces, into electricity using photovoltaic (PV) cells. These heat sources typically emit radiation across a broad wavelength range, resembling blackbody radiation. However, conventional PV cells can efficiently convert only IR light with wavelengths around $2\text{ }\mu\text{m}$ into electrical energy. Radiation outside this wavelength range can hardly contribute to power generation, leading to not only thermal energy loss but also increased temperature of the PV cells, which degrades their photoelectric conversion efficiency. To address this issue, bandpass filter (BPF), also known as a wavelength-selective transmission thin film, has been proposed. By introducing a BPF between the heat source and the PV cells, only infrared radiation

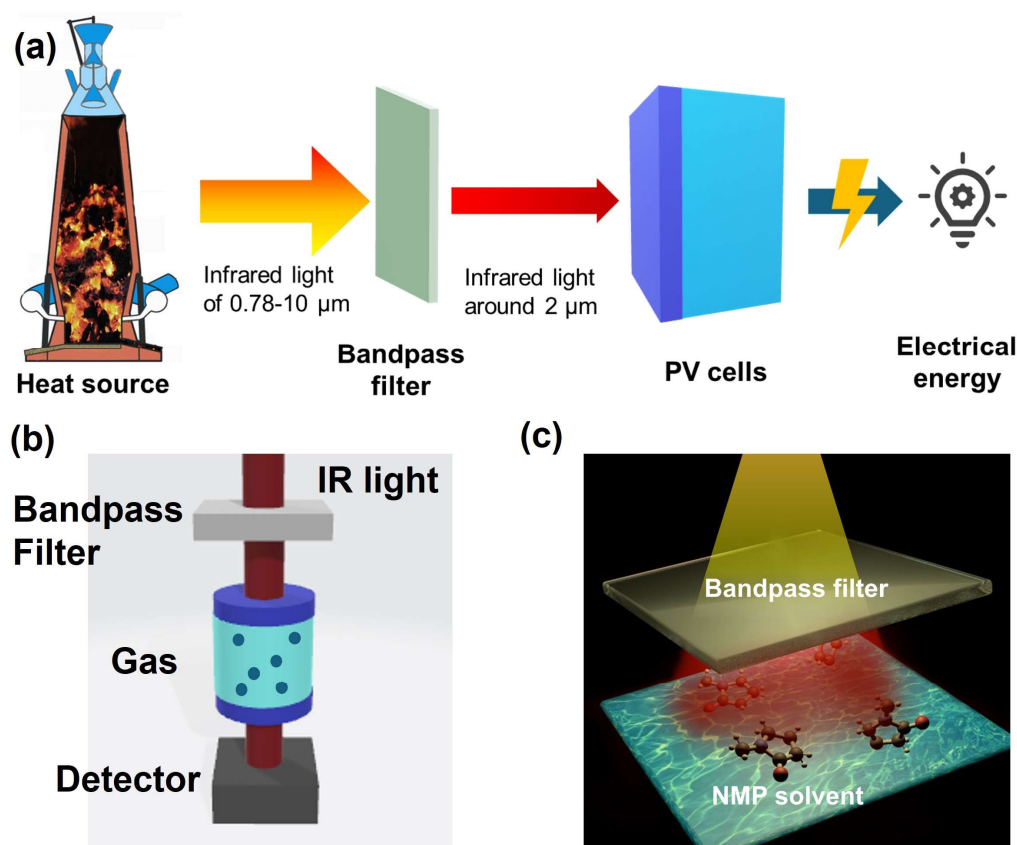


Figure 1.1 The applications of wavelength selective radiation. (a) TPV system; (b) Gas sensor; (c) Wavelength selective drying system.

around 2 μm can pass through while other wavelengths are blocked. This selective transmission reduces energy loss and enhances overall power generation efficiency. Additionally, wavelength control technology is also important in the measurement of gas concentrations, such as carbon dioxide and methane (Figure 1.1 (b)). Because these gas molecules possess characteristic absorption wavelengths in the mid-infrared region, their concentrations can be measured by utilizing a BPF designed at those wavelengths, based on the magnitude of their infrared absorption. [10, 11]

In addition to the above applications, wavelength-selective radiation technology has also been proposed for use in solvent-drying processes.[12-14] Conventional drying methods, such as hot air method and infrared heating, often face issues related to safety of solvents and thermal damage under high-temperature conditions. By employing a bandpass filter to irradiate only infrared wavelengths that precisely match the absorption band of the solvent (Figure 1.1(c)), both drying efficiency and system safety can be improved. Therefore, in all of the wavelength-selective radiation applications described above, BPFs capable of precisely controlling the emitted wavelength play a critical role in achieving high-efficiency operation.

1.2 Previous studies and challenges

Numerous micro- and nanostructures have been developed to realize ideal BPFs with narrow and high transmittance peaks at the required wavelengths. Among them, the most widely used approach is multilayer thin films. These filters, composed of alternating high and low refractive index materials that are transparent in the infrared region, provide well-defined transmittance spectra and are commonly available in commercial products. However, the high refractive index materials commonly used in multilayer thin films, such as Si and TiO_2 , is not sufficiently high, typically in the order of 2–3.[15-18] In such cases, an increase in the thickness of the thin film and the number of layers is required to achieve ideal optical functions. Other studies have suggested that two-dimensional[19, 20] and three-dimensional photonic crystals[21, 22] can effectively control the shape and position of the peak by precisely tuning the wavelength of the photonic bandgap using their periodic structures. However, challenges remain in scaling up production and reducing the high costs. Therefore, for systems that require wavelength control of radiation over large areas, it is essential to employ multilayer stack structures with fewer layers, enabled by the use of materials with higher refractive indices.

Figure 1.2 shows the refractive indices of several commonly used optical thin film materials.[23] It can be observed that $\beta\text{-FeSi}_2$ ($n > 5$) exhibits a much higher refractive index than these conventional optical thin film materials including Si, TiO_2 , and Ta_2O_5 . Although PbTe also possesses a high refractive index, its toxicity and limited chemical stability significantly restrict its practical use. Therefore, we focus on $\beta\text{-FeSi}_2$ as a promising candidate material.

$\beta\text{-FeSi}_2$ is well known for its remarkable optical and electrical properties. It has a direct bandgap of 0.87 eV and a significant optical absorption coefficient ($\alpha > 10^5 \text{ cm}^{-1}$), [24, 25] and has been extensively studied as a thermoelectric material,[26] as well as for

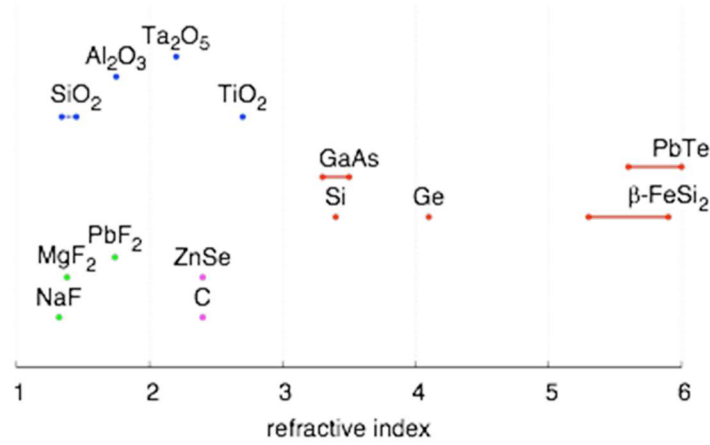


Figure 1.2 Refractive indices of typical optical thin film materials.

applications in LEDs[27] and photovoltaic devices.[28] However, despite possessing one of the highest refractive indices among semiconductor materials, it has not been utilized as an optical thin-film material. Since bulk β -FeSi₂ is transparent and has a high refractive index of above 5 (for wavelength $> 1.55 \mu\text{m}$), it is suitable for the application of an optical thin film in the infrared region.[29] By utilizing β -FeSi₂ as a high-refractive-index layer, it can be expected to realize BPFs with reduced film thickness and fewer layers, thereby enabling applications in wavelength-selective radiation.

1.3 Aims of this thesis

The purpose of this thesis is to develop a novel BPF based on β -FeSi₂ and to investigate its potential for wavelength-selective radiation applications. To achieve this, this thesis is divided into the following three steps:

- 1) Investigate the optical properties of β -FeSi₂ thin films and develop β -FeSi₂ thin film which is transparent in the infrared region.
- 2) Design and fabricate infrared BPFs with a high and narrow peak at the desired wavelengths.
- 3) Evaluate the effectiveness of fabricated BPFs in wavelength-selective radiation applications in lab scale—in this thesis, we focused on wavelength-selective drying as the target application. Mainly, we investigated the effect of using such bandpass filters on the evaporation rate of organic solvents in wavelength selective drying.

1.4 Outline of this thesis

This study focuses on developing novel β -FeSi₂-based BPFs that meet the requirements for high performance, large-area manufacturability, and low cost in wavelength-selective radiation applications. In addition, the potential of these BPFs for applied to wavelength-selective drying was explored at the laboratory scale.

Chapter 2 investigates the composition and optical properties of β -FeSi₂ thin films fabricated by co-sputtering, focusing on reducing infrared absorptance for use in BPFs. By adjusting the Fe/Si ratio through RF power control, films with nearly zero extinction coefficient ($k \approx 0$) and high refractive index were successfully obtained. The content of this chapter is based on the article: X. Zhang, S. Kumar, K. Namura, and M. Suzuki, "Studies on Composition and Optical Properties of β -FeSi₂ Thin Film Prepared by Co-sputtering," *Surface and Vacuum*, **64**, 418 (2021).

Chapter 3 presents the design and fabrication of a β -FeSi₂-based infrared BPF with a simple three-layer structure (β -FeSi₂/SiO₂/ β -FeSi₂), demonstrating high transmittance (> 80%) and narrow spectral selectivity at the target wavelength of 2 μ m. The experimental results confirm that β -FeSi₂, owing to its high refractive index and low extinction coefficient, enables efficient and low cost BPF fabrication, offering significant advantages over conventional materials in both optical performance and manufacturing simplicity. The content of this chapter is based on the article: X. Zhang, K. Namura, and M. Suzuki, " β -FeSi₂: A high refractive index candidate material for infrared bandpass filters " *J. Appl. Phys.*, **134**, 185302 (2023).

Chapter 4 investigates the effect of wavelength-selective IR irradiation on solvent evaporation using β -FeSi₂-based BPFs tuned to the absorption band of NMP at 3.4 μ m. Experimental results demonstrated that aligning the IR wavelength with the solvent's absorption peak significantly enhanced evaporation efficiency at lower bulk temperatures,

with an evaporation rate approximately six times higher than that under broad-spectrum IR, highlighting the potential of this approach for energy-efficient drying in industrial applications. The content of this chapter is based on the article: X. Zhang, K. Namura, and M. Suzuki, "Application of β -FeSi₂-based bandpass filters in wavelength-selective infrared drying systems " Jpn. J. Appl. Phys., **64**, 11SP16 (2025).

Chapter 5 summarizes the entire thesis and highlights the significance of this research.

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Chapter 2 Composition and Optical Properties of β -FeSi₂ Thin Film Prepared by Co-sputtering

Abstract

β -FeSi₂ is a promising candidate for high-performance BPF for its bulk is transparent and has a high refractive index for wavelengths above 1.55 μm . However, previous study revealed that the sputtered β -FeSi₂ thin film differ from the bulk material, showing a higher extinction coefficient and significant absorptance in the infrared region. To address this, we investigated the relationship between absorptance and composition by fabricating β -FeSi₂ films via RF co-sputtering, controlling the Si atomic fraction through the applied power on FeSi₂ and Si targets. By maintaining the FeSi₂ target at 100 W and adjusting the Si target power, we achieved stoichiometric β -FeSi₂ (1:2 ratio) at 10–12 W, yielding minimal absorptance (~ 0) in the infrared range. These films exhibited both a high refractive index and low extinction coefficient, demonstrating that co-sputtering is an effective method for producing β -FeSi₂ films suitable for BPF applications.

2.1 Introduction

β -FeSi₂, also known as iron disilicide, is a semiconductor composed of elements that are abundantly available in natural resources. Due to its direct bandgap of approximately 0.87 eV and high optical absorption coefficient ($\alpha > 10^5 \text{ cm}^{-1}$), β -FeSi₂ has been extensively studied for various advanced optical applications, including light-emitting diodes (LEDs) and solar cells.[1-5] Additionally, β -FeSi₂ exhibits excellent thermal and corrosion resistance, along with a high Seebeck coefficient, making it a promising candidate for thermoelectric energy conversion.[6, 7] Here, we focus on the optical properties of β -FeSi₂. Given that bulk β -FeSi₂ is transparent and possesses a high refractive index in the infrared region (for wavelengths above 1.55 μm),[8, 9] it is particularly suitable for applications as optical thin films in infrared-related technologies. (We have also explored several applications of β -FeSi₂ in the ultraviolet and visible wavelength ranges, such as solar-blind photodetectors and laser-induced bubble resonators. Interested readers may refer to Refs.[10, 11] for details.)

Figure 2.1 shows a portion of the phase diagram of the Fe–Si binary system.[12] Three crystalline phases can be identified: tetragonal α -Fe₂Si₅, orthorhombic β -FeSi₂, and cubic ϵ -FeSi.[13] Among them, β -FeSi₂ is a semiconducting phase and exhibits significant potential for practical applications. It can also be seen that β -FeSi₂ exhibits a very narrow compositional stability range and is stable only near the stoichiometric composition of Fe: Si = 1:2. Various fabrication methods for β -FeSi₂ thin films have been reported, including ion beam synthesis, molecular beam epitaxy, sputtering, and high-vacuum vapor deposition.[14] Our group has primarily focused on the development of β -FeSi₂ thin films using the sputtering method. When a FeSi₂ alloy target is sputtered onto substrates heated above 400 °C, the β -FeSi₂ phase can be formed, whereas deposition at lower substrate temperatures results in an amorphous FeSi₂ phase.

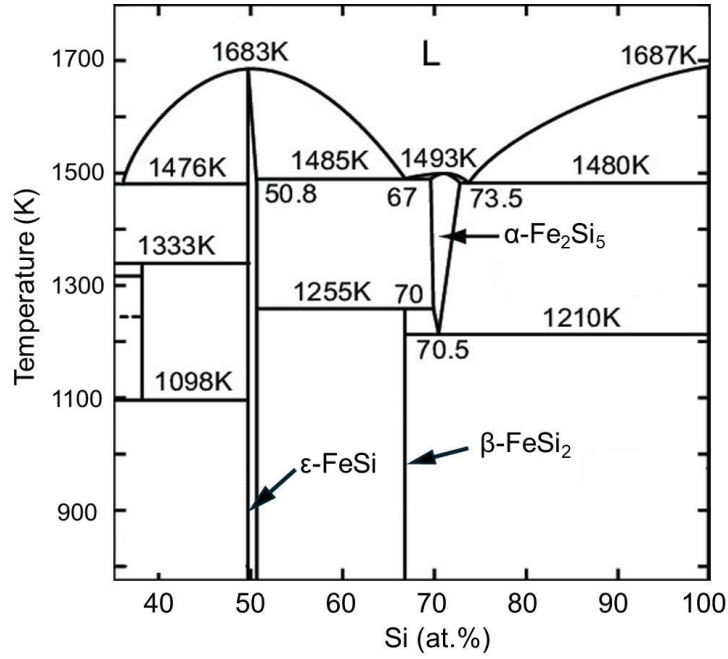


Figure 2.1. Phase diagram of the Fe-Si binary system.[12]

Utilizing this approach, we successfully developed β -FeSi₂ thin films that selectively absorb sunlight using a FeSi₂ alloy target, in which a multilayer structure composed of β -FeSi₂ and SiO₂ was fabricated on a tungsten layer to serve as an efficient solar-selective absorption coating.[15] This structure demonstrated a solar absorption rate exceeding 90% for wavelengths $\leq 2 \mu\text{m}$ while maintaining an emissivity below 10% in other wavelength regions. However, optical characterization of the β -FeSi₂ layers revealed that the extinction coefficient k for wavelengths above $2 \mu\text{m}$ was approximately 0.3, which is notably higher than that of bulk β -FeSi₂. Although the value of k enabled the realization of an efficient solar-absorber coating, it will lead to a substantial degradation in the performance of the bandpass filter.

To utilize β -FeSi₂ in a BPF, it is essential to eliminate film absorption; in other words, the extinction coefficient k must be reduced to 0. Multiple factors could contribute to this discrepancy in the extinction coefficient k , including variations in film composition, crystallinity, and the presence of impurities. Based on prior observations that Si-

containing films readily form SiO through oxidation and then volatilized during deposition, the most plausible explanation is a change in the composition of the β -FeSi₂ thin film during sputtering. While previous studies have investigated the properties of β -FeSi₂ thin films with varying Fe/Si ratios,[16, 17] to the best of the authors' knowledge, no research has specifically explored the relationship between the Fe/Si ratio and the infrared optical properties of β -FeSi₂ thin films prepared via sputtering. Therefore, the objective of this chapter is to clarify the origin of the extinction coefficient k becoming 0.3 and to develop transparent β -FeSi₂ thin films suitable for use in infrared bandpass filters.

2.2 Modeling for the transmittance and reflectance spectrum of the thin film and the complex reflective index

2.2.1 Reflectance and transmittance of single-layer thin film

As shown in Figure 2.2, the model of a single-layer thin film with refractive index N and thickness d on a substrate with refractive index N_s is considered when calculating reflectance R and transmittance T . The interface between air (refractive index N_0) and the thin film is defined as boundary a, while the interface between the thin film and the substrate is boundary b. Light incident from air undergoes reflection and transmission at boundaries a and b, respectively. The corresponding electric and magnetic fields at the interfaces are E_a , H_a and E_b , H_b . Since the tangential components of the electric and magnetic fields must remain continuous across interfaces, the following relationship is established.[18, 19]

At boundary b, the tangential components of $\mathbf{E}$ and $\mathbf{H}$ are

$$E_b = E_{1b}^+ + E_{1b}^- \quad (2.1)$$

$$H_b = \eta E_{1b}^+ - \eta E_{1b}^- \quad (2.2)$$

Hence

$$E_{1b}^+ = \frac{\eta E_b + H_b}{2\eta} \quad (2.3)$$

$$E_{1b}^- = \frac{\eta E_b - H_b}{2\eta} \quad (2.4)$$

$$H_{1b}^+ = \eta E_{1b}^+ = \frac{\eta E_b + H_b}{2} \quad (2.5)$$

$$H_{1b}^- = -\eta E_{1b}^- = \frac{H_b - \eta E_b}{2} \quad (2.6)$$

where η is the admittance of the thin film and symbol “+” means waves in the direction of incidence and “-” means waves in the opposite direction.

