ABSTRACT

WANG, YAN. Switching Applications Based on Reversible Insulator-Metal Transition of Vanadium Dioxide Thin Films Synthesized by Pulsed Laser Deposition. (Under the direction of Dr. John F. Muth).

Vanadium dioxide (VO₂) is a phase transition metal oxide that has attracted the attention of researches because of its reversible and abrupt insulator to metal transition. Upon heating through a critical temperature of \( T_c \approx 68 \, ^\circ\text{C} \), VO₂ undergoes a structural transformation of the crystalline lattice, from a monoclinic (M₁) phase for the low temperature insulating state to a tetragonal/rutile (R) phase for the high-temperature metallic state. There are several ways to trigger this transition other than increase the temperature, including photonic excitation and electric excitation. The purpose of this dissertation is to synthesize high quality VO₂ thin films by pulsed laser deposition, utilize its insulator to metal transition to design and fabricate different electronic and optical devices. The devices include thermochromic devices, optical modulators, radio frequency switches, and reconfigurable dipole antennas.

Thermochromic devices were fabricated by depositing a metal layer on top of VO₂ thin films. We observed that the magnitude of the reflectivity increases for metal coated VO₂ films, but decreases for uncoated VO₂ thin films in the near infrared. The measured reflectance results matched well with our calculation results obtained from a double layer model using the optical transfer matrix method. We demonstrate that the magnitude of the reflected color change in that visible portion of the spectrum as VO₂ undergoes the insulating to metallic phase transition can be controlled by changing the type of metal, the thickness of the metal and by patterning the metal at the nano scale. The changing dielectric
properties of VO$_2$ also suggest interactions with plasmons in the nano patterned metal films and plasmonic crystals can lead to new devices.

Optical modulators based on joule heating mechanisms were fabricated with VO$_2$ thin films. The device switches from semiconductor phase to metal phase by applying a constant voltage across two metal contacts. The transition is caused by joule heating from the current flowing through the VO$_2$ thin films. We have improved the performance of the devices by fabricating them on SiN$_x$ membranes. Compared to the devices fabricated on the normal substrates, such as sapphire, silicon or glasses, the switching speed of the devices on the membrane is an order of magnitude faster. Decreasing the area and thickness of VO$_2$ on top of thinner membranes allows kHz bandwidths to be achieved.

Applying VO$_2$ to radio frequency (RF) applications were investigated by designing and fabricating RF switches and reconfigurable dipole antennas. The propagation of the RF signal was controlled by the insulating to metal transition of VO$_2$. Simulated results were obtained using the RF simulation software SONNET before fabrication. The measured results show a high contrast between the insertion loss of the on state and isolation of the off state for both of series and shunt configuration switches. The measured return loss of the reconfigurable dipole antennas confirmed the change of the resonance frequency because of the phase transition of VO$_2$. 
Switching Applications Based on Reversible Insulator-Metal Transition of Vanadium Dioxide Thin Films Synthesized by Pulsed Laser Deposition

by
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DEDICATION

To my loving parents Haiping Wang and Xiuling Liu and my beautiful, intelligent and kind hearted wife Yihe Wang.
BIOGRAPHY

Yan Wang was born in Jiaohe, which is a small town in the northeast of China. He grew up there and then went to Zhejiang University in Hangzhou to pursue his Bachelor’s degree in Physics. In 2008, he came to U.S. and became a PhD student in the Physics Department at North Carolina State University. Yan joined Dr. John Muth’s research group at Electrical and Computer Engineering Department in 2009 and started his research on vanadium dioxide. In 2009, Yan married Yihe Wang who came to U.S. to accompany him and start her own graduate study in 2010. Yan received his Master’s degree in Physics and Master’s degree in Electrical Engineering in spring 2012 and fall 2012. He graduated from North Carolina State University with his PhD in Physics in the summer 2013.
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CHAPTER 1
INTRODUCTION

1.1 Overview

Vanadium dioxide (VO$_2$) is well known for its reversible and abrupt insulator to metal transition at a temperature close to 68 °C, and attracted attention for its potential in various electrical and optical applications since it was first reported by Morin in 1959.[1] VO$_2$ is distinguished among all the transition metal oxides because of the distinct insulator-to-metal transition and near room temperature occurrence. The transition temperature can be modified by doping other metals into VO$_2$ or stress due to the lattice mismatch between VO$_2$ films and the substrates.[2,3] Below the transition temperature, the film is a monoclinic structure insulator with high near infrared transmission. Above that temperature, the film undergoes a phase transition, transforming it into rutile tetragonal structure metal with much lower near infrared transmission.[4] The magnitude of the resistivity change is 4–5 orders for single bulk crystal and 3–4 orders for thin films.[5] The transition can be simply triggered by heating the VO$_2$ over the transition temperature. Joule heating due to the current flow through thin films will also cause the temperature increase and hence trigger the transition. Electrical and optical triggered transitions within picoseconds range have also been reported recently.[6–13] The characteristics associated with the insulator to metal transition in VO$_2$ are of technological importance for potential application in future electrical and optical devices.
Thermochromic thin films whose reflectivity depends on temperature can be used as coating materials for smart windows and switchable glass.[14] The use of smart windows can save power for heating, air-conditioning and lighting by controlling the heat and light passing through. VO₂ has been one of the most interesting thermochromic materials because of its high infrared transmission in the insulating phase and high infrared reflectivity in the metallic phase. Thermochromics in infrared region have been observed from single VO₂ films or VO₂ films coated with oxides.[15, 16]