When light travels from boundary a to boundary b within a thin film, the phase difference of the electric field δ is given by:

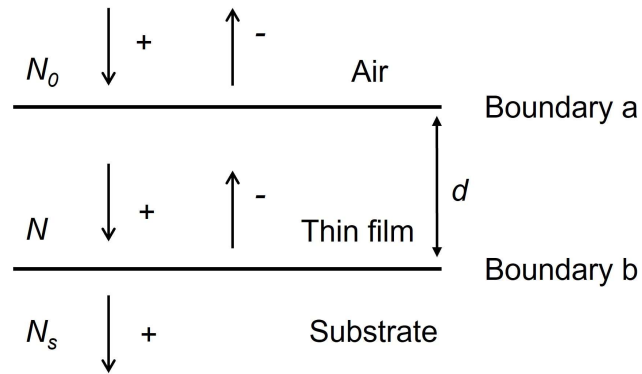


Figure 2.2. Optical model of the single-layer thin film.

$$\delta = \frac{2\pi}{\lambda}Nd \quad (2.7)$$

In this way, at boundary a

$$E_{1a}^+ = E_{1b}^+ e^{i\delta} = \frac{\eta E_b + H_b}{2\eta} e^{i\delta} \quad (2.8)$$

$$E_{1a}^- = E_{1b}^- e^{-i\delta} = \frac{\eta E_b - H_b}{2\eta} e^{-i\delta} \quad (2.9)$$

$$H_{1a}^+ = H_{1b}^+ e^{i\delta} = \frac{\eta E_b + H_b}{2} e^{i\delta} \quad (2.10)$$

$$H_{1a}^- = H_{1b}^- e^{-i\delta} = \frac{H_b - \eta E_b}{2} e^{-i\delta} \quad (2.11)$$

Therefore,

$$\begin{aligned} E_a &= E_{1a}^+ + E_{1a}^- \\ &= E_b \left(\frac{e^{i\delta} + e^{-i\delta}}{2} \right) + H_b \left(\frac{e^{i\delta} - e^{-i\delta}}{2\eta} \right) \\ &= E_b \cos \delta + H_b \left(\frac{i \sin \delta}{\eta} \right) \end{aligned} \quad (2.12)$$

$$\begin{aligned} H_a &= H_{1a}^+ + H_{1a}^- \\ &= E_b \eta \left(\frac{e^{i\delta} - e^{-i\delta}}{2} \right) + H_b \left(\frac{e^{i\delta} + e^{-i\delta}}{2} \right) \\ &= E_b i \eta \sin \delta + H_b \cos \delta \end{aligned} \quad (2.13)$$

It can be represented as a matrix notation:

$$\begin{bmatrix} E_a \\ H_a \end{bmatrix} = \begin{bmatrix} \cos \delta & \frac{i \sin \delta}{\eta} \\ i \eta \sin \delta & \cos \delta \end{bmatrix} \begin{bmatrix} E_b \\ H_b \end{bmatrix} \quad (2.14)$$

The 2×2 matrix M in equation 2.14 is known as the characteristic matrix of the thin film:

$$M = \begin{bmatrix} \cos \delta & \frac{i \sin \delta}{\eta} \\ i\eta \sin \delta & \cos \delta \end{bmatrix} \quad (2.15)$$

and it can represent the relationship between the electromagnetic fields of the boundary a and b. Meanwhile, on the air side of boundary a, the following equation can be derived:

$$E_{0a}^+ = \frac{\eta_0 E_a + H_a}{2\eta_0} \quad (2.16)$$

$$E_{0a}^- = \frac{\eta_0 E_a - H_a}{2\eta_0} \quad (2.17)$$

where η_0 is the admittance of the incident medium.

We define the input optical admittance of the assembly as:

$$Y = \frac{H_a}{E_a} \quad (2.18)$$

and the reflection coefficient and the transmission coefficient are:

$$\rho = \frac{E_{0a}^-}{E_{0a}^+} = \frac{\eta_0 E_a - H_a}{\eta_0 E_a + H_a} = \frac{\eta_0 - Y}{\eta_0 + Y} \quad (2.19)$$

$$\tau = \frac{E_b}{E_{0a}^+} = \frac{2\eta_0 E_b}{\eta_0 E_a + H_a} = \frac{2\eta_0 \left(\frac{E_b}{E_a}\right)}{\eta_0 + Y} \quad (2.20)$$

Since $Y_b = H_b/E_b$ is the admittance of the substrate, we can transform equation 2.14 as:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} \cos \delta & \frac{i \sin \delta}{\eta} \\ i\eta \sin \delta & \cos \delta \end{bmatrix} \begin{bmatrix} 1 \\ Y_s \end{bmatrix} \quad (2.21)$$

and the admittance Y is

$$Y = \frac{C}{B} \quad (2.22)$$

The reflection coefficient ρ and the transmission coefficient τ can be represented as:

$$\rho = \frac{\eta_0 B - C}{\eta_0 B + C} \quad (2.23)$$

$$\tau = \frac{2\eta_0 E_b}{\eta_0 E_a + H_a} = \frac{2\eta_0}{\eta_0 B + C} \quad (2.24)$$

The reflectance and the transmittance are:

$$R = |\rho|^2 = \left(\frac{\eta_0 B - C}{\eta_0 B + C} \right) \left(\frac{\eta_0 B - C}{\eta_0 B + C} \right)^* \quad (2.25)$$

$$T = \frac{Re(y_s)}{y_0} |\tau|^2 = \frac{4\eta_0 Re(y_s)}{(\eta_0 B + C)(\eta_0 B + C)^*} \quad (2.26)$$

2.2.2 Calculation for the complex reflective index of β -FeSi₂ thin films

The optical constants of bulk β -FeSi₂ have been reported in detail by Udono et al.,[20] however, there are no reports on the optical constants of polycrystalline β -FeSi₂ thin films. To design the multilayer thin film that meets the BPF requirement, a complex reflective index of the single layer β -FeSi₂ thin film on Si substrate was obtained as follows.

By replacing the film with a single surface shown in Figure 2.2, the method of solving the transmittance T_a and reflectance R_a of the air/thin film/substrate part on boundary a using the optical admittance concept is shown in Section 2.2.1. However, the reflection R_b caused by the high refractive index Si substrate at boundary b between the substrate and air also accounts for a large proportion of the measured reflectance. Therefore, the

calculated transmittance T and reflectance R spectrum of the thin film were considered using an air/thin film/substrate/air model (Figure 2.3).

When calculating n and k of a β -FeSi₂ thin film, light is vertically incident on a single-layer film. On boundary a, the reflectance R_a and transmittance T_a (from equation 2.25 and 2.26) as the light passes from air to the substrate and R'_a , T'_a as the light passes from the substrate to air in the opposite direction of the thin film assembly can be computed by the optical admittance concept. Furthermore, R_b and T_b are the reflectance and transmittance, respectively, as light passes from the substrate to the air on boundary b. It is possible to ignore the interference caused by the reflected light at each substrate interface because the thickness of the substrate is significantly greater than the infrared wavelength. Therefore, transmittance T and reflectance R of the entire system can be theoretically calculated using the following equations:

$$\begin{aligned} R &= R_a + T_a T'_a R_b e^{-2\alpha d} + T_a T'_a R'_a R_b^2 e^{-4\alpha d} + \dots \\ &= R_a + \frac{T_a T'_a R_b e^{-2\alpha d}}{1 - R'_a R_b e^{-2\alpha d}} \end{aligned} \quad (2.27)$$

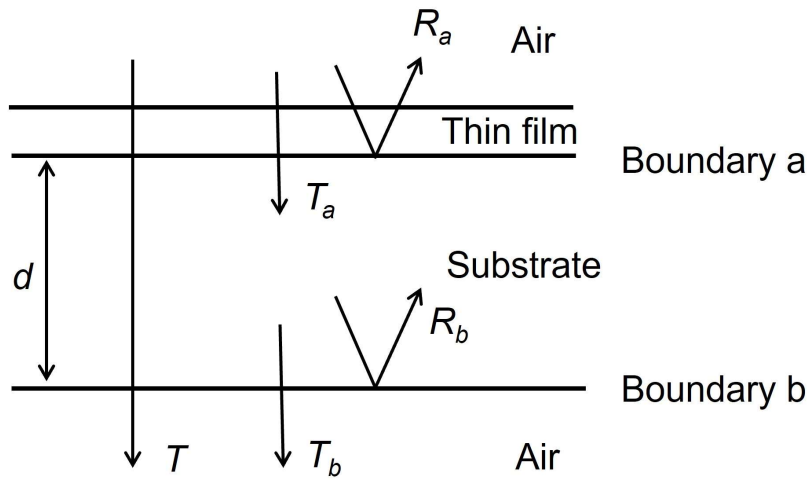


Figure 2.3. Optical model of air/thin film/substrate/air structure.

$$\begin{aligned}
T &= T_a T_b e^{-\alpha} + T_a T_b R_b R'_a e^{-3\alpha d} + \dots \\
&= \frac{T_a T_b e^{-\alpha d}}{1 - R'_a R_b e^{-2\alpha d}}
\end{aligned} \tag{2.28}$$

where the substrate's absorption coefficient $\alpha = \frac{4\pi k}{\lambda}$. λ is the wavelength of the incident light, and d is the substrate thickness. n and k values of a single-layer thin film can be obtained by solving the following simultaneous equations using the Newton-Raphson method:

$$\begin{cases} T(n, k) = T_{\text{exp}} \\ R(n, k) = R_{\text{exp}} \end{cases} \tag{2.29}$$

where T_{exp} and R_{exp} are the measured values. These nonlinear simultaneous equations were solved through a self-developed Scilab program.

2.3 Experiment

2.3.1 Preparation of β -FeSi₂ thin film

In this study, thin films were fabricated by co-sputtering, in which multiple targets were simultaneously deposited using radio frequency (RF) magnetron sputtering. RF magnetron sputtering is a physical vapor deposition (PVD) technique that utilizes high-frequency alternating electric fields to generate plasma between a target and substrate in a vacuum chamber. Argon ions (Ar^+), produced by glow discharge plasma (Figure 2.4(a)), are accelerated towards the target, causing atoms or molecules to be ejected from the target surface and deposited onto a substrate, forming a thin film. The addition of a magnetron arrangement enhances plasma density by confining electrons through

perpendicular magnetic fields, thus increasing ionization efficiency and deposition rates. This method enable control over film composition, thickness, crystallinity, and density by adjusting parameters such as sputtering time, power, gas pressure, and substrate temperature.

In contrast, co-sputtering involves the simultaneous sputtering of two or more target materials to fabricate films. The actual co-sputtering apparatus used in this study is shown in Figure 2.4(b). It mainly consists of a vacuum chamber, three sputter guns, a turbomolecular pump, a rotary pump, vacuum gauges, a substrate heater, a water-cooling system, and a gas inlet system. In this chapter, we utilized co-sputtering to control the composition of β -FeSi₂ thin films. The approach is based on first measuring the individual sputtering rates of FeSi₂ and Si targets under identical deposition conditions—the same gas pressure and substrate temperature—across a range of applied RF powers. During film deposition, the applied power to the FeSi₂ target was fixed at 100 W, while the Si content in the thin film was controlled by varying the applied power to the Si target. This method enables precise tuning of the Fe/Si ratio in the resulting thin films.

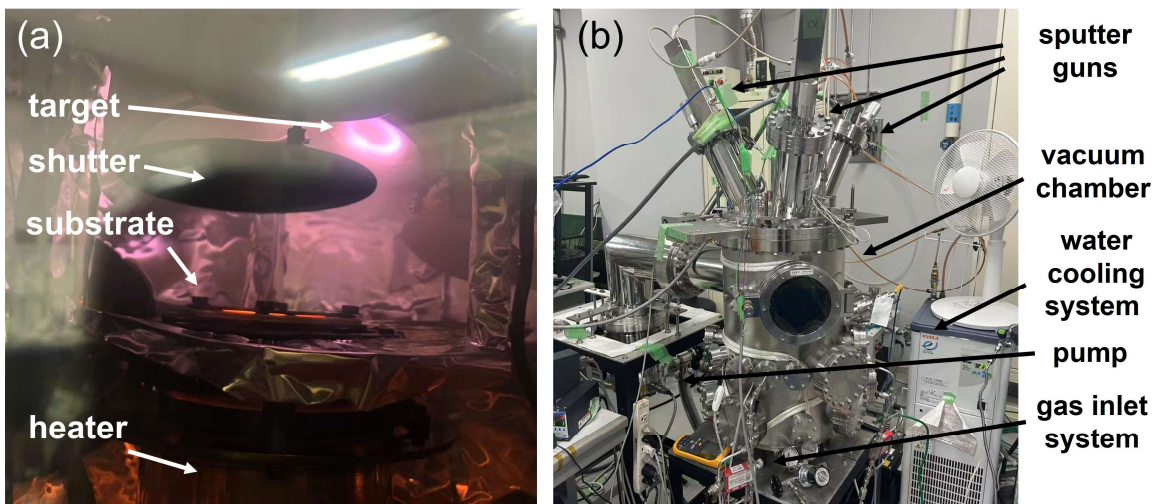


Figure 2.4. Photographs of (a) glow discharge plasma during sputtering and (b) the co-sputtering equipment.

The β -FeSi₂ thin films were deposited onto double-sided polished Si substrates via RF magnetron sputtering at high temperatures. The deposition chamber, with an inner diameter of 350 mm and a height of 600 mm, was evacuated using a rotary pump for rough pumping, followed by a cryopump to achieve high vacuum. Three sputter guns were mounted at the top of the chamber, each equipped with a sputtering target and a magnet positioned at the gun's base. In this study, FeSi₂, SiO₂, and Si targets were used. Material was ejected from each target under applied RF power and deposited onto the substrate. The sputter guns were angled at 28° relative to the substrate, with a target-to-substrate center distance of approximately 80 mm. Substrate heating was provided by a light-collecting lamp heater positioned beneath the substrate, ensuring uniform temperature distribution. To achieve uniform film thickness, the substrate was continuously rotated by a motor during deposition.

Prior to deposition, the substrate was cleaned using UV/ozone treatment (Mercury lamp, 4.5 W × 3, ozone generation rate 5 mg/h × 3) for 30 minutes to remove organic contaminants. The deposition chamber was then evacuated to a vacuum of at least 3.0×10^{-4} Pa, after which the substrate was heated. After maintaining the substrate temperature above 430 °C at least 1 hour, pure Argon gas was then introduced at a flow rate of 9 sccm and the pressure was maintained at 0.86 Pa. Before initiating the sputtering process, the FeSi₂ and Si targets were pre-cleaned for approximately 5 minutes to remove surface impurities. During sputtering, the RF power applied to the FeSi₂ target was fixed at 100 W, while the Fe/Si composition ratio was controlled by adjusting the RF power applied to the Si target. The film thickness was maintained at 100 nm by precisely adjusting the deposition time.

2.3.2 β -FeSi₂ thin film optical measurements

In this study, the IR transmittance and reflectance spectrum of the thin films were

measured using Fourier Transform Infrared (FT-IR) spectroscopy (SHIMADZU, IRAffinity-1). In the FT-IR system, light emitted from the source is collimated and directed into an interferometer, where it is incident obliquely on a beam splitter. The beam is divided into two paths: a transmitted beam and a reflected beam (see Figure 2.5). These two beams are reflected by a fixed mirror and a moving mirror, respectively, and then recombined at the beam splitter to generate an interference signal. Because the position of the moving mirror changes the optical path difference, different interference patterns are produced. By recording the signal intensity of the interferogram at each mirror position, the spectral intensity at each wavenumber can be obtained computationally. This calculation is performed using a Fourier transform, which can be rapidly processed by a computer. The transmittance and reflectance spectra of the thin film can be determined through measurements. The absorbance spectrum were then calculated using:

$$A = 1 - T - R \quad (2.30)$$

The part of spectra in the wavelength range around 1.9 μm and 4.3 μm were excluded to remove the effects from CO_2 and H_2O in the air.

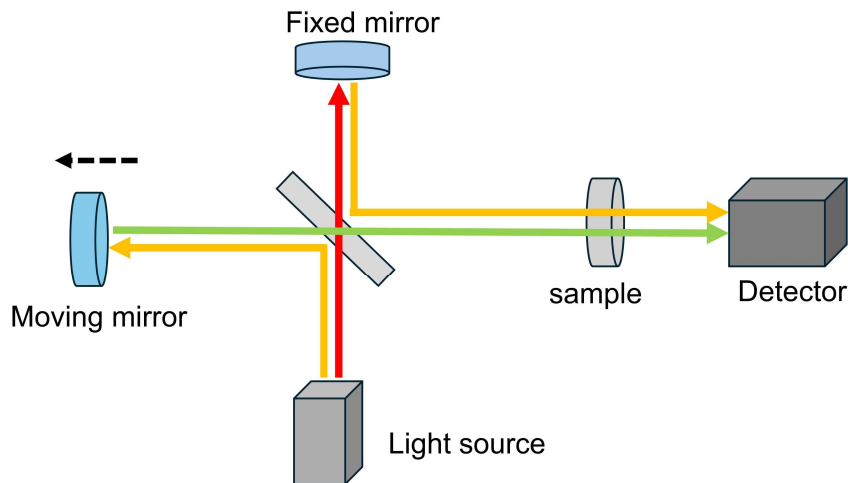


Figure 2.5. Structure of the FT-IR spectroscopy.

2.3.3 β -FeSi₂ thin film crystalline structure measurements

We employed X-ray diffraction (XRD, Rigaku, smartlab) to analyze the crystalline structure of the thin films. The measurements were based on 2θ scans with an incident angle of 0.5° using Cu $K\alpha$ radiation. The principle of XRD is based on Bragg's law:

$$2d\sin\theta = n\lambda \quad (2.31)$$

As illustrated in Figure 2.6, when radiation is incident on parallel crystal planes, the path difference between beams reflected from two adjacent planes is $2d\sin\theta$. Constructive interference occurs when this path difference is an integer multiple of the wavelength λ . The XRD patterns of the thin film samples were measured using Cu $K\alpha$ radiation ($\lambda = 0.15406$ nm) in a 2θ scan mode, with the incident angle θ fixed at 0.5° .

In this study, the target material, β -FeSi₂, has been reported to possess an orthorhombic crystal structure, with lattice parameters $a = 9.86$ Å, $b = 7.79$ Å, and $c = 7.83$ Å.[21] Typical calculated diffraction patterns for β -FeSi₂ crystals are summarized in Figure 2.7.

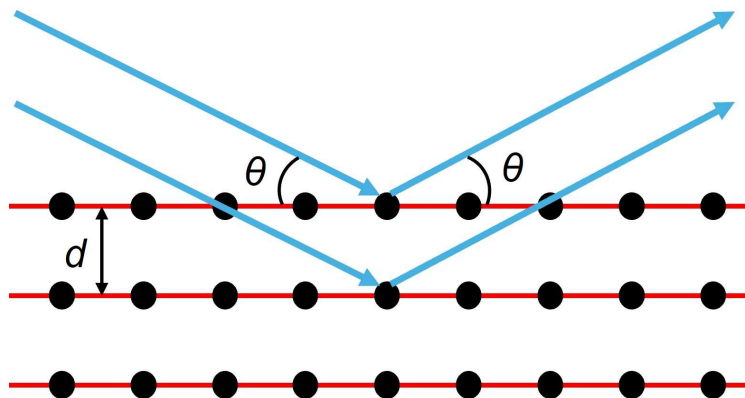


Figure 2.6. Bragg diffraction.

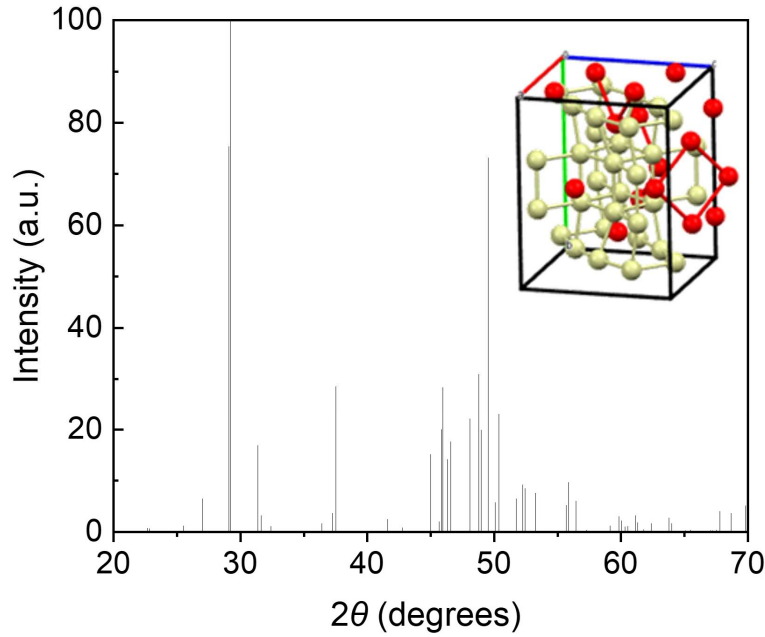


Figure 2.7. Typical XRD diffraction patterns for β -FeSi₂ crystals.

2.3.4 β -FeSi₂ thin film composition measurements

X-ray photoelectron spectroscopy (XPS, ULVAC-Phi, PHI 5000) analysis was used to confirm the chemical state of the elements and the composition of the β -FeSi₂ thin film. Figure 2.8 shows the photograph of the XPS apparatus used in this study, which employed Al K α radiation as the X-ray source. The basic principle of XPS involves irradiating the sample surface with X-rays and measuring the kinetic energy of the emitted photoelectrons. The binding energy E_B of the electrons can then be calculated using the following equation:

$$E = h\nu - E_B - \Phi \quad (2.32)$$

where E is the kinetic energy of the photoelectrons and Φ is the work function of the spectrometer. This allows for the analysis of the elemental composition and electronic

states of the sample.

To ensure accurate quantitative analysis of the β -FeSi₂ thin films, the sample surfaces were first subjected to 1 min of Ar⁺ ion etching to remove surface contamination and oxides. Subsequently, we performed scans again for the Fe2p and Si2p regions. Data processing was performed using CasaXPS software. The background types applied for Fe2p and Si2p regions are Shirley and linear, respectively. The atomic concentration is given by the following formula:[22]

$$X_i \text{ atomic percent (\%)} = 100\% \times \frac{A_i / \text{ASF}_i}{\sum_{j=1}^m (A_j / \text{ASF}_j)} \quad (2.33)$$

where A_i is the measured peak area and ASF_i is the atomic sensitivity factor for the element X_i . Here, the atomic sensitivity factors for Fe2p and Si2p are 3.0 and 0.27, respectively.[23]

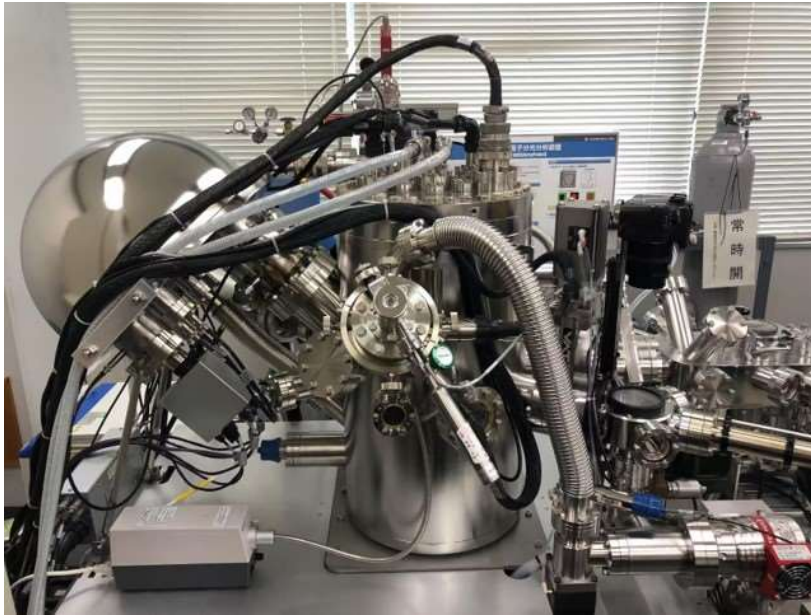


Figure 2.8. Photograph of the XPS apparatus.

2.4 Results and discussion

2.4.1 Changes in optical properties and composition of β -FeSi₂ thin film due to Si addition

The transmittance and reflectance spectrum, measured using FT-IR, as well as the calculated absorbance spectrum (Eq. 2.30) for β -FeSi₂ thin films under different Si target power (P_{si}) conditions, are presented in Figure 2.9(a–c). Additionally, the refractive index n and extinction coefficient k , derived from the transmittance and reflectance

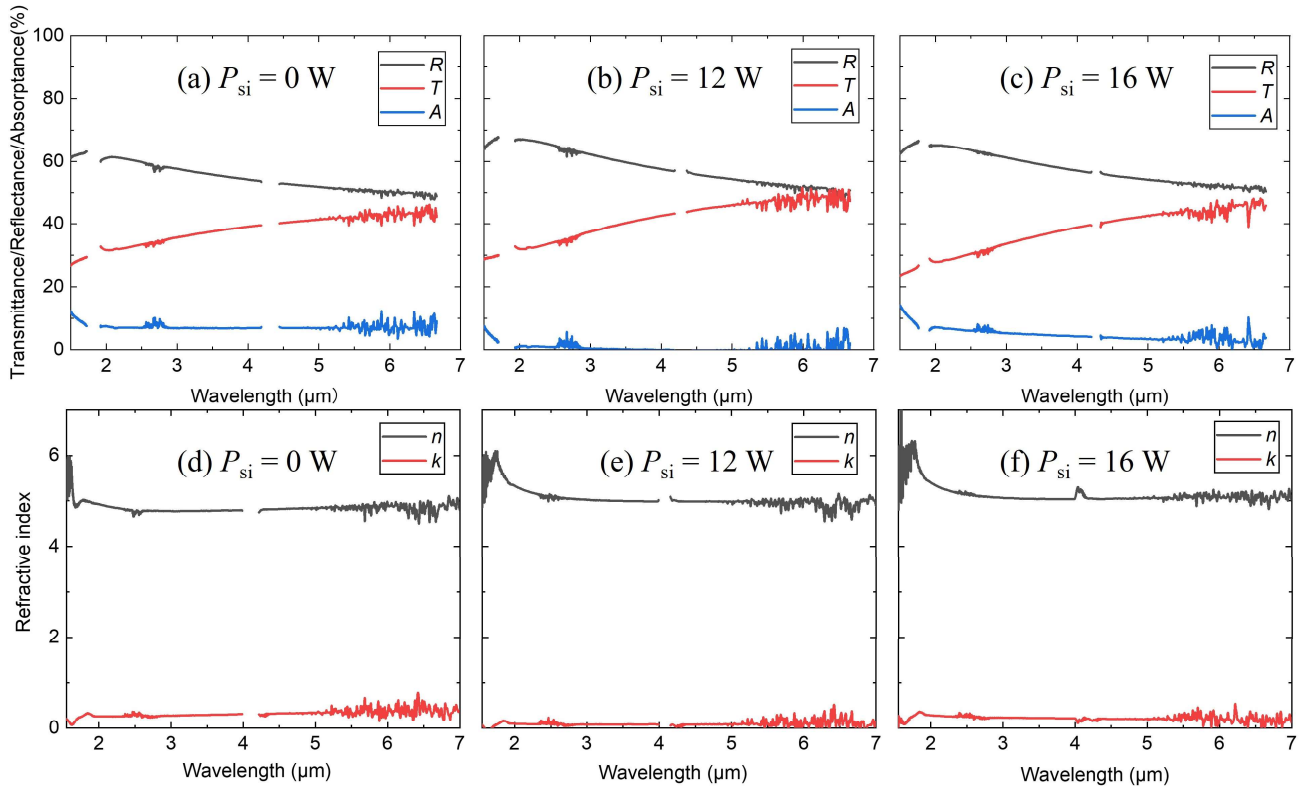


Figure 2.9. Optical properties of β -FeSi₂ thin film with varying P_{si} . Transmittance(T), Reflectance(R) and Absorbance(A) spectra of β -FeSi₂ thin film for P_{si} = (a) 0 W, (b) 12 W and (c) 16 W. n and k for P_{si} = (d) 0 W, (e) 12 W and (f) 16 W.

measurements, are shown in Figure 2.9(d–f). As depicted in Figure 2.9(a) and (d), when $P_{\text{Si}} = 0$ W, the β -FeSi₂ thin film exhibits high absorptance ($\sim 7\%$) in the infrared region. The corresponding refractive index and extinction coefficient are approximately 5.0 and 0.3, respectively, which are consistent with values reported in our previous study. In Figure 2.9(b), at $P_{\text{Si}} = 12$ W, the absorptance of the β -FeSi₂ thin film decreases significantly, reaching 0 for wavelengths above 3 μm . As shown in Figure 2.9(e), k drops to below 0.1. However, as P_{Si} increases further to 16 W, the absorptance of the β -FeSi₂ thin film begins to rise again, as illustrated in Figure 2.9(c) and (f).

To investigate how the absorptance of β -FeSi₂ thin films vary with increasing P_{Si} from 0 to 20 W, we incrementally increased P_{Si} by 2 W and measured the optical properties of the deposited thin films. The absorbance of the samples at a wavelength of 2 μm is summarized in Figure 2.10. When $10 \text{ W} \leq P_{\text{Si}} \leq 12 \text{ W}$, β -FeSi₂ thin film with minimum absorptance of about 0 were successfully fabricated. Replication experiments were performed at $P_{\text{Si}} = 12$ W to provide support for the reliability of the results. The primary reason for infrared absorption in β -FeSi₂ thin films is the Si deficiency in polycrystalline β -FeSi₂, where the Si content is lower than the stoichiometric ratio (Fe:Si = 1:2). By introducing an appropriate amount of additional Si, the stoichiometry is balanced, effectively reducing optical absorption. However, when P_{Si} exceeds 12 W, excess Si incorporation leads to an increase in absorption, suggesting that an optimal Si content exists for minimizing infrared absorptance in β -FeSi₂ thin films.

To better understand how the crystal structure and composition of the β -FeSi₂ thin films evolve with varying Si content, XRD and XPS analyses were performed. The results of the XRD analysis are presented in Figure 2.11. In all samples, diffraction peaks corresponding to orthorhombic β -FeSi₂ were successfully observed,[21] and no Si-related peaks were detected even at P_{Si} as high as 99 W. Additionally, compared to other samples, the β -FeSi₂ peaks were less intense at $P_{\text{Si}} = 99$ W, whereas for P_{Si} below 16 W, no

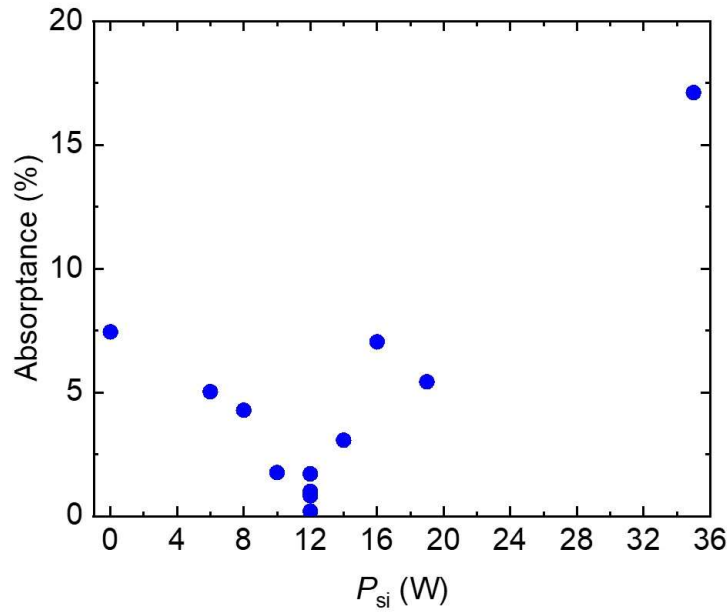


Figure 2.10. Absorbance at wavelength 2 μm of $\beta\text{-FeSi}_2$ thin film prepared as different P_{si} .

significant differences were observed in either peak position or intensity. These findings indicate that variations in composition within the investigated range had no substantial impact on the crystallinity of the $\beta\text{-FeSi}_2$ thin films, suggesting that crystallinity is not the primary factor responsible for the elevated extinction coefficient k .

The XPS analysis was conducted on samples with $P_{si} = 0, 12$, and 16 W. It is well known that a natural oxide film of SiO_2 is formed on the surface of the $\beta\text{-FeSi}_2$ thin film, and that Si is preferentially etched during depth profiling using Ar^+ ion sputtering.[24] Therefore, to remove surface contamination and the oxide film, it was essential to irradiate Ar^+ for the shortest possible duration to minimize unintended material removal. As shown in Figure 2.12(a), the O1s and C1s peaks almost disappear after 1 min Ar^+ ion sputtering in XPS survey spectrum, which means that the impurities on the sample's surface were effectively removed.[25, 26] Subsequently, Fe2p and Si2p regions were

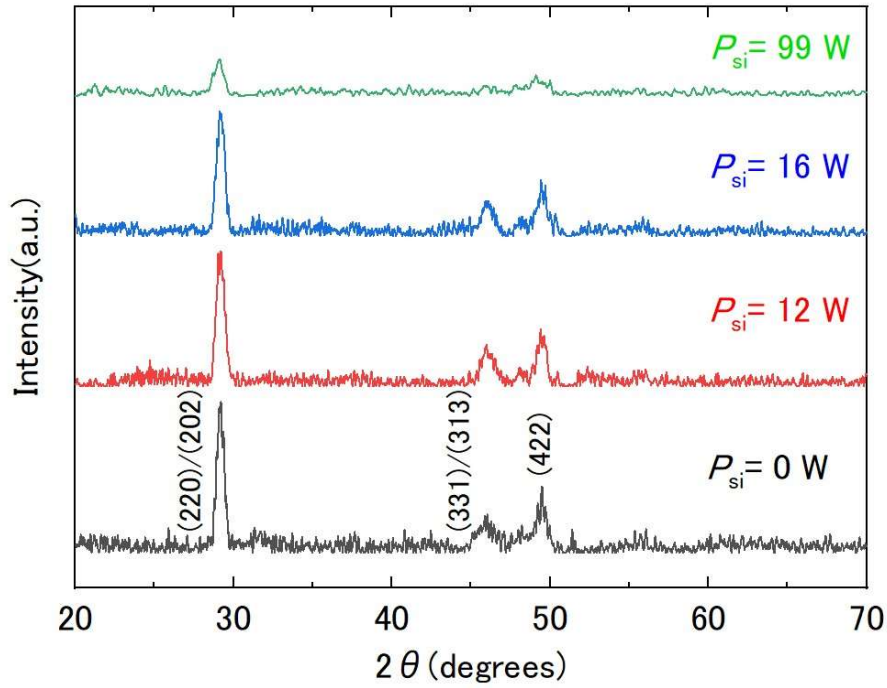


Figure 2.11. XRD patterns of β -FeSi₂ thin film prepared when $P_{\text{si}} = 0, 12, 16, 99$ W.

rescanned for quantitative analysis, as shown in Figure 2.12 (b) and (c). The calculated Si concentrations for each sample are summarized in Table 2.1.

The "without SiO₂ barrier" row in Table 2.1 represents the Si composition of samples deposited on the Si substrates (the "with SiO₂ barrier" results are discussed later). The "Cal." row denotes the nominal Si atomic ratio, which was calculated based on the sputtering yield and atomic density of β -FeSi₂ and Si, respectively. If all deposited atoms were fully incorporated into the thin film, the film composition would match these nominal values. As expected, the Si composition increased with increasing P_{si} . However, for all samples, the measured Si content was lower than the nominal values. This discrepancy may partly be attributed to a slight preferential etching of Si during Ar⁺ ion sputtering, introducing an estimated measurement uncertainty of ± 0.5 at%. For $P_{\text{si}} < 12$ W, the Si composition remained lower than the stoichiometric Fe:Si = 1:2 ratio. At $P_{\text{si}} = 12$ W, the Si composition was closest to the ideal 1:2 ratio, whereas for $P_{\text{si}} > 12$ W, deviations from stoichiometry reappeared. These results suggest that in films deposited

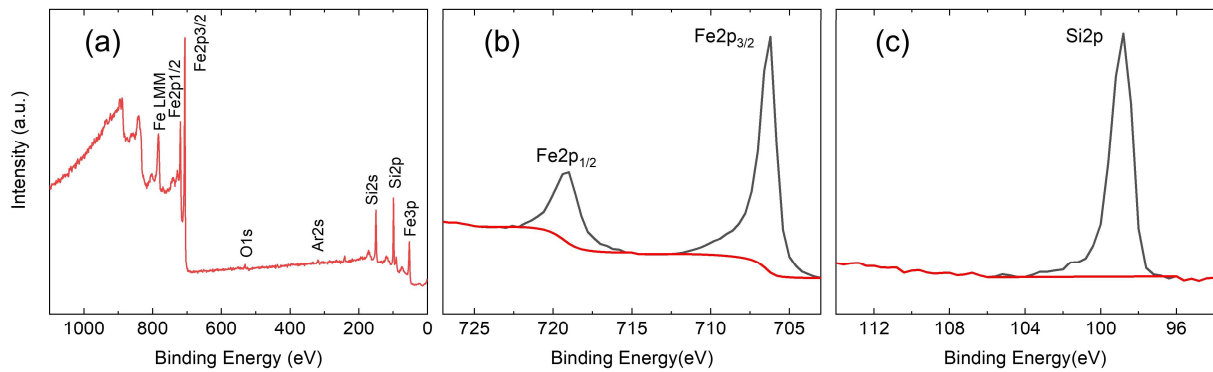


Figure 2.12. (a) Survey, (b) Fe2p and (c) Si2p XPS spectra of β -FeSi₂ thin film prepared as $P_{\text{Si}} = 12$ W.

using an FeSi₂ alloy target, the Si content is initially lower than the stoichiometric value, but the Si atoms supplied from the Si target compensate for the Si lost from the thin film. At $P_{\text{Si}} = 12$ W, the amount of Si added from the Si target precisely balances the Si loss from the film, resulting in a stoichiometric Fe:Si ratio of 1:2. This stoichiometric balance is considered to be the key factor behind the minimum absorptance observed.

Table 2.1 The concentration of Si atoms (%) from the results of theoretically calculation as well as the XPS quantitative analysis of β -FeSi₂ thin film prepared as $P_{\text{Si}} = 0, 12, 16$ W with or without a SiO₂ barrier.

	$P_{\text{Si}} = 0$ W	$P_{\text{Si}} = 12$ W	$P_{\text{Si}} = 16$ W
Without SiO ₂ barrier	64.0	67.1	67.7
With SiO ₂ barrier	65.9	66.3	67.9
Cal.	66.7	68.3	68.8

2.4.2 Investigation of Si loss mechanism and substrate influence on Si composition

It is well known that when Fe is deposited onto a heated Si substrate, Si atoms diffuse from the substrate, leading to the formation of β -FeSi₂. [27] However, there have been no reported cases of Si diffusing back into the Si substrate after β -FeSi₂ formation. Therefore, it is reasonable to assume that the decrease in Si content at $P_{\text{si}} = 0$ W is due to Si loss to the vacuum side during film formation rather than diffusion into the substrate. In addition to the Ar gas used for sputtering, the residual atmosphere within the vacuum chamber contains traces of water, as well as oxygen and hydrogen generated from water decomposition. If the thin film surface undergoes oxidation due to these residual gases,

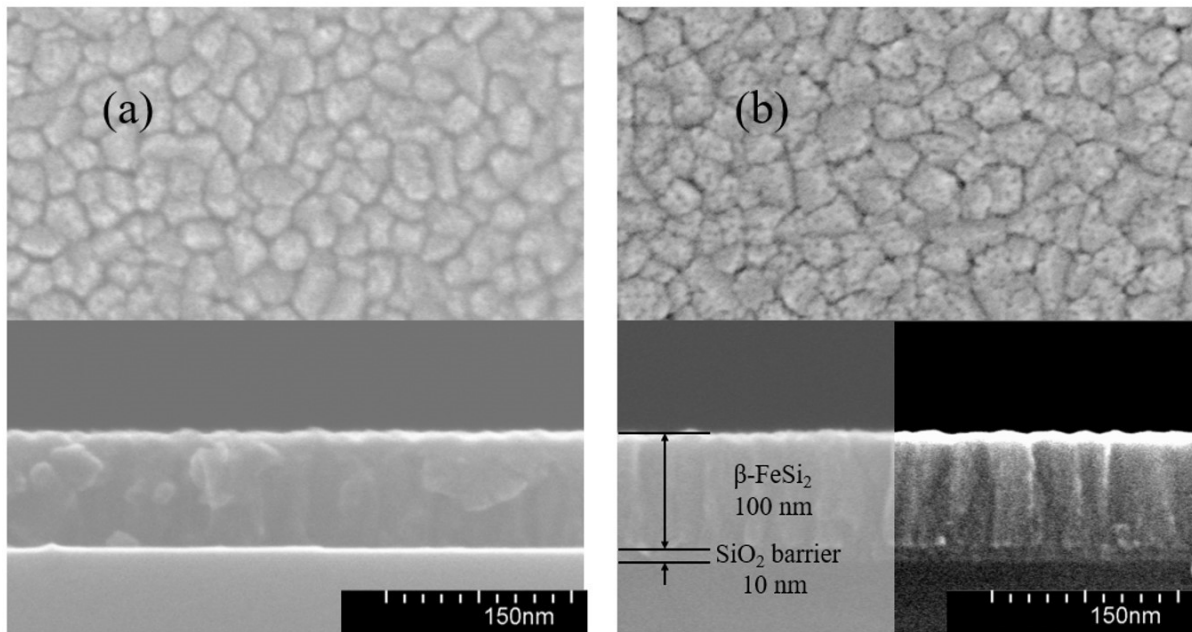


Figure 2.13. Cross-sectional and top view SEM images of samples ($P_{\text{si}} = 12$ W) (a) without and (b) with SiO₂ barrier.