Modern communication systems rely on high performance devices using conventional electrical materials, but can be improved by novel materials with new photonic functionality. The dielectric constants of VO₂ thin films are hugely increased during the phase transition, which can be used to control infrared light for communication systems or even the terahertz radiation transmitted through it.[17–20] Radio frequency switches based on VO₂ thin films integrated with coplanar waveguides have also been realized.[21–24]

The large magnitude of the resistance change and the fast switching response to the electrical and optical excitations make VO₂ thin films a high potential material for future optical and logic devices. Field effect devices with VO₂ thin films as the channel layer have been reported by several groups.[9, 10] Understanding the excitations mechanism of the phase transition is especially critical for using VO₂ thin films in electronic applications, as well as distinguishing VO₂ as Mott or Peierls insulator.

During the last few decades the research trends on the topic of VO₂ are mainly focused on:
(1) highly crystalline structured VO$_2$ thin film growth and deposition, including sol-gel dip-coating method\cite{25}, reactive ion-beam sputtering\cite{26} and pulsed laser deposition\cite{27}.

(2) VO$_2$ phase transition mechanism, debate between electron-electron correlations-Mott-Hubbard and lattice instability-Peierls\cite{4, 12, 28–34}.

(3) study on the ultrafast insulator to metal transition, such as ultrafast time-resolved x-ray diffraction (XRD) method, femtosecond laser and ultrafast terahertz response to the photo excitation\cite{11–13, 35–37}.

(4) device fabrication based on the optical and electrical properties associated with the insulator to metal transition of VO$_2$, optical modulator, field effect thin film transistors and memory type applications\cite{9, 10, 38}.

Our research interests are focused on depositing highly crystalline structured VO$_2$ thin films and developing novel optical and electrical devices utilizing the unique insulator to metal transition of VO$_2$. The deposition conditions and substrates affect the films quality and the transition characterization. In this research we successfully find the optimal conditions to grow highly crystalline structured VO$_2$ thin films with larger magnitude of resistivity change and narrower hysteresis loop on different substrates using the Pulsed Laser Deposition (PLD) method. The films optical and electrical properties have been characterized and the substrates effect on the films quality has also been studied.

We are also specifically looking at applications that can utilize the insulator to metal transition properties of VO$_2$. As the VO$_2$ undergoes the insulator to metal transition, the optical properties of the films also has tremendous changes. In this research we studied the thermochromic effect based on VO$_2$ thin films and fabricated the thermochromic devices.
with VO₂. The enhancement of the thermochromic effect due to the structured metal layers has also been investigated. Optical modulators utilizing the properties of VO₂ were fabricated and tested. We improved the device performance by fabricating the devices on top of silicon nitride membranes. The change of the electrical properties associate with the insulator to metal transition has also been used to make application devices in this research. The radio frequency (RF) signal can propagate through metals but not an insulator. The reversible insulator to metal transition makes VO₂ a potential candidate material for RF switches. We fabricated switches using this property to turn on and off an incoming electromagnetic field propagating in a microwave planar waveguide. Reconfigurable dipole antennas have also been realized based on this idea. The performance of RF applications based on VO₂ thin films have also been studied in this research.

The work in this dissertation covers the deposition and characterization of VO₂ thin films and also the application devices utilizing the optical and electrical properties associated with the insulator to metal transition of VO₂.

**1.2 Dissertation Organization**

The structure of this dissertation is as follows. Chapter 2 gives a brief review of the literature related to the recent research about VO₂. The fundamental physical and electrical structure of VO₂ was reviewed. The phase transition mechanism has been discussed throughout a decade long debate. Different excitation methods and most recent application studies based on the transition properties were introduced.
Chapter 3 provides a description of the deposition and characterization tools used in this study. The VO\textsubscript{2} thin films in this study were deposited by Pulsed Laser Deposition. Films were characterized by different tools and the devices were fabricated in the cleanroom with standard semiconductor processes.