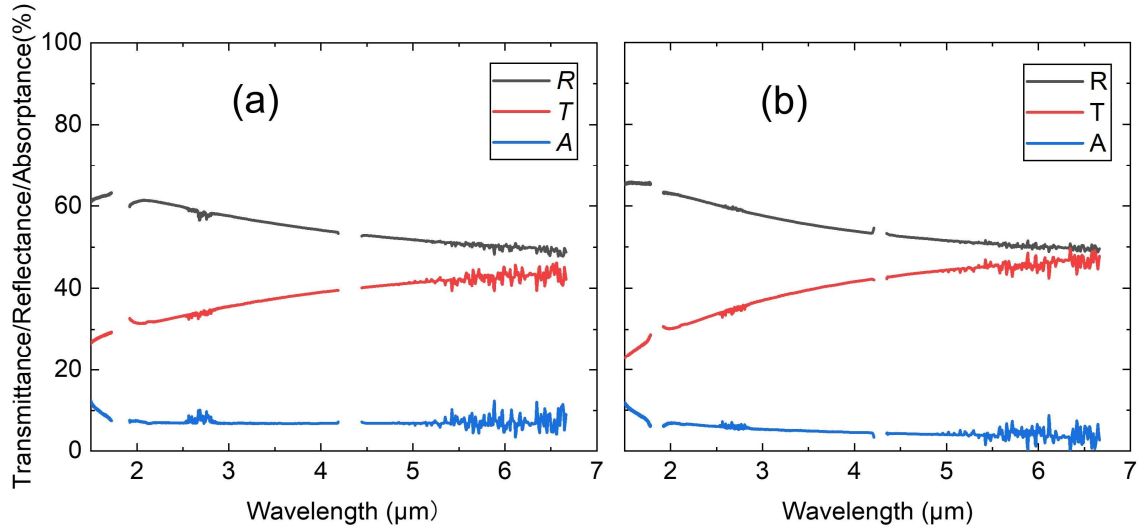


Figure 2.14. Transmittance(T), Reflectance(R) and Absorptance(A) spectra of β -FeSi₂ thin film for $P_{\text{si}} = 0$ W (a) without and (b) with a SiO₂ barrier.

forming SiO, the relatively high vapor pressure of SiO could result in the evaporation of SiO molecules, ultimately leading to a Si deficiency in the thin film. When an Si substrate is used, the missing Si may be replenished from the substrate. However, in practical applications such as infrared bandpass filters, quartz substrates may be used instead of Si, which could further exacerbate Si depletion. To investigate the effect of the substrate on Si composition, a 10-nm-thick SiO₂ barrier layer was introduced between the Si substrate and the β -FeSi₂ thin film to prevent Si diffusion from the substrate, allowing for a more precise evaluation of the intrinsic Si loss mechanism.

Figure 2.13 presents the cross-sectional and top-view SEM images of β -FeSi₂ thin films deposited at $P_{\text{si}} = 12$ W, both with and without the SiO₂ barrier. In Figure 2.13(b), the right half of the cross-sectional view has been image-processed to enhance the visibility of the SiO₂ barrier layer. When the SiO₂ barrier thickness was 10 nm, the β -FeSi₂/ SiO₂ barrier/Si substrate structure was clearly observed. A comparison of the SEM images of

samples with and without the SiO₂ barrier revealed no significant differences in surface morphology or thin film thickness.

To further investigate the effect of the SiO₂ barrier, we measured the optical characteristics of β -FeSi₂ thin films deposited on SiO₂ barrier/Si substrates under the same sputtering conditions to those without SiO₂ barrier. Figure 2.14(a) and (b) present the transmittance, reflectance, and absorptance spectrum for $P_{\text{si}} = 0$ W, comparing samples with and without the SiO₂ barrier. In the absence of additional Si supply ($P_{\text{si}} = 0$ W), the presence of the SiO₂ barrier led to a slight reduction in absorptance, yet the β -FeSi₂ thin film still exhibited high absorptance. Figure 2.15(a) and (b) compare the absorptance at 2 μm and 3 μm wavelengths for β -FeSi₂ thin films with and without the SiO₂ barrier, under conditions where Si atoms were supplied. The absorptance of the β -FeSi₂ thin film reached a minimum at $P_{\text{si}} = 10$ –12 W, consistent with the trend observed in SiO₂ barrier

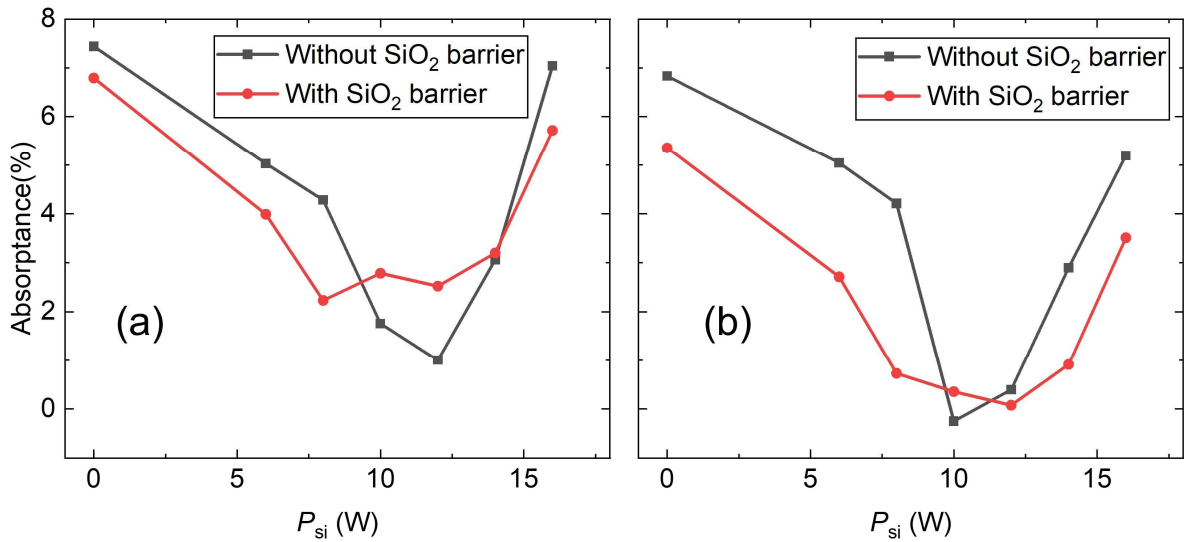


Figure 2.15. Comparison of the absorptance at (a) 2 μm and (b) 3 μm wavelength for β -FeSi₂ thin film with and without SiO₂ barrier as different P_{si} .

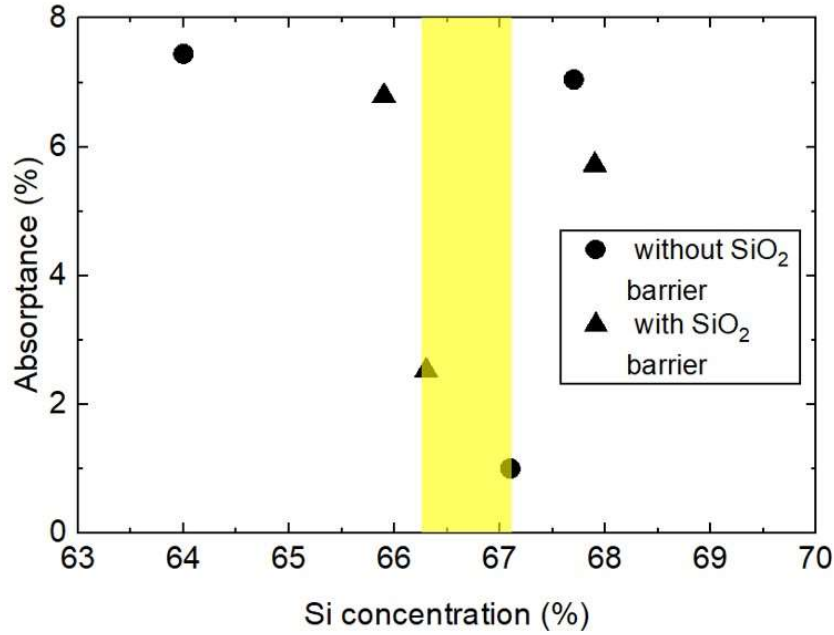


Figure 2.16. Comparison of the absorptance at (a) 2 μm and (b) 3 μm wavelength

for $\beta\text{-FeSi}_2$ thin film with and without SiO_2 barrier as different P_{si} .

free samples. Furthermore, in the range of $P_{\text{si}} \approx 12$ W, the absorptance of the $\beta\text{-FeSi}_2$ thin film approached zero, irrespective of the presence of the SiO_2 barrier.

XPS analysis was also conducted on samples with SiO_2 barrier, and the corresponding Si concentrations are listed in the "with SiO_2 barrier" row in Table 2.1. The results indicate that the Si concentration in thin films with the barrier is nearly identical to that of films without the barrier, suggesting that the presence of the SiO_2 layer does not significantly affect Si incorporation during deposition. Additionally, Figure 2.16 illustrates the relationship between Si concentration and the absorptance of $\beta\text{-FeSi}_2$ thin films, both with and without the SiO_2 barrier. The yellow region represents the range of Si concentration in which the minimum absorptance was achieved in this study. A more precise determination of this optimal composition range can be obtained by increasing the applied power of the FeSi_2 target and investigating the effect of finer adjustments to P_{si} . The data reveals that, regardless of the substrate type, when the Si concentration

approaches 66.7% (Fe:Si = 1:2), the absorptance of the thin film is minimized, approaching zero. These findings suggest that in the fabrication of β -FeSi₂ layers for BPF, the choice of substrate material (e.g., quartz substrate) does not pose a significant issue, as long as P_{Si} is maintained within the range of 10–12 W.

2.5 Conclusion

In this chapter, we investigated the composition and optical properties of β -FeSi₂ thin films prepared by co-sputtering. The results demonstrate that β -FeSi₂ thin films with nearly zero absorptance in the infrared region were successfully fabricated under deposition conditions of $P_{\text{Si}} = 10\text{--}12$ W. XPS analysis revealed that under these conditions, Si loss due to reactive evaporation was effectively compensated, leading to a Fe:Si ratio in β -FeSi₂ thin films closer to the ideal 1:2 stoichiometry. Furthermore, this conclusion holds even when the substrate material is changed from Si to quartz, indicating that the Si supply mechanism is independent of the substrate type.

These findings suggest that β -FeSi₂ thin films with a high refractive index and a low extinction coefficient in the infrared spectrum can be successfully produced using this method. Such films can be integrated into multilayer structures to develop bandpass filters with fewer layers and reduced film thickness, thereby be applied to the wavelength-selective radiation systems.

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Chapter 3 Design and Fabrication of Infrared bandpass filter using β -FeSi₂

Abstract

Bandpass filters (BPFs) are optical filters with significantly high transmittance in a specific wavelength range and low transmittance on both sides. Infrared (IR) BPFs can reduce system losses and overheating caused by other light wavelengths owing to their ability to selectively transmit infrared light of the desired wavelength. This chapter describes the development of a novel BPF using the high refractive index material β -FeSi₂. Based on the findings of β -FeSi₂ thin film in chapter 2, simulation results showed that the high refractive index of β -FeSi₂ enable the realization of the excellent performance of the BPF using a multilayer thin film structure with only three layers. Additionally, a β -FeSi₂/SiO₂/ β -FeSi₂ multilayer film structure was designed to fabricate the BPF. The fabricated BPF exhibited a narrow peak and achieved a peak transmittance exceeding 80%. This suggested that β -FeSi₂ is a promising material for fabricating infrared BPFs. Utilizing these filters is expected to yield significant efficiency improvements and reduce losses across various applications.

3.1 Introduction

Bandpass filters (BPFs), also known as wavelength-selective transmission thin films, are optical filters with significantly high transmittance in a specific wavelength range and low transmittance on both sides. Owing to their ability to selectively transmit light of the desired wavelength, BPFs are widely employed in applications such as spectroscopic analysis, laser systems, and imaging. In particular, Infrared BPFs have attracted considerable attention because they can reduce system losses and mitigate overheating induced by unwanted wavelengths. These advantages have motivated increasing interest in utilizing infrared BPFs to improve the power-generation efficiency of thermophotovoltaic (TPV) systems, which are expected to surpass the Shockley–Queisser limit.[1-4] Furthermore, infrared BPFs are critical in developing infrared heaters[5, 6] and gas sensor devices.[7, 8]

The most commonly used BPFs are based on Fabry–Pérot filter structures. [9] As schematically illustrated in Figure 3.1, such a structure consists of a central spacer layer (resonant cavity) sandwiched between two reflectors (mirrors). The spacer layer has an optical thickness of $\lambda/2$ and can be composed of either a high- or low-refractive-index



Figure 3.1. The structure of a Fabry–Pérot filter structure.

material. Each reflector is formed by multiple alternating thin-film layers with high and low refractive indices, each having an optical thickness of $\lambda/4$, where λ denotes the center wavelength of the BPF, i.e., the wavelength at which the transmittance reaches its maximum. The operating principle is based on optical interference. Incident light entering the resonant cavity through the front mirror undergoes multiple reflections between the two mirrors. During this process, constructive and destructive interference occurs. When the optical thickness of the spacer layer matches an integer multiple of half the wavelength, the phases of the incident and reflected waves are aligned, resulting in constructive interference and enhanced transmission. In contrast, wavelengths that do not satisfy this resonance condition experience destructive interference and are suppressed. Consequently, only light within a narrow wavelength range is selectively transmitted through this filter. Figure 3.2 shows a portion of the cross-sectional structure of a commercially available 1.3 μm BPF, in which the multilayer configuration can be seen to follow the design principles described above.

In such structures, the refractive index of the high refractive index layer is a critical parameter, as it determines the reflectivity at the interfaces between adjacent quarter-wave layers and directly influences the overall structural complexity required to achieve

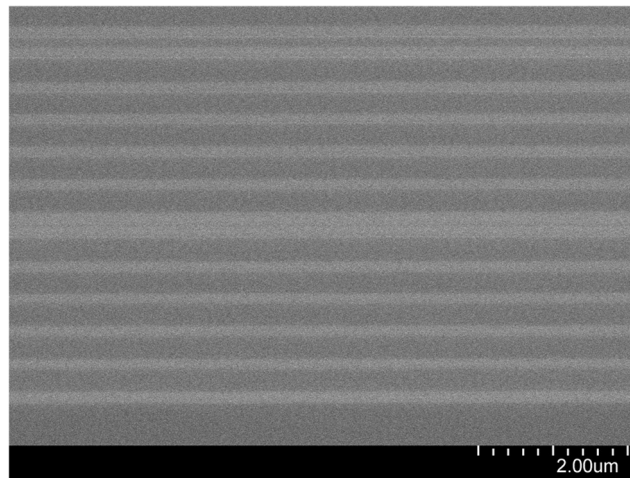


Figure 3.2. Cross-sectional structure of a commercially available BPF.

the desired optical performance. However, the refractive index of materials commonly used in infrared BPFs, such as Si and TiO₂, [10, 11] is not sufficiently high, typically in the order of 2–3. In such cases, an increase in the thickness of the thin film and the number of layers is required to achieve ideal optical functions. As shown in Figure 3.2, more than 20 layers with a total thickness exceeding 5 μm are employed to realize a bandwidth of 12 nm at 1.3 μm . Even greater structural complexity and higher manufacturing costs are expected when targeting longer infrared wavelengths.

In Chapter 2, the optical properties of $\beta\text{-FeSi}_2$ thin films deposited by co-sputtering using FeSi₂ and Si targets were investigated. The results revealed that when an appropriate amount of Si was added during deposition, the refractive index n and extinction coefficient k of the $\beta\text{-FeSi}_2$ thin film reached 5 and 0, respectively. Furthermore, the high refractive index and transparency in the infrared region ($\lambda > 1.55 \mu\text{m}$) indicate that $\beta\text{-FeSi}_2$ is a promising material for the fabrication of infrared BPFs. Thus, in this chapter, we aim to develop infrared BPFs using $\beta\text{-FeSi}_2$. The fabricated BPF should exhibit a high and narrow transmission peak at the desired wavelength. Furthermore, due to its low cost and structure suitable for large-scale production, $\beta\text{-FeSi}_2$ -based BPFs have the potential for practical applications in wavelength-selective radiation systems.

3.2 Design of the multilayer bandpass filters

3.2.1 Calculation of the reflectance and transmittance of multilayer thin films

The essence of a multilayer film lies in the superposition of multiple single-layer thin films. Therefore, when calculating the reflectance and transmittance of a multilayer thin film, it is sufficient to consider the characteristic matrix of the multilayer structure as the

product of the characteristic matrices of its individual layers. As shown in Figure 3.3, in the case where light is vertically incident on a multilayer film consisting of l thin layers. The Optical admittance of j^{th} layer is

$$Y_j = \sqrt{\frac{\epsilon_0}{\mu_0}} N_j \quad (j = 0, 1, 2, \dots, l+1) \quad (3.1)$$

where the optical properties $N_j = n_j - ik_j$, ϵ_0 and μ_0 are permittivity permeability of a vacuum, respectively. The layer ($j = 0$) is air ($n_0 = 1$, $k_0 = 0$). The phase shift occurs every time as light pass through the j^{th} layers. And the phase factor

$$\delta_j = \frac{2\pi}{\lambda} N_j d_j \quad (j = 1, 2, \dots, l) \quad (3.2)$$

where λ is wavelength of light and d_j is thickness of each layer. Characteristic matrix can be defined according to equation 2.15:

$$[M_j] = \begin{bmatrix} \cos \delta_j & \frac{i \sin \delta_j}{Y_j} \\ Y_j \cdot i \sin \delta_j & \cos \delta_j \end{bmatrix} \quad (j = 1, 2, \dots, l) \quad (3.3)$$

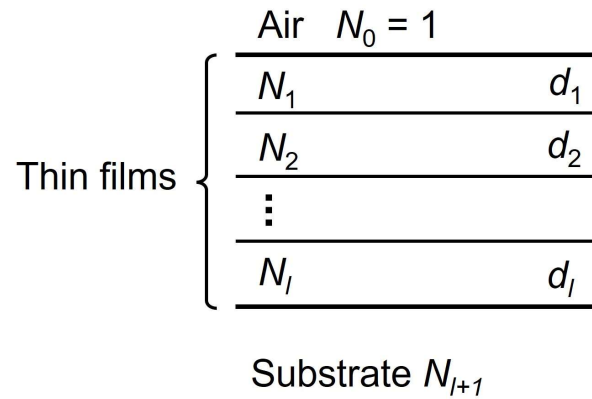


Figure 3.3. Optical model of the multilayer thin film.

And the total characteristic matrix of the multilayer film can be defined as

$$[M] = \prod_{j=1}^l [M_j] = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \quad (3.4)$$

As a result, the transmittance T and reflectance R of multilayer film can be written as

$$T = \frac{n_{l+1}}{n_0} \left| \frac{2Y_0}{Y_0(m_{11} + Y_{l+1}m_{12}) + (m_{21} + Y_{l+1}m_{22})} \right|^2 \quad (3.5)$$

$$R = \left| \frac{Y_0(m_{11} + Y_{l+1}m_{12}) - (m_{21} + Y_{l+1}m_{22})}{Y_0(m_{11} + Y_{l+1}m_{12}) + (m_{21} + Y_{l+1}m_{22})} \right|^2 \quad (3.6)$$

In Section 2.2.2, we discussed how the high reflectance at the bottom surface of the substrate affects the overall optical measurements. For the optical calculations of multilayer films, the similar air / multilayer film / substrate / air structure was adopted, because the absorption of the substrate in the infrared region must be taken into account. Therefore, when calculating the transmittance spectrum of the multilayer film, the results obtained from Eqs. (3.5) and (3.6), together with the optical constants of the substrate, are substituted into Eq. (2.28).

3.2.2 Structure and simulated optical performance of the β -FeSi₂-based bandpass filter

We utilized a β -FeSi₂/SiO₂/ β -FeSi₂/quartz three-layer structure (Figure 3.4) to achieve the infrared BPF. The transmittance spectrum of the designed multilayer BPF was calculated using equation 2.28. The refractive index of the β -FeSi₂ layer was set to 5 based

on the optical properties of β -FeSi₂ thin film discussed in Chapter 2. The refractive index of the SiO₂ layer was fixed at 1.4.[12] The thickness of each layer was determined by

$$\lambda = 4n_1d_1 = 2n_2d_2 \quad (3.7)$$

where n_1 and d_1 represent the refractive index and thickness of the β -FeSi₂ layer, respectively, and n_2 and d_2 represent those of the SiO₂ layer (see Table 3.1). The transmittance and reflectance of the quartz substrate were determined by FT-IR measurements. This analysis is conducted at a desired wavelength of 2 μ m, as infrared radiation at this wavelength has a wide range of applications.[13, 14]

The pink curve in Figure 3.5(a) shows the transmittance spectrum of the multilayer structure in which the β -FeSi₂ layers have optical constants that are the same as those of the bulk ($k = 0$). The calculated transmittance reaches 95%, with a sideband transmittance lower than 5%. Therefore, high transmittance and selectivity bandpass filters can theoretically be realized through this multilayer structure.

The transmittance spectra in other cases, where k is more extensive than zero, are also showed in Figure 3.5(a). As the value of k increases to 0.3, there is a significant decrease in the transmittance at the peak. This observation highlights the importance of minimizing

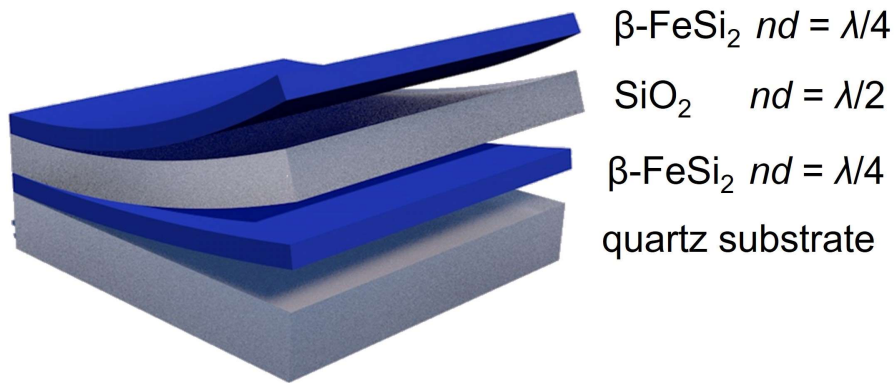


Figure 3.4. β -FeSi₂/SiO₂/ β -FeSi₂/quartz multilayer thin film.

the k -value of the β -FeSi₂ layer when it is utilized in a BPF. Therefore, reducing the imaginary part of the refractive index is crucial.

Furthermore, we conducted two additional calculations for the BPFs using Si ($n = 3.3$) and TiO₂ ($n = 2.4$) within the same multilayer structure. The details and results are summarized in Table 3.1 and Figure 3.5(b), respectively. Compared with the β -FeSi₂-based filter, the multilayer film using TiO₂ and Si requires a thicker film with same number of layers, resulting in a wider full width at half maximum (FWHM) in the transmittance spectrum. Moreover, the higher transmittance on both sides of the peak wavelength degrades the overall wavelength selectivity. Achieving a narrow peak with these materials requires a significant number of layers and an increase in the thickness, leading to higher costs. Therefore, achieving β -FeSi₂ with $n \approx 5$ and $k \approx 0$ is crucial for the realization of high-performance bandpass filters.

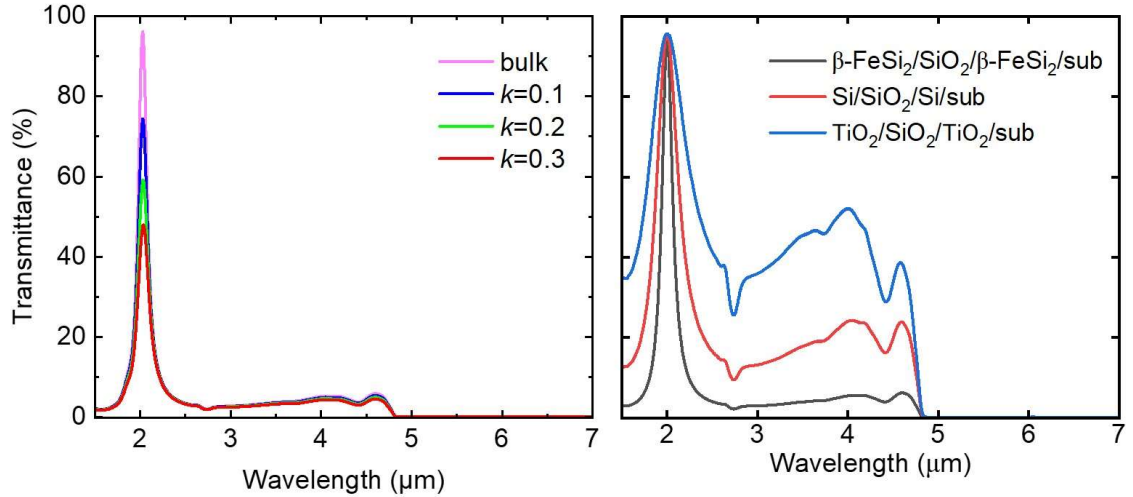


Figure 3.5. Transmittance spectrum of the multilayer thin films calculated for (a) various values of k of the β -FeSi₂ layers and (b) various values of n for high refractive index layers.

Table 3.1. Details for each layer of the designed BPFs

Layer	BPF 1		BPF 2		BPF 3	
	material	thickness[nm]	material	thickness[nm]	material	thickness[nm]
1	β -FeSi ₂	100	Si	151	TiO ₂	208
2	SiO ₂	714	SiO ₂	714	SiO ₂	714
3	β -FeSi ₂	100	Si	151	TiO ₂	208

3.3 Experiment

In Chapter 2, we discussed the structural design of the BPF. Based on this design, β -FeSi₂/SiO₂/ β -FeSi₂ multilayer films were prepared on a 1-mm-thick quartz substrate. The substrate was cleaned by ultrasonic cleaning in acetone for 10 min and by UV/ozone cleaning for 30 min before deposition. The β -FeSi₂ layers were produced in the same way as described in Section 2.3.1. The SiO₂ layer was produced after completion of the first β -FeSi₂ layer. After the heating was stopped and the substrate was returned to room temperature, pure Argon gas was introduced at a flow rate of 9 sccm and the pressure was changed to 1.0 Pa. Sputtering was initiated after cleaning the surface of the SiO₂ target for approximately 10 min. The applied power of the SiO₂ target was fixed at 150 W during the sputtering deposition process. The second β -FeSi₂ layer was repeated after the completion of the SiO₂ layer. Thickness of each layer was based on the principle that the optical thickness is one-quarter of the wavelength for the high-refractive-index layer of β -FeSi₂ and one-half of the wavelength for the low-refractive-index layer of SiO₂. The samples were maintained under vacuum from the time the substrate was set until they were removed after deposition.

3.4 Results and discussion

Figure 3.6 shows the transmittance spectra of the multilayer thin films fabricated under $P_{\text{Si}} = 0$ and 12 W, as measured using FT-IR. Compared with the calculation results in Figure 3.5 (a), the measured spectra is almost identical to that calculated for $k = 0.3$. At $P_{\text{Si}} = 12$ W, owing to the addition of Si atoms, the absorptance of the β -FeSi₂ layer was reduced, and a BPF with a transmittance at the peak exceeding 80% was achieved.

Figure 3.7 is the top and cross-sectional view SEM image of the fabricated BPF. The cross-sectional view SEM image (Figure 3.7(b)) confirms that the multilayer structure was properly formed, and the thicknesses of the individual layers closely matched the design values. In other studies, Szeghalmi et al. utilized a 15-layer TiO₂/Al₂O₃ structure to attain a peak transmittance of 70% within a BPF[15]. Similarly, Kumar et al.[16] and Sullivan et al.[17] achieved satisfactory BPF performance using 43-layer and 10-layer Si/SiO₂ structures, respectively. Pérez et al. employed ten layers of Ge/SiO to achieve a BPF with a peak transmittance of 70%.[18] Comparatively, the BPF we developed exhibited a comparable peak transmittance while featuring a simpler structure with only

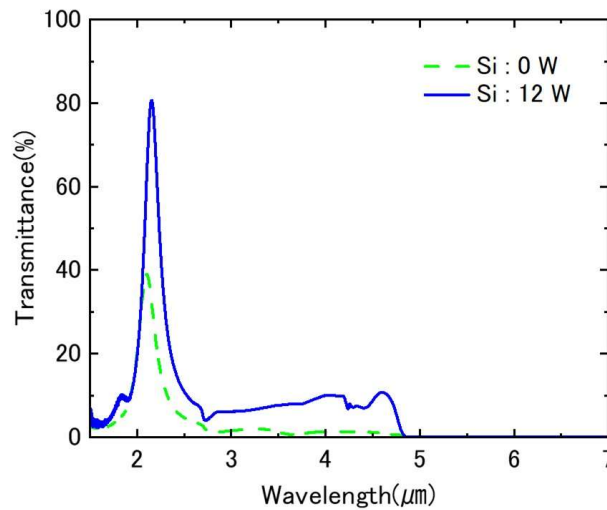


Figure 3.6. Transmittance spectrum of the multilayer thin films fabricated under the condition of $P_{\text{Si}} = 0$ and 12 W.

three layers and a thinner film thickness. This 3-layer structure is not only more cost-effective to fabricate due to the shorter deposition time but is also superior from a practical standpoint, as it minimizes the increase in light scattering typically associated with thick films.

The position of the BPF peak in this multilayer film structure can be easily controlled by adjusting the thickness of each layer. To demonstrate this, we fabricated the BPFs at other wavelengths using Equation 3.8. The transmittance spectrum of only the peak part of the BPFs at 1.6, 2 and 3.3 μm wavelength are shown in Figure 3.8. The transmission peaks of all the produced BPFs exceeded 75%. Therefore, it can be concluded that this

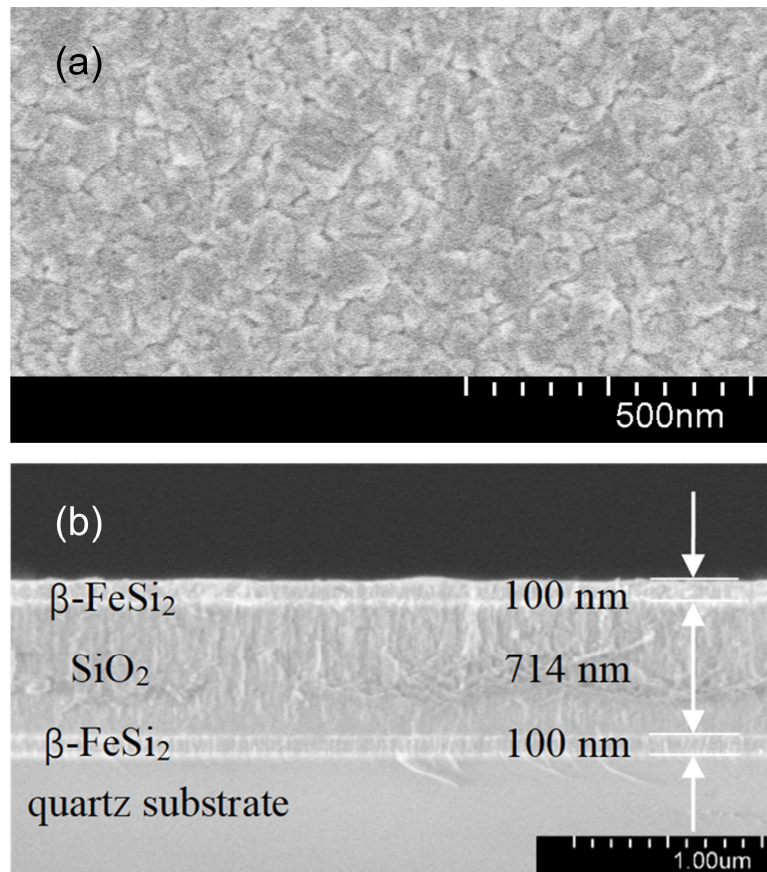


Figure 3.7. (a) Top and (b) cross-sectional view SEM image of the multilayer thin film.

multilayer structure can produce BPFs that perform well in the wavelength range from 1.55 μm ($\beta\text{-FeSi}_2$ band gap) to 3.5 μm (point where the transmittance of the quartz substrate begins to decrease).

Our results show that $\beta\text{-FeSi}_2$ is a suitable candidate material for infrared BPFs. Owing to the high n , and the low k achieved by adding Si atoms, the BPFs produced using this multilayer film structure achieved the expected narrow and high peaks with a small number of layers and a significantly thin film. Further improvements in the peak transmittance can be achieved by selecting other intermediate layer materials and exploring more suitable film-forming conditions. In addition, because of the high heat resistance and oxidation resistance of $\beta\text{-FeSi}_2$, the infrared BPF prepared using this material is expected to be practically applicable in various fields such as TPV and infrared drying systems.

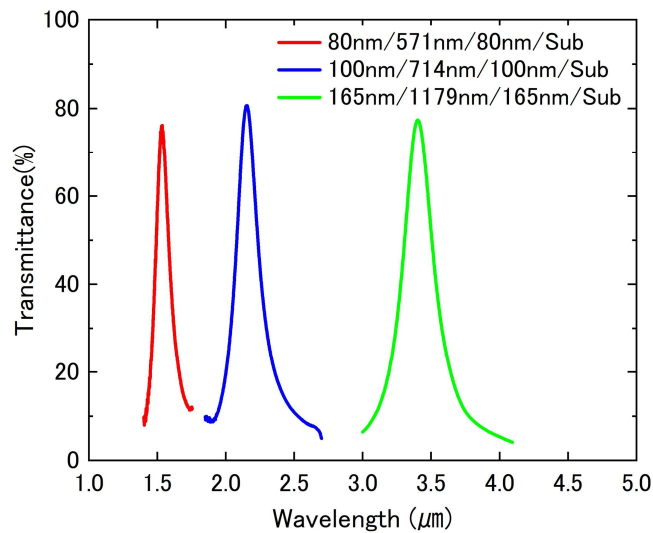


Figure 3.8. Measured transmittance spectrum of the peak part of the BPFs at 1.6, 2 and 3.3 μm wavelength.

3.5 Conclusion

This chapter investigated the performance of BPFs fabricated using β -FeSi₂ thin film prepared by co-sputtering. Our results demonstrate that the BPFs prepared with the β -FeSi₂ layer under the applied power of the Si target is 12 W exhibited the highest transmittance, exceeding 80%. The experimental results demonstrate that β -FeSi₂ is a promising material for the fabrication of infrared BPFs. Using such filters is expected to significantly enhance the efficiency and reduce losses in a variety of applications, such as TPV and infrared drying systems.

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Chapter 4 Application of the β -FeSi₂-based Bandpass Filter: Enhancement of Solvent Evaporation in Wavelength-selective Drying System

Abstract

This chapter investigates the enhancement of solvent evaporation rates using wavelength-selective IR drying based on a simple tri-layered β -FeSi₂-based bandpass filter. Experimental results demonstrate that IR irradiation at 3.4 μm , corresponding to the absorption band of N-methyl-2-pyrrolidone (NMP), significantly increases evaporation efficiency compared to other wavelengths or broad-spectrum IR irradiation. Notably, wavelength-selective IR heating achieves an evaporation rate up to six times higher than broad-spectrum IR irradiation while improving overall energy efficiency. Numerical simulations clarify the critical role of localized heating caused by near-complete absorption of IR energy within a 0.05 mm depth beneath the liquid surface, which substantially increases vapor pressure and thereby accelerates evaporation. These results underscore the advantages of the BPF's optimized transmittance characteristics and present a promising approach for efficient drying processes in applications such as lithium-ion battery electrode fabrication.

4.1 Introduction

Control of solvent evaporation rates is crucial in advanced technologies, including coating film fabrication,[1-5] microfluidics,[6, 7] printed electronics,[8, 9] and chemical synthesis.[10, 11] For instance, in the production of lithium-ion battery (LIB) cathodes, active electrode materials are dispersed in a solvent (commonly N-methyl-2-pyrrolidone, NMP) and coated onto a substrate, followed by solvent evaporation to form a solid film.[12-16] The NMP drying process directly influences the porous structure and properties of electrode films, as well as the overall performance of the cell.[14, 15] Conventional drying systems, such as hot air, present several limitations, including low energy efficiency due to heat losses to non-target components (e.g., surrounding environment and substrate), thermal damage risk to the coating film, and increased explosion hazards at high temperatures—particularly for solvents like NMP with a low flash point of 93 °C. Alternative advanced drying techniques, such as microwave-assisted drying, vacuum drying, and laser drying, have been explored.[17-20] However, their implementation in electrode coating processes remains limited as these techniques suffer from drying defects, high scale-up costs, and limited process flexibility.

Wavelength-selective IR drying systems are proposed as an alternative drying technology.[21] By controlling the IR irradiation wavelength and minimizing emission outside the absorption bands of the solvents, these systems enhance the drying efficiency while maintaining a low overall system temperature, which can help improve the LIB electrodes qualities. A wavelength-selective IR drying system using a quartz optical filter to selectively transmit radiation approximately from 0.7 μm to 3.5 μm for drying NMP has been reported in industrial settings.[21] While this approach successfully reduced thermal damage and shortened drying time, significant heat energy loss still occurred due to IR irradiation outside NMP's absorption band.

Consequently, efforts to improve the drying efficiency have highlighted the importance of selective IR transmission. Enhanced energy efficiency and drying performance can be achieved by optimizing the selectivity of the IR transmission. However, research that specifically explores the efficient drying of solvents using IR irradiation tuned to the absorption band of the solvent remains scarce. Bandpass filters (BPFs) are typically fabricated using multilayer optical thin films. Recently, multilayer thin films that produce narrow BPFs with bandwidths below 50 nm have been reported.[22, 23] However, such extreme narrowness is often excessive for solvent absorption bands. More importantly, the materials commonly used for IR BPFs, such as Si and TiO₂, have refractive indices typically in the order of 2–3. Achieving the desired wavelength selectivity to match solvent absorption bands requires a large total thickness and a high number of layers, which presents challenges in scalability and manufacturing cost, particularly for large-scale LIB cathode drying applications. In chapter 3, we developed a sputtered multilayer thin film structure composed of β -FeSi₂ and SiO₂. Owing to the exceptionally high refractive index (exceeding 5) and transparency of β -FeSi₂, prepared via co-sputtering of FeSi₂ and Si, this structure achieved BPFs with high transmittance and appropriate bandwidth using only three layers. This simple three-layer structure significantly reduces production costs while remaining highly suitable for large-scale applications, where the BPF coverage may need to extend over several meters or even tens of meters. Moreover, the transmitted wavelength can be easily adjusted by modifying the film thickness, allowing adaptation for drying various solvents with different absorption characteristics.

The purpose of this chapter is to investigate the effect of wavelength-selective IR irradiation on solvent evaporation rates using β -FeSi₂-based BPFs. These BPFs are expected to be applied in practical wavelength-selective drying systems and enhance solvent drying efficiency.