Chapter 4 introduces the electrical and optical properties of VO\textsubscript{2} thin films deposited by our Pulsed Laser Deposition system. We successfully deposited highly crystalline structured VO\textsubscript{2} thin films on sapphire and ITO glass. The resistivity, reflectance and transmission data were obtained by measurement. The relationship between the transition properties and the substrates has been discussed.

Chapter 5 discusses the thermochromic effect of VO\textsubscript{2} thin films. We investigate metallic thin films on VO\textsubscript{2} and show that the magnitude of the reflected color change in that visible portion of the spectrum as VO\textsubscript{2} undergoes the insulating to metallic phase transition can be controlled by changing the type of metal, the thickness of the metal and by patterning the metal at the nano scale. We consider the role of surface plasmons in the metal film and show that in the near infrared, the magnitude of the reflectivity increases for metal coated VO\textsubscript{2} films, but decreases for uncoated VO\textsubscript{2} thin films. This is explained in the context of Fresnel equations and considers the large change in the imaginary part of the dielectric constant as the VO\textsubscript{2} changes state from the insulating to metallic phase.

Chapter 6 presents the optical modulator fabricated on silicon nitride membranes. Joule heating devices fabricated on silicon nitride membranes switches from semiconductor phase to metal phase by applying a constant voltage across two metal contacts. Compared to the devices fabricated on the normal substrates, such as sapphire, silicon or glasses, the switching
speed of the devices on membrane is an order of magnitude faster. Decreasing the area and thickness of VO$_2$ on top of thinner membranes allows kHz bandwidths to be achieved.

Chapter 7 reports the design, fabrication and the performance of RF switches and reconfigurable dipole antennas based on VO$_2$ thin films. We utilize the insulator to metal transition of VO$_2$ to control the propagation of RF signals. The designed structures were first simulated in RF simulation software. The fabricated switch devices, both of series and shunt configuration show a high contrast between the insertion loss of on state and isolation of off state. The measured return loss of the reconfigurable dipole antennas confirmed the change of the resonance frequency because of the phase transition of VO$_2$. Both of the simulated and measurement results present the high application potential of VO$_2$ in radio frequency and microwave systems.

Chapter 8 concludes this research by summarizing the results and discussions presented through this work and providing some suggestions for future work.

Two appendices, A and B are included. Appendix A details the optical transfer matrix method used in Chapter 5 to calculated the reflectance of the thermochromic devices. Appendix B contains MATLAB code written to implement the method described in Appendix A.
CHAPTER 2
LITERATURE REVIEW

The phenomena of the insulator to metal transition have attracted the attention of many research groups in recent years. The research has been focused on the preparation and characterization of transition oxides that undergo a transition by heating or cooling the material. Among those phase transition metal oxides, vanadium dioxide (VO$_2$) has been one of the most studied strong correlated metal compounds which has the remarkable insulator to metal transition at the critical temperature around 68°C.[1] Although other oxides of vanadium, such as VO, V$_2$O$_3$ and V$_2$O$_5$ also exhibit insulator to metal transition,[39] VO$_2$ stands out to be interesting because its transition temperature is near room temperature and can be lowered by using the appropriate doping materials. The transition could also be triggered by electrical field or by optical excitation.[6, 11, 40] The resistivity change is of order $\sim$10$^3$-10$^5$ with a hysteresis width of $\sim$ 1°C for bulk single crystals and is of the order $\sim$10$^3$-10$^5$ with a hysteresis width of $\sim$ 5°C-10°C for thin films.[5, 27] Vanadium dioxide has been extensively investigated and implemented in several applicable devices that utilize the change in optical and electrical properties associated with its insulator to metal transition, but the physical mechanism whether the electron-electron correlations or lattice instabilities dominate the transition is still under debate.
2.1 Physical and Electrical Structure of VO₂

During the metal-insulator transition, VO₂ also undergoes a structural transformation of the crystal lattice, from a monoclinic (M1) phase for the low-temperature insulator to a tetragonal/rutile (R) phase for the high-temperature metal.[4] The two structures are listed in Figure 2.1. The rutile structure can be alternatively visualized in terms of a body-centered tetragonal lattice formed by the metal atoms, where each metal atom is surrounded by an oxygen octahedron. Octahedron is centered at the corners and the center of the cell is rotated by 90° about the tetragonal c axis relative to each other. The monoclinic phase is derived after pairing and tilting V-V along the c axis resulting in a doubled sized unit cell with distortion of the oxygen cages.[4, 28]