4.2 Experiment

4.2.1 Measurement of the transmittance spectrum of solvents

The Infrared transmittance spectrum of the solvents was measured using a Fourier transform infrared (FT-IR) spectroscopy (SHIMADZU, IRAffinity-1) equipped with a liquid cell (S.T. JAPAN, 162-1100). The liquid cell, consisting of two 3 mm-thick KBr windows and a replaceable spacer, enabled precise adjustment of the optical path length for the injected solvents.

4.2.2 Preparation of bandpass filters

The BPFs were designed and fabricated based on the characteristic absorption spectrum of NMP, which was selected as the representative solvent. Figure 4.1 (black line) shows the transmittance spectrum of pure NMP (Sigma-Aldrich) with a 0.05 mm path length, exhibiting a strong absorption peak near 3.4 μm . Accordingly, Filter 1 was designed with a multilayer structure of $\beta\text{-FeSi}_2/\text{SiO}_2/\beta\text{-FeSi}_2/\text{quartz}$, providing a bandpass

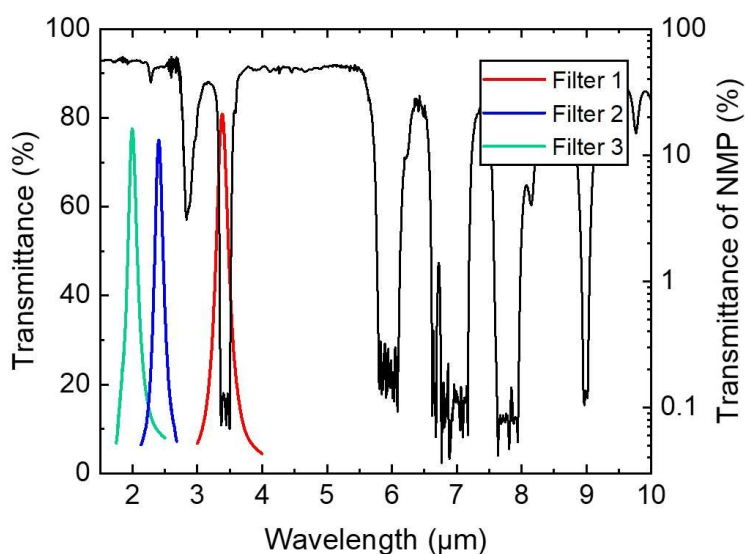


Figure 4.1 Transmittance spectra of 0.05 mm thickness pure NMP and Filter 1, 2, and 3.

centered at 3.4 μm . Details of the fabrication method are provided in Chapter 3. For comparison, Filter 2 (at 2.4 μm) and Filter 3 (at 2 μm) were tuned to shorter wavelengths. The layer stacks and the expected bandwidths of Filters 1 to 3 are summarized in Table 4.1.

Table 4.1. Details of Filter 1, 2, and 3.

	Layer structure	Peak wavelength (μm)	Full width at half maximum (μm)
Filter 1	$\beta\text{-FeSi}_2$ (170 nm)/ SiO_2 (1214 nm) / $\beta\text{-FeSi}_2$ (170 nm)	3.4	0.2
Filter 2	$\beta\text{-FeSi}_2$ (120 nm)/ SiO_2 (857 nm) / $\beta\text{-FeSi}_2$ (120 nm)	2.4	0.2
Filter 3	$\beta\text{-FeSi}_2$ (100 nm)/ SiO_2 (714 nm) / $\beta\text{-FeSi}_2$ (100 nm)	2.0	0.2

4.2.3 Experimental setup

The setup of solvent drying experiments is illustrated in Figure 4.2, and a photograph of the actual experimental apparatus is shown in Figure 4.3. Drying experiments were conducted by filtering the halogen lamp (Ushio, UL-SH-01) emission through one of the BPFs (50 mm $\times$ 50 mm $\times$ 1 mm) and irradiating the solvent in an aluminum container featured a central cavity with a 25-mm diameter and a 4-mm depth. The lamp position was adjustable via an XYZ stage and the output power was controlled via a variable transformer. To minimize the thermal load on BPF, a quartz plate was installed between the lamp and BPF. In addition, airflow was introduced above the BPF to provide cooling,

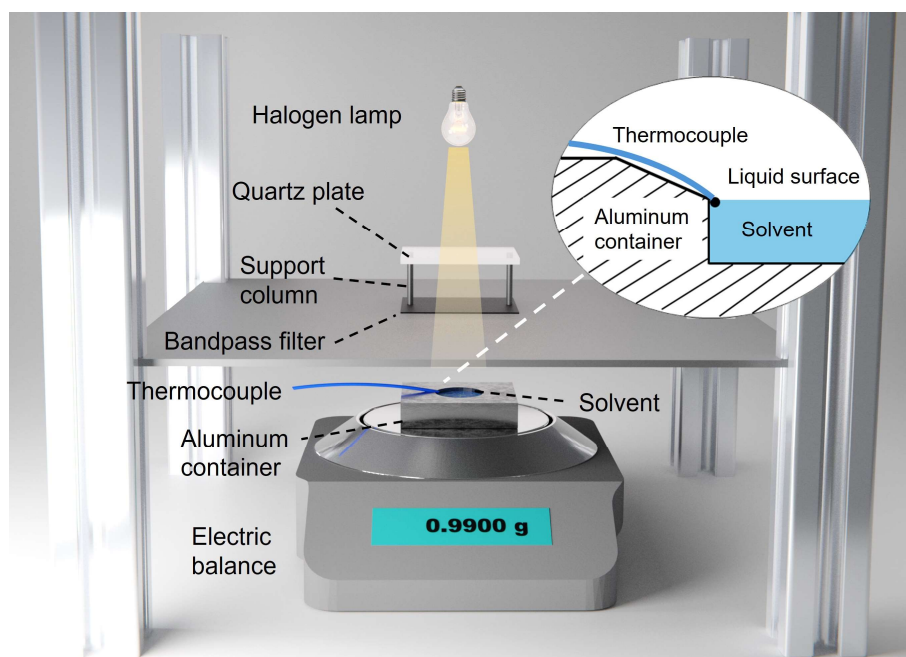


Figure 4.2. Schematic of the experimental setup.

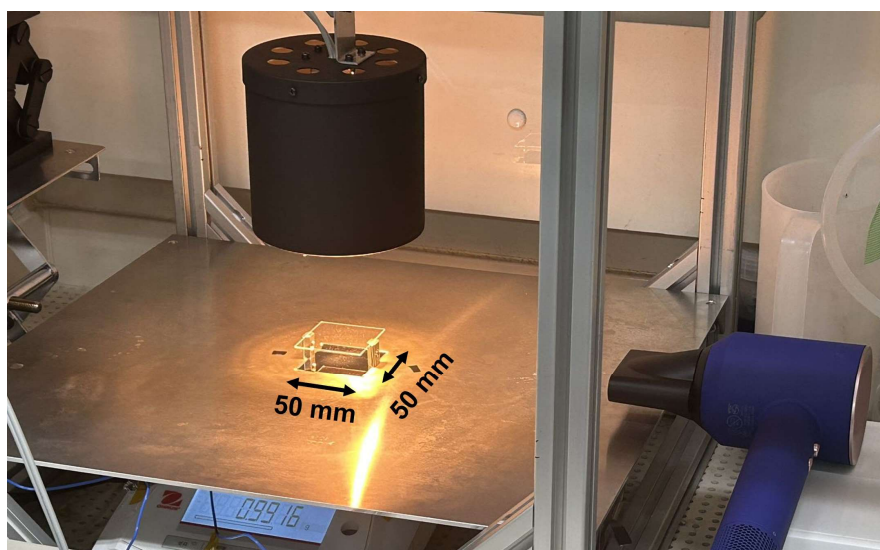


Figure 4.3. A photograph of the actual experimental apparatus.

while the airflow velocity below the BPF was maintained at ≤ 0.1 m/s to minimize its influence on the measurement of solvent evaporation behavior. The distance between the container surface and the halogen heater was approximately 120 mm. The intensity of IR radiation incident at the solvent surface was pre-measured using a power meter (Thorlabs,

S322C) positioned at the same location. An electronic balance (OHUAS, PX224, precision: 0.1 mg) and a thermocouple (TC) were used to record the changes in solvent mass and the apparent temperature at the solvent surface (T_{exp}), respectively.

Notably, owing to various factors such as finite TC size, steep temperature gradients near the surface, and interference from IR radiation, it is extremely challenging to accurately measuring the temperature at the free liquid surface during evaporation. To ensure uniform irradiation on the liquid surface, the TC was not placed near the center of the surface. Therefore, in this study, a 0.5 mm-diameter TC junction was positioned adjacent to the inner wall of the container and immersed just below the liquid surface (see inset of Figure 4.2). A small aluminum shutter was placed above the junction to protect it from direct IR heating. These efforts allowed us to monitor T_{exp} associated with the surface temperature, and to perform numerical simulations to estimate the localized temperature field based on the measured data.

4.2.4 Drying experiments

All drying experiments were conducted using approximately 1 g of pure solvent in a container. The lamp was turned on one minute after adding the solvent, and the weight and temperature of the solvent were recorded. Mass and temperature data were collected every second and stored on a computer using LabVIEW (Figure 4.4). The entire setup was placed in a draft chamber to ensure controlled conditions. The lamp was turned off after 5 min of irradiation, followed by ventilation for at least another 5 min. Once the surrounding environment had cooled, the used solvent was discarded, and the fresh solvent was added to prepare for the next drying experiment. Each measurement was repeated at least three times to ensure reproducibility.

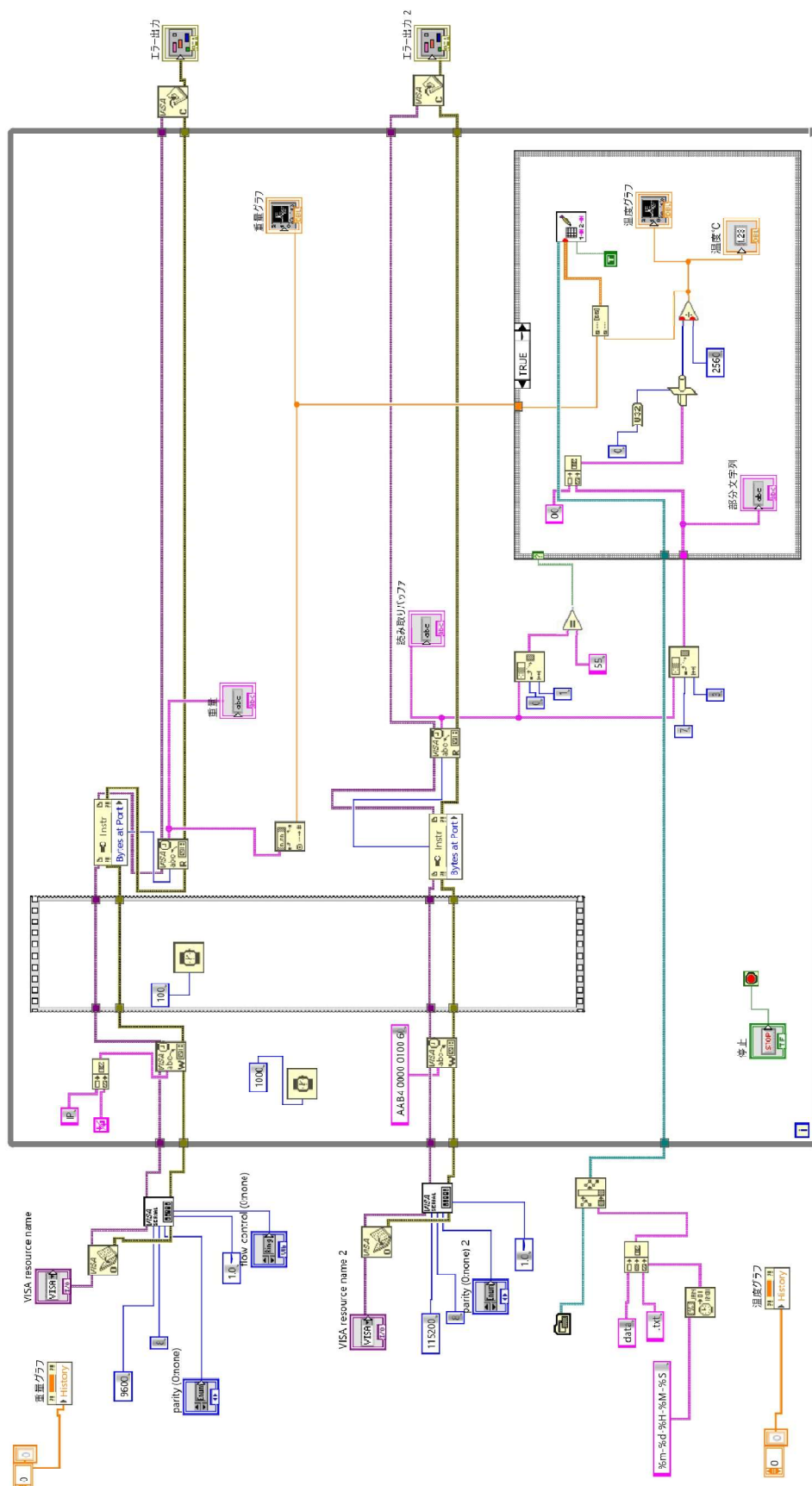


Figure 4.4. LabVIEW program for real-time logging and plotting of mass and temperature change.

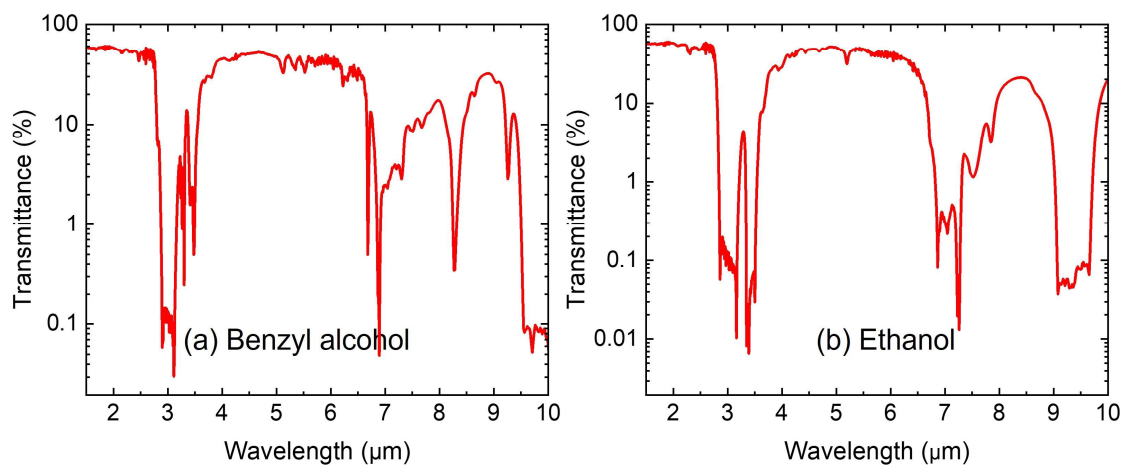


Figure 4.5. The transmittance spectrum of benzyl alcohol and ethanol, measured with a FT-IR spectrometer equipped with a liquid cell at a 0.05-mm optical pathlength.

Two additional solvents, benzyl alcohol and ethanol (both sourced from Fujifilm Wako), were also employed in the drying experiments. Figure 4.5 presents the transmittance spectrum of benzyl alcohol and ethanol, measured using an FT-IR spectrometer equipped with a liquid cell with an optical path length of 0.05 mm. Similar to the transmittance spectrum of NMP shown by the black curve in Figure 4.1, both solvents exhibit distinct absorption bands around 3.4 μm . These solvents were selected not only because of this shared absorption feature but also due to their widespread industrial use and their significantly different vapor pressures, which allow them to represent different classes of solvents with distinct drying behaviors.

4.2.5 Simulation of the NMP evaporation model

1. Model description

To investigate the mechanism of evaporation enhancement by infrared radiation at a wavelength of $3.4\ \mu\text{m}$, we employed a simplified axisymmetric model, as illustrated in Figure 4.6, to simulate the temperature distribution and evaporation rate of NMP solvent. All elements shown in the figure, including air, NMP, and the Al container, were included in the model. The blue region represents the liquid NMP domain, with an initial height set to 2 mm and radius set to 12.5 mm. The geometric dimensions of the Al container are nearly identical to those shown in Figure. 4.2. Under axisymmetric model, the shape of the container is modeled as a cylinder, which introduces negligible error for the purposes of evaporation simulation in this study. The NMP solvent and the container are placed in an air environment. To approximate the surrounding environment, we used a finite air domain coupled with an infinite domain, where the temperature at infinity is set to the initial room temperature and the NMP vapor concentration is assumed to be zero. The

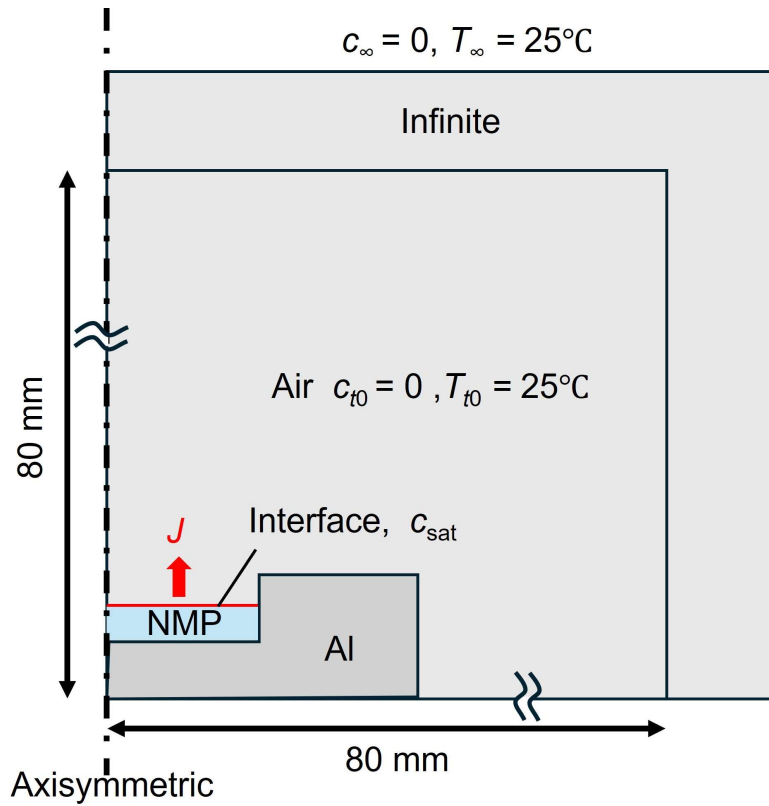


Figure 4.6. Schematic of the model geometry.

presence of the thermocouple was omitted from the model. Instead, to represent the temperature measured by the thermocouple in the actual experiment, we calculated the average temperature within a $0.5\text{ mm} \times 0.5\text{ mm}$ region at the upper right corner of the NMP domain, corresponding to the actual location of the thermocouple.

The absorption of infrared radiation by the solvent and its subsequent conversion into thermal energy was modeled as a heat source acting on the NMP domain. As discussed later in Figure 4.12, the irradiation by the $3.4\text{ }\mu\text{m}$ infrared wavelength can be approximated as a surface heat source with a power of 1.9 W applied at the liquid surface of the NMP. In contrast, broadband infrared irradiation was approximated as a domain heat source with a power of 2.1 W distributed throughout the entire NMP domain.

In this model, the entire evaporation process involves the following coupled phenomena:

- a) The heat source acting on the solvent induces a temperature rise.
- b) At the liquid–gas interface (indicated in red in the figure), a phase change occurs as NMP transitions from liquid to vapor, with a corresponding mass flux denoted by J .
- c) The saturated vapor at the interface diffuses into the air due to the concentration gradient, and this diffusion-driven mass transport determines the evaporation rate J .
- d) The mass loss due to evaporation causes the liquid–gas interface to move.
- e) The mass loss from evaporation also removes latent heat from the interface.

These phenomena occur simultaneously throughout the evaporation process. Therefore, our analysis is based on numerical simulations using COMSOL Multiphysics, incorporating the following modules: two-phase laminar flow, transport of diluted species, heat transfer in fluids and solids, moving mesh, and non-isothermal flow.[24, 25]

2. Assumption

The following assumptions were made to construct the numerical model:

- a) External convection above the solvent was neglected.
- b) The gas phase was assumed to behave as an ideal gas, and gravitational effects were ignored.
- c) Gas–liquid equilibrium was assumed at the interface.
- d) The thermal effects caused by infrared absorption in the surrounding environment and the aluminum container were neglected.

3. Governing Equations

In the two-phase laminar flow module, the NMP liquid domain and the air (gas) domain were considered. Both the liquid and vapor phases were treated as compressible fluids. Accordingly, the continuity equation is given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (4.1)$$

where $\mathbf{u}$ denotes the fluid velocity vector and ρ represents density. The Navier–Stokes equations for compressible laminar flow (neglecting gravitational effects) were employed to describe the relationships among fluid velocity, pressure, and density:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \left[-P \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] \quad (4.2)$$

where P denotes the pressure, μ is the dynamic viscosity and $\mathbf{I}$ represents the identity matrix.

In the Transport of Diluted Species module, only the diffusion of NMP vapor in the air domain was considered. The concentration distribution is governed by the diffusion

equation:

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot (D \nabla c) \quad (4.3)$$

where c is NMP vapor concentration and D is the diffusion coefficient of NMP in air.

Heat transfer in the entire model is described by the following energy equation:

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (t_c \nabla T) + Q \quad (4.4)$$

where C_p is the heat capacity at constant pressure, t_c is the thermal conductivity and Q is the heat energy form the heating source.

4. Initial and boundary conditions

Initially, the fluid was at rest. The initial temperature throughout the entire model was set to be uniform and equal to room temperature (25 °C), as summarized in Figure 4.6.

At the liquid–gas interface, evaporation causes continuous mass transfer from the liquid domain to the gas domain. The mass flux from the liquid phase to the gas phase is defined as J . Based on mass balance at the interface, the following relation can be obtained:

$$u_{l,n} = u_{v,n} + J \left(\frac{1}{\rho_l} - \frac{1}{\rho_v} \right) \quad (4.5)$$

where n represents the unit normal unit and l, v represent liquid and vapor, respectively. Furthermore, the liquid–gas interface is assumed to remain horizontal throughout the evaporation process. The downward velocity of the liquid surface, u_l , resulting from evaporation is calculated as J/ρ .

For the transport of diluted species, the initial NMP vapor concentration c_{i0} within the air domain is set to zero, and the concentration at infinity c_{∞} is also assumed to be zero. The saturation vapor concentration c_{sat} at the interface is considered as the ideal gas law:

$$c_{\text{sat}} = \frac{p_{\text{sat}}}{RTM_{\text{NMP}}} \quad (4.6)$$

where R is the specific gas constant, M_{NMP} is the molecular weight of NMP, T is the temperature, and p_{sat} is the saturation vapor pressure. The saturation vapor pressure is given by Antoine equation:[26]

$$\ln(p_{\text{sat}}) = A - \frac{B}{T + C} \quad (4.7)$$

The Antoine constants A , B , and C for NMP are listed in Table 4.2.

The evaporation mass flux at the interface is determined by diffusion of NMP vapor, following Fick's law of diffusion:

$$J = M_{\text{NMP}} \mathbf{n} \cdot (-D \nabla c) \quad (4.8)$$

where $\mathbf{n}$ is the surface normal vector. The diffusion coefficient D is estimated using the empirical correlation proposed by Fuller et al. :[27, 28]

$$D = \frac{1.43 \times 10^{-7} T^{1.75}}{PM_{\text{NMP,air}}^{0.5} \left[(\sum v)_{\text{NMP}}^{\frac{1}{3}} + (\sum v)_{\text{air}}^{\frac{1}{3}} \right]^2} \quad (4.9)$$

where P is the pressure, $M_{\text{NMP,air}}$ is defined as $2(M_{\text{NMP}}M_{\text{air}})/(M_{\text{NMP}} + M_{\text{air}})$, M_{air} is the molar mass of air, and $\sum v$ represents the diffusion volume. $\sum v_{\text{air}}$ and $\sum v_{\text{NMP}}$ are equal to 19.7 and 76.74, respectively.

For the heat transfer in solids and fluids module, the latent heat of evaporation was considered at the interface to accurately determine the saturation vapor pressure.

Additionally, as previously described, IR irradiation was approximated as a heat source applied to the NMP domain.

The material properties of air and aluminum were predefined in the COMSOL material library. The values used for NMP in the model are listed in Table 4.2.

Table 4.2. Values of the parameters of NMP.

Parameter	Value
Molecular weight, M_{NMP}	99.13 g/mol
Density, ρ	1.03 g/cm ³
Thermal conductivity, t_c	0.179 W/m K
A	14.66
B	4112.28
C	-66.87
Dynamic viscosity, μ	1.65 mPa·s
Constant pressure heat capacity, C_p	307.8 J/mol K
Specific gas constant, R	83.89 J/kg K
Latent heat of vaporization, L_H	44.5 kJ/mol

4.3 Results

4.3.1 Comparison of the solvent evaporation under same power IR irradiation and different wavelengths

Figure 4.1 shows the measured transmittance spectrum of Filters 1, 2, and 3. It can be observed that Filter 1 (red line) exhibits a sharp, high-transmission peak at $3.4\ \mu\text{m}$ and low transmittance at other wavelengths. In addition, the filter's bandwidth is approximately $0.2\ \mu\text{m}$ as designed, which matches well with the width of the absorption spectrum of NMP. Therefore, the IR light transmitted through this filter is expected to be efficiently absorbed by NMP.

Before the drying experiments under IR irradiation, we measured the mass changes of approximately 1 g of NMP placed at room temperature ($25\ ^\circ\text{C}$) under various relative humidity conditions in 400 seconds, as shown in Figure 4.7. Due to the hygroscopic nature of NMP and its low vapor pressure at room temperature, the observed mass change at higher humidity levels was predominantly attributed to moisture absorption. Therefore,

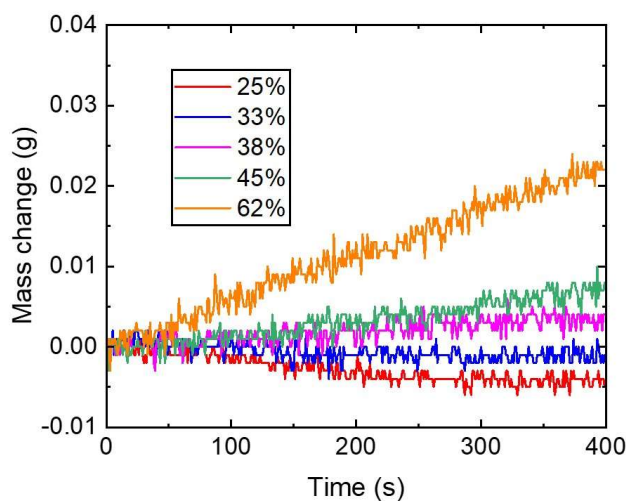


Figure 4.7. The 400 seconds mass change of NMP under different humidity levels.

the experiments in this study were conducted under controlled conditions with indoor humidity maintained below 40%, where the mass variation of NMP under ambient conditions was minimal.

The changes in the mass and T_{exp} of 1 g of pure NMP solvent over 300 s with IR irradiation filtered by Filters 1-3 and without irradiation, are summarized in Figures 4.8(a) and (b), respectively. To ensure a consistent IR power of approximately 1.9 W across all wavelengths, the power applied to the halogen lamp was carefully adjusted. Considering the hygroscopic nature of NMP, all experiments were conducted in an environment with relative humidity below 40 %. Airflow velocity above the solvent container was maintained at a minimum (≤ 0.1 m/s). The black line in Figure 4.8(a) indicates that the mass of NMP remained nearly unchanged in the absence of IR radiation under these conditions.

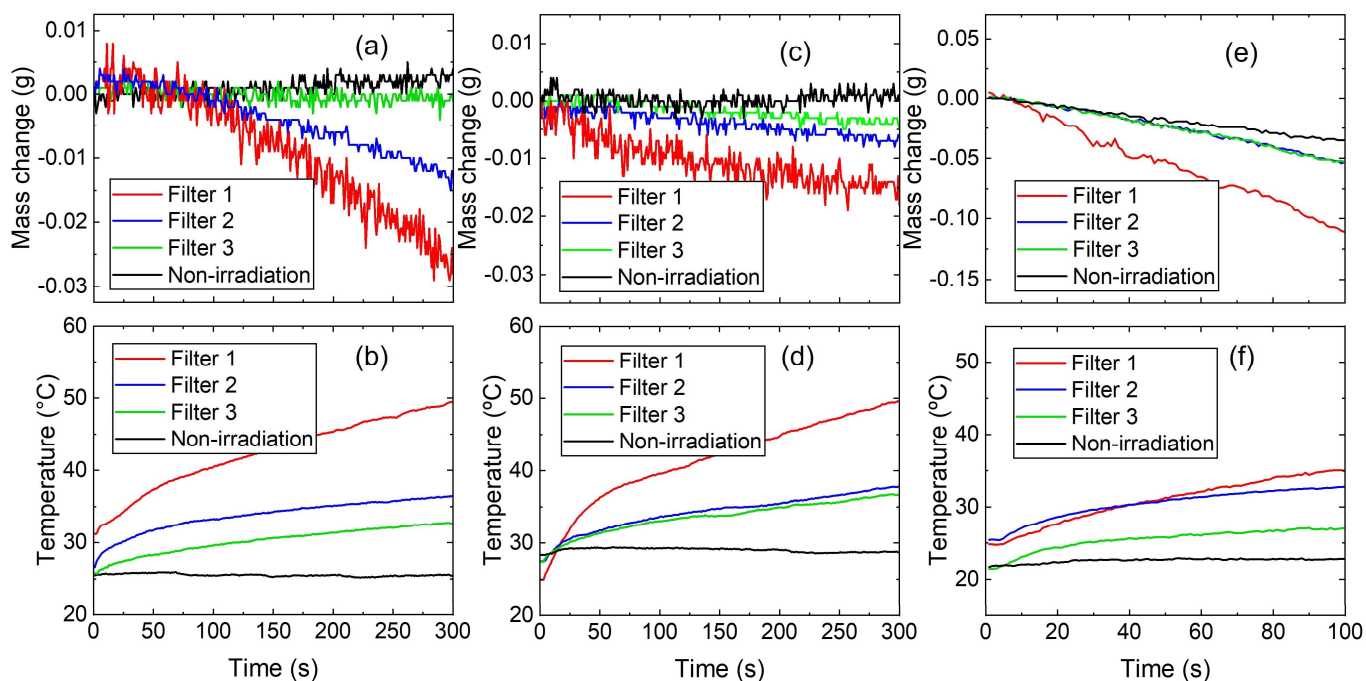


Figure 4.8. Changes in mass and temperature of the solvent (a, b) NMP, (c, d) Benzyl alcohol and (e, f) ethanol under IR irradiation at different wavelengths.

In contrast, under IR irradiation at 3.4 μm , which corresponds to the absorption band of the solvent, significant evaporation was observed, as indicated by the notable mass decrease shown by the red line in Figure 4.8(a). The measured temperature T_{exp} progressively increased to approximately 50 $^{\circ}\text{C}$, further accelerating the evaporation rate with continued IR heating. Conversely, irradiation at wavelengths of 2 and 2.4 μm resulted in considerably lower evaporation rates and slower temperature increases. Under 2- μm irradiation, the mass change was nearly identical to that observed under non-irradiated conditions. The mass and temperature changes in benzyl alcohol and ethanol under the same experimental conditions as those for NMP are summarized in Figures 4.8(c)–(f). Due to the rapid mass loss of ethanol, the observation period for mass and temperature variations was limited to 100 s to ensure that the TC remained immersed in the solvent throughout the temperature measurement. Similar to NMP, IR irradiation at 3.4 μm , corresponding to the absorption band of the solvent, induced the fastest evaporation and temperature increase. Deviations from this wavelength caused significant differences in the mass loss and temperature changes, even under the same IR power.

4.3.2 Comparison of the solvent evaporation under wavelength-selective IR irradiation and broad-spectrum IR irradiation

To clarify the effect of wavelength selectivity provided by the BPF, drying experiments were also conducted under broadband infrared irradiation without wavelength selection, using a double-side-polished Si wafer as the filter. A schematic of the experimental setup is shown in Fig. 4.9(a). Figure 4.9(b) presents the transmittance spectrum of the Si wafer measured by FT-IR, demonstrating a nearly uniform transmittance over a wide infrared wavelength range from 2 to 20 μm . In these experiments, the irradiation intensity was adjusted so that T_{exp} would remain the same regardless of wavelength selectivity. Specifically, the irradiation intensity was set to 1.9 W for the drying experiment using

Filter 1 and to 4.4 W for the non-selective drying experiment. The blue lines in Figures. 4.10(a) and (b) illustrate the mass and temperature changes of NMP over 300 s under 4.4 W IR irradiation, while the red lines are the same as the Filter 1 data shown in Figures. 4.8(a) and (b). The temperature increases in the NMP of the two experiments were nearly the same (Figure 4.10(b)). As shown in Figure 4.10(a), the mass change under wavelength-selective IR irradiation was significantly greater than that under broad-spectrum IR irradiation. The evaporation rate was calculated using $J = \dot{m}/A$, where A is the solvent surface area and $\dot{m}$ is the rate of mass change obtained by differentiating the polynomial fit of the mass–time curve with respect to time. At 300 s, the evaporation rate under wavelength-selective IR irradiation was $3.2 \times 10^{-4} \text{ kg/m}^2\cdot\text{s}$, which was approximately six times higher than that observed under broad-spectrum IR irradiation ($0.5 \times 10^{-4} \text{ kg/m}^2\cdot\text{s}$).

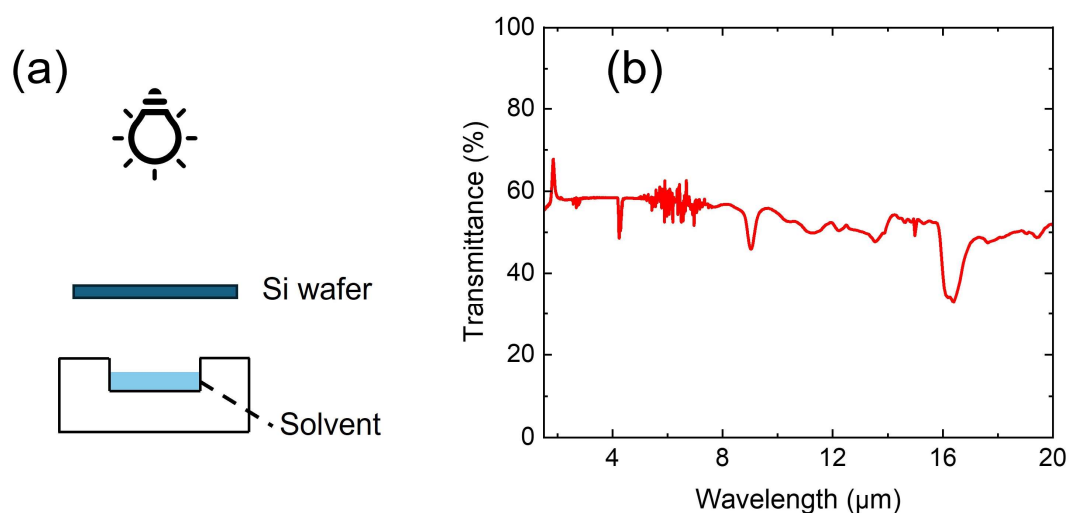


Figure. 4.9. A double-side-polished Si wafer used as a filter to transmit broad-spectrum (over 1 μm) IR light for drying. (a) Schematic of the experimental set up using Si wafer filter. (b) Transmittance spectrum of the Si wafer.

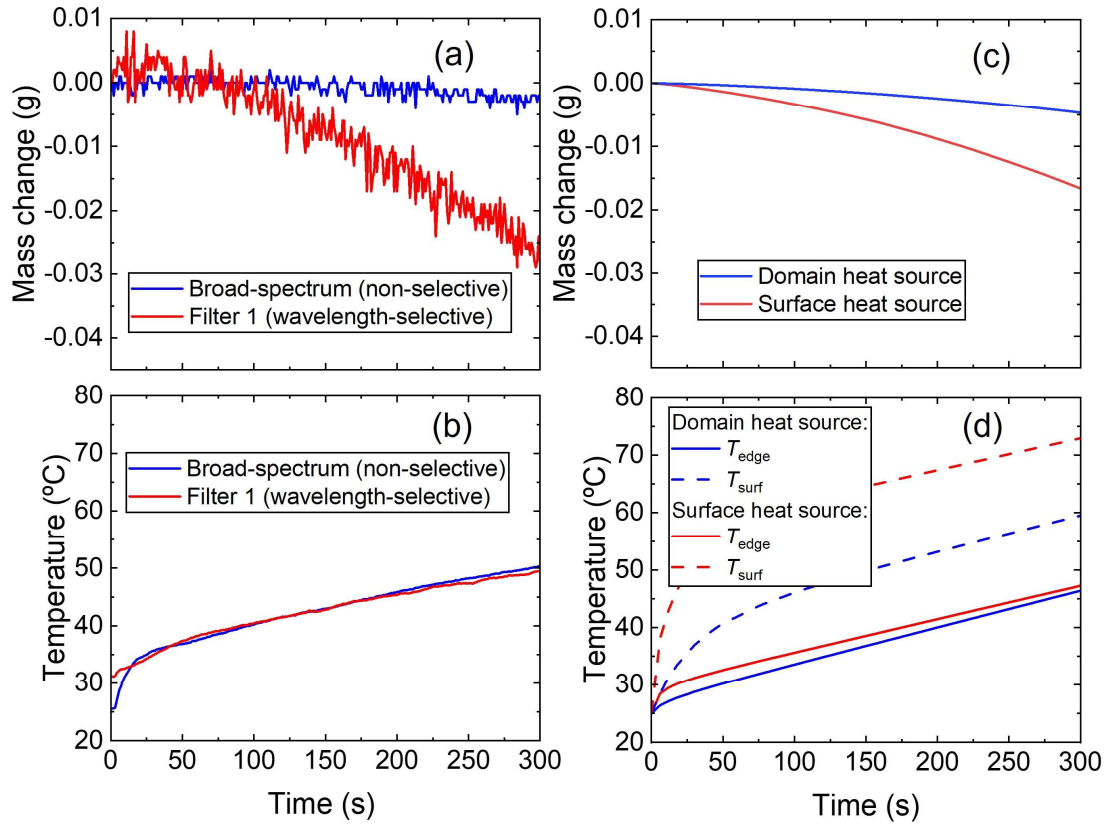


Figure 4.10. The 300-second changes in (a) mass and (b) temperature of the NMP under wavelength-selective and broad-spectrum IR irradiation. Simulation results of the 300-second changes in (c) mass and (d) temperature of the NMP under domain and surface heat source.

T_{edge} corresponds to the temperature at the TC location and T_{surf} represents the average temperature on the liquid surface.

4.4 Discussion

Under the same surface temperature conditions, the theoretical evaporation rate must be the same. However, the experimental results revealed that the use of the BPF resulted in an evaporation rate nearly six times higher, even at a lower irradiation power. This discrepancy appears to be attributed to localized temperature increases at the liquid–gas interface. Such temperature spikes, occurring within a narrow interfacial region, cannot

be accurately captured by the TC used in the experiments. Therefore, we developed a coupled heat and mass transfer model in COMSOL Multiphysics to further elucidate the temperature distribution and mechanisms underlying the enhanced evaporation behavior.

In this simulation model, the axisymmetric geometry and boundary conditions were configured to closely replicate the experimental setup (Figure 4.6). Wavelength-selective and broad-spectrum IR irradiation was approximated as heat sources acting at different depths within the NMP domain based on the spectral absorption characteristics of NMP. At a depth d beneath the liquid surface, the IR energy intensity $I(d, \lambda)$ at wavelength λ can be expressed using the Lambert–Beer law:

$$I(d, \lambda) = I_0 \cdot e^{-ad} \quad (4.10)$$

where I_0 represents the incident IR intensity at the liquid surface, and a is the absorption coefficient of NMP, both of which are wavelength dependent. Based on the transmittance spectrum of NMP with different thickness (Figure 4.11), the absorption coefficient a near the wavelength of $3.4 \mu\text{m}$ was estimated to be approximately 10^5 m^{-1} . Thus, the intensity

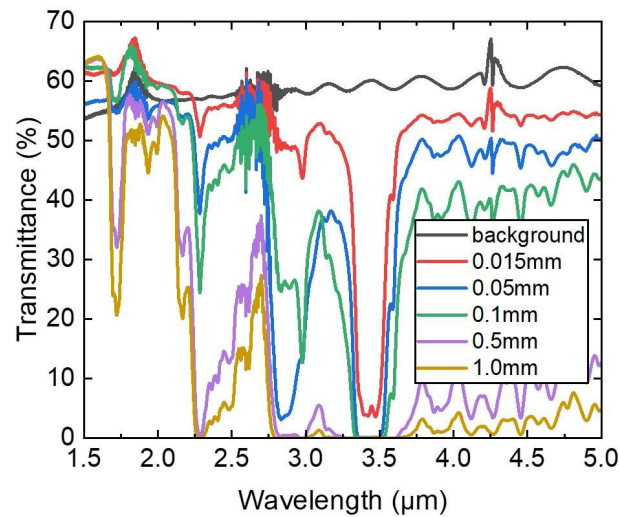


Figure 4.11. Transmittance spectra of NMP liquid film with 0.015 mm, 0.05 mm, 0.1 mm, 0.5 mm and 1.0 mm optical path lengths.

of 3.4 μm irradiation at 0.05 mm depth dropped to $I_0 e^{-5}$, which was nearly zero. In contrast, at wavelengths with minimal absorption, such as 2 μm , it was less than 10^2 m^{-1} . The intensity of 2 μm irradiation at a depth of 2 mm remained approximately $I_0 e^{-0.2} \approx 0.8 I_0$. This indicates that IR light near 3.4 μm was almost entirely absorbed and converted into heat at the solvent surface, whereas IR light at other wavelengths penetrated deeper and resulted in more uniform heating. A portion of the IR radiation outside the NMP absorption band was either absorbed by the aluminum container or escaped from the solvent, making it challenging to precisely quantify the amount of IR power absorbed by the solvent under broad-spectrum irradiation. To investigate the effect of heating caused by absorption within the solvent and container, broad-spectrum IR irradiation was roughly modeled as a domain heat source with a power lower than 4.4 W (a value of 2.1 W was selected to ensure that the simulated temperature closely matched T_{exp}), uniformly distributed throughout the solvent. In contrast, wavelength-selective IR radiation was approximated as a surface heat source with a power of 1.9 W applied at the NMP liquid surface. On this basis, we computed the temporal evolution of temperature distributions and mass changes over 300 s.

The calculated temperature distributions at $t = 30, 150$, and 300 s under the surface and domain heating conditions are summarized in Figure 4.12(a–f). While a more uniform temperature distribution was observed with the domain heat source, the simulation results for the surface heat source revealed a steep temperature gradient near the surface and a large temperature difference between the surface and the bottom throughout the entire heating process. Moreover, the temperature at the center region of the solvent surface was higher than at the edges. This phenomenon may be attributed to the heat absorption of the aluminum container.

We estimated the temperature at the TC location (T_{edge}), defined as the average temperature within a $0.5 \text{ mm} \times 0.5 \text{ mm}$ region located at the upper right corner of the NMP domain, corresponding to the actual position of the TC used in the experiments, and

the temperature at the liquid surface (T_{surf}), defined as the average temperature at the NMP liquid surface. The time-dependent variations of these temperatures are shown in Figure 4.10(d), where the red and blue lines represent the surface and domain heat source conditions, respectively. Solid lines indicate T_{edge} , and dashed lines represent T_{surf} . The corresponding mass change over time is presented in Figure 4.10(c). The simulated temperature rise rates and values for T_{edge} under both heating conditions were nearly identical in the simulation results, closely aligning with T_{exp} . Moreover, the computed mass change in the surface heat source case was significantly greater than that in the domain heat source scenario, exhibiting a trend consistent with experimental observations.

A comparison between the simulated and experimental mass changes and temperature rises under different power levels was also performed. In Figure 4.13, the red symbols

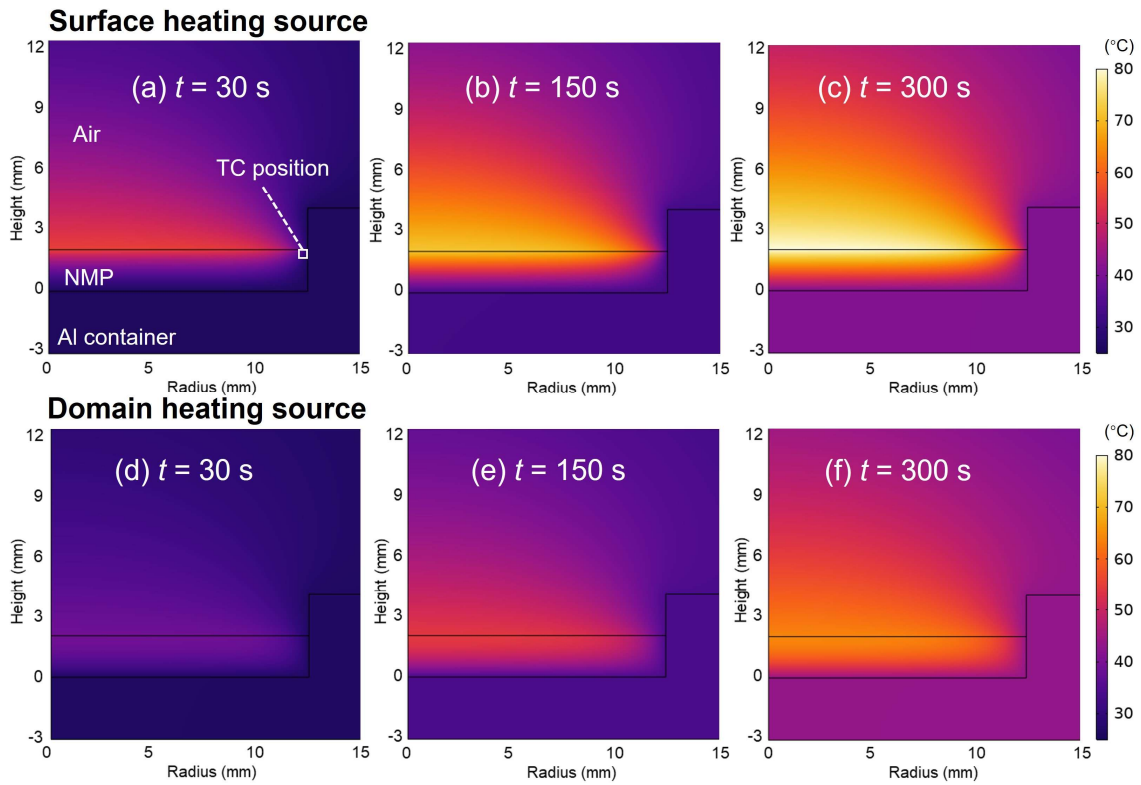


Figure 4.12. Simulated temperature distributions at $t = 30, 150$, and 300 s under (a–c) surface heating at 1.9 W and (d–f) domain heating at 2.1 W.

represent the simulated 5-min mass loss of NMP and the corresponding T_{edge} under surface heating conditions, while the black symbols indicate the experimentally measured averages obtained from three independent experiments. The error bars represent the minimum and maximum measured values. Good agreement between the simulated and experimental results was observed for both temperature and mass change across different power levels of wavelength-selective IR irradiation.

However, under surface heat source conditions, a noticeable temperature difference exceeding 25 °C between T_{surf} and T_{edge} was observed, as shown in Figure 4.10(d). This

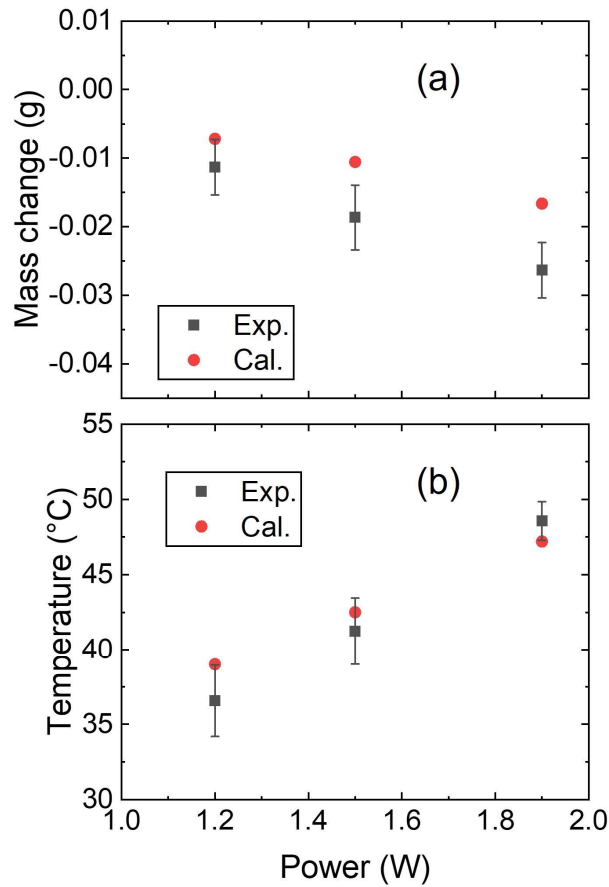


Figure 4.13. Comparison of the simulated mass change (a) and temperature (b) under different power levels with the experimental data. The experimental data show the average of three experiments. The corresponding error bars show the minimum and maximum measured values.

indicates that under wavelength-selective IR heating, the solvent surface was locally and efficiently heated, resulting in substantially higher temperatures than those measured by the TC. This localized high temperature at the surface generated higher saturation vapor pressure, thereby accelerating evaporation. The optimized transmittance spectrum of the BPFs employed in this study matches the absorption band of the solvent, ensuring that almost all IR radiation energy is absorbed at the liquid interface, resulting in localized heating and enhanced solvent evaporation.

Since it is difficult to measure the temperature at the bottom of the solvent using a thermocouple without disturbing the evaporation experiments, numerical simulations were employed to evaluate the bottom temperature. Figure 4.14 shows the time evolution of the 300 seconds averaged temperature at the bottom surface of the solvent with a depth of 2 mm. Although the liquid surface temperature under surface heating is significantly higher than that under domain heating, the temperature at the solvent bottom remains lower during the whole heating. This advantage becomes even more pronounced in practical drying processes involving thicker solvent layers. Because only a negligible fraction of IR radiation at wavelengths outside the absorption band can penetrate deeply into the solvent and heat the bottom, substrate materials can prevent thermal damage in practical drying applications.

As shown in Figures 4.10 and 4.13, the mass changes predicted by the simulations are slightly lower than the experimental results. The observed discrepancies are primarily attributed to air convection. In our simulation, convection was neglected, and evaporation was assumed to be purely diffusion-controlled. Due to the relatively low diffusion coefficient of NMP vapor,[28] a high concentration of NMP vapor accumulated near the liquid–gas interface. However, in experiments, despite efforts to minimize air convection effects and ensure reproducibility, airflow above the solvent container (≤ 0.1 m/s) enhanced vapor transfer near the interface, consequently increasing the evaporation rate. In practical applications, environmental factors such as humidity, airflow, and solvent

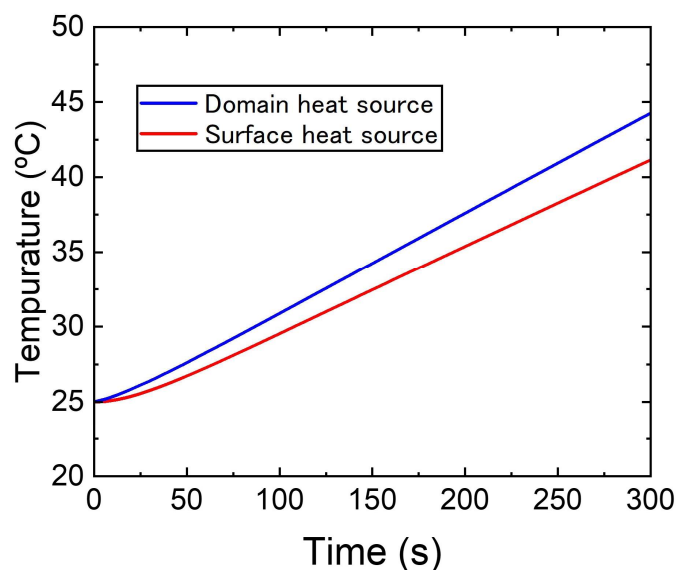


Figure 4.14. Simulated 300-seconds averaged temperature at the bottom surface of the solvent.

concentration can significantly influence the evaporation rate of organic solvents.[14, 29] In future experiments and simulations, investigating these factors and identifying their optimal values can further improve the evaporation rate and overall energy efficiency.

By employing optimized BPFs, our laboratory scale wavelength-selective IR heater demonstrated evaporation rates comparable to conventional hot-air drying methods ($\leq 4.2 \times 10^{-4} \text{ kg/m}^2 \cdot \text{s}$ at drying temperature 90°C).[30, 31] This study demonstrates that aligning IR irradiation wavelengths with the solvent's absorption band significantly enhances evaporation efficiency. It also highlights the potential of a wavelength-selective drying system utilizing BPFs to achieve rapid evaporation while maintaining low temperatures in deeper regions of solvents. Furthermore, the BPFs developed in this study offer flexibility in tuning their peak transmittance wavelength. By designing BPFs to match the absorption wavelengths of target solvents, these findings can be extended to a broader range of drying systems.

4.5 Conclusion

This chapter investigated the effect of IR wavelength selectivity on solvent evaporation rates and explored the potential of BPFs for IR drying. By aligning the IR irradiation wavelength with the absorption band of the solvent, significant enhancements in evaporation rate were achieved. Simulation results confirmed that selective absorption near the liquid surface plays a critical role in accelerating evaporation. These findings demonstrate that wavelength optimization using β -FeSi₂-based BPFs enhances the evaporation rate and overall energy efficiency. A drying system incorporating this BPF, which is suitable for large-scale and cost-effective production, presents a promising alternative to conventional solvent drying methods, such as NMP drying in LIB cathode fabrication.

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Chapter 5 Conclusion

In this study, we developed and evaluated a novel infrared bandpass filter (BPF) based on β -FeSi₂ for use in wavelength-selective radiation systems. First, β -FeSi₂ thin films with high refractive index and negligible extinction coefficient ($k \approx 0$) in the infrared region were successfully fabricated via co-sputtering by optimizing the Fe/Si ratio. These films were then used to construct simple tri-layer BPFs (β -FeSi₂/SiO₂/ β -FeSi₂), which demonstrated high transmittance (>80%) and narrow spectral selectivity around the target wavelengths. Finally, the fabricated BPFs were applied to a wavelength-selective drying system in lab scale, where infrared light matched to the absorption band of NMP (3.4 μ m) was used to enhance solvent evaporation. Experimental results confirmed that selective irradiation significantly improved evaporation efficiency, achieving an evaporation coefficient approximately six times higher than that of broad-spectrum IR. These findings demonstrate the feasibility of using β -FeSi₂ as a high-performance, scalable, and low-cost material for infrared optical applications. Moreover, this research highlights the potential of these BPFs in advancing energy-efficient processes, particularly in the field of precision drying for battery electrode manufacturing.

In the future, β -FeSi₂ is expected to serve as a novel high-refractive-index optical thin-film material, enabling the development of a wide range of optical devices and advancing research in photonics, such as metasurfaces. In particular, by leveraging its exceptionally high refractive index and transparency in the infrared region, β -FeSi₂ has the potential to realize broadband optical functionalities with a high degree of design freedom that are difficult to achieve using conventional materials. In addition, the effectiveness of β -FeSi₂-based BPFs in promoting solvent evaporation was demonstrated at the laboratory scale in

this study. Future work will focus on large-area fabrication and process scale-up, followed by systematic evaluations of evaporation enhancement, practical feasibility, and energy efficiency in real industrial-scale processes.

List of Publications

Journal Papers

Publications concerning this thesis

1) Co-sputter による β -FeSi₂ 薄膜の組成と光学特性の制御に関する研究

Xuanwei Zhang, Samir Kumar, 名村 今日子, 鈴木 基史

表面と真空, **64**, 9, 2021

2) β -FeSi₂: A high refractive index candidate material for infrared bandpass filters

X. Zhang, K. Namura, M. Suzuki

Journal of Applied Physics **134**, 185302, 2023

3) Application of β -FeSi₂-based bandpass filters in wavelength-selective infrared drying systems

X. Zhang, K. Namura, M. Suzuki

Japanese Journal of Applied Physics, **64**, 11SP16, 2025.

Publications concerning other studies

4) Microbubble oscillation on localized heat source affected by dissolved gases in water

N. Hiroshige, S. Okai, X. Zhang, S. Kumar, K. Namura, M. Suzuki

Journal of Applied Physics **135**, 094701, 2024

5) Configurable Vibrational Coupling in Laser-Induced Microsecond Oscillations of Multi-Microbubble System

X. Zhang, R. Matsuo, Y. Yahano, J. Nishida, K. Namura, M. Suzuki

small, **21**, 2408979, 2025

6) Reverse-bias driven anomalous polarity switching in FeSi₂/Ga₂O₃-NRs heterojunction based solar-blind photodetector

R. Dahiya, D. Kaur, X. Zhang, B. Gatadi, K. Bhatt, R. Singh, M. Suzuki, M. Kumar
Applied Surface Science, **720**, Part C, 2026.

Conferences

1) Co-sputter による β -FeSi₂ 薄膜の組成と光学特性の制御に関する研究

Zhang Xuanwei, 舩中 翔馬, 名村 今日子, 鈴木 基史

2020 年日本表面真空学会学術講演会, 3Ba11, 11 月 2020 年

2) Co-sputtering による赤外域で透明な多結晶 β -FeSi₂ 薄膜の作製

Zhang Xuanwei, 名村 今日子, 鈴木 基史

第 68 回応用物理学会春季学術講演会, 16a-Z23-3, 3 月 2021 年

3) Wavelength Selective Transmission Thin Film using β -FeSi₂ for Infrared heating

X. Zhang, S. Kumar, K. Namura, M. Suzuki

The 9th International Symposium on Surface Science, 01PS-64, Nov. 2021.

4) Wavelength Selective Transmission Thin Film using β -FeSi₂ for Thermophotovoltaic system

Xuanwei Zhang, Kyoko Namura, Motofumi Suzuki

The 6th Asia-Pacific Conference on Semiconducting Silicides and Related Materials, C42, July, 2022

5) Mg₂Si 短波長赤外線センサーのための反射防止膜の設計と作製

Xuanwei Zhang, 植田 香菜, 今泉 尚己, 名村 今日子, 鵜殿 治彦, 鈴木 基史

第 84 回応用物理学会秋季学術講演会, 22a-B202-3, 9 月 2023 年

6) 鉄シリサイドの狭帯域フィルターを用いた波長選択乾燥に関する研究

Xuanwei Zhang, 名村 今日子, 鈴木 基史

第 85 回応用物理学会秋季学術講演会, 17p-B1-10, 9 月 2024 年

7) Vibrational interaction of two vapor-rich microbubbles in degassed water

Kyoko Namura, Xuanwei Zhang, Ryu Matsuo, Motofumi Suzuki

Bulletin of the American Physical Society, Nov. 2024

8) Application of β -FeSi₂-Based Bandpass Filters in Wavelength-Selective Infrared Drying Systems

Xuanwei Zhang, Kyoko Namura, Motofumi Suzuki

The 7th Asia-Pacific Conference on Semiconducting Silicides and Related Materials,
Sun-a-O6, July, 2025