Figure 2.1 Crystallographic structures of vanadium dioxide (VO₂): (a) Metallic (Rutile) above the transition temperature, and (b) Insulating (monoclinic) below transition temperature. Large and small spheres denote vanadium (V) and oxygen (O) atoms respectively.[28]
The detailed band structure of VO$_2$ was first demonstrated by Goodenough in 1971.[4] The structure was constructed based on V$^{4+}$:3d orbitals and O$^{2-}$:2p orbitals. The 4s$^2$3d$^5$ V atoms, each bound to two 1s$^2$2s$^2$2p$^4$ O atoms, contribute four electrons to fill the O 2p shells, leaving V$^{4+}$ cations with a single valence electron near the Fermi level. The closed-shell O 2p electrons now stay quite below the Fermi level, not contributing significantly to the conductivity. The cubic component of the V$^{4+}$ ion octahedral sites splits the 3d$_{\parallel}$ energies into higher energy twofold-degenerate states of e$_g$ symmetry and lower energy threefold-degenerate states of t$_{2g}$ symmetry. The t$_{2g}$ states which are near the Fermi energy, are split into a 3d$_{\parallel}$ state and 3d$_\pi$ state. 3d$_{\parallel}$ states are aligned along the rutile c-axis with metal-metal bonding. Rutile phase VO$_2$ is metallic because of the single electron in the lowest vanadium 3d$_{\parallel}$ band. In the low temperature insulating phase, the V-V paring and tilting with respect to the rutile c-axis causes the splitting of the 3d$_{\parallel}$ band into filled bonding and empty antibonding states and the 3d$_\pi$ band shift away from the Fermi level. As a result, the band gap between the bonding 3d$_{\parallel}$ band and the other t$_{2g}$ bands is ~0.7eV; the 2d$_{\parallel}$ band splitting is ~2.5eV and the rise of the 3d$_\pi$ band is ~0.5eV.
Figure 2.2 (a) Structure of VO$_2$: Side view: Only the vanadium sublattice is shown, which undergoes pairing and tilting along the c-axis in the cell-doubled M1 structure. Top view: Each V$^{4+}$ cation lies within an octahedron of six oxygen atoms. (b) Diagram of the crystal field-split V 3$d$ states in VO$_2$. (C) Energy-level diagram of VO$_2$. [41]
\textbf{2.2 Electrical Properties}

Vanadium dioxide (VO$_2$) has been well known for its metal-to-insulator transition and the abrupt change of its resistance at 68°C. It has been reported the magnitude of the resistivity can change on the order of $10^5$ over the transition temperature. Thermal hysteresis exists because of the different transition temperatures for heating and cooling through the transition. As shown in Figure 2.3, VO$_2$ films demonstrate a transition of electrical resistance by as much as $10^3$-$10^5$ at 68°C with a thermal hysteresis of 2-10°C upon heating and cooling down.[27]

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.3.png}
\caption{(a) Electrical resistance as a function of temperature for VO$_2$ thin films on (0001) and (1010) sapphire substrates.[27] (b) The phase diagram of VO$_2$ and the resistance-temperature curve showing the insulator-to-metal transition.[42]}
\end{figure}

Qazilbash et al. measured the electromagnetic response of a VO$_2$ film on a spatial scale of 20 nm, using scattering scanning near field infrared microscopy (s-SNIM) in conjunction with far field infrared spectroscopy.[42] They observed that the transition occurs
via nucleation of the nanoscale metallic puddles in the insulating VO$_2$ host. As temperature increases these puddles grow in size, percolate, and eventually lead to a nominally homogeneous metallic film. As shown in Figure 2.4, as the temperature increases, the resistance of the VO$_2$ films decreases. The near field scattering amplitude is higher (light blue) at high temperature low resistance state, which means that the films are at metallic phase. At low temperature, the near field scattering amplitude is lower (dark blue) because of the films are in insulating phase. During the transition, these two phases are mixed together.

Figure 2.4 The resistance of the VO$_2$ film is plotted with increasing temperature. Also shown are maps of near-field scattering amplitude of a VO$_2$ film for three temperatures (from left to right): insulating regime, phase coexistence, and rutile metal. The scanned area is 2×2 µm$^2$. The near-field scattering amplitude is higher (light blue and white light gray) for the metallic regions compared to the insulating phase (dark blue and dark gray).[42]
Yong Wook Lee et al. measured the I-V hysteresis loops in a two terminals VO$_2$ device by using V mode and I mode at room temperature(Figure 2.5 (a)).[43] In V mode, the voltage applied on the devices is in the range of 0-11 volts. Two threshold voltages $V_{t1}$ and $V_{t2}$ were measured at 9.7 and 4.0 V, where a current abruptly rises and falls, respectively. In I mode, the current flowing through the device is in the range of 0-3mA. As the current increases, the voltage across the devices increase exponentially until it reaches $V_{t1}$. After that, the voltage starts to decrease until it reaches $V_{t2}$, where the voltage maintains a constant value irrespective of the current increase. The currents at $V_{t1}$ and $V_{t2}$ were designated as $I_{t1}$ and $I_{t2}$, which are 0.43mA and 1.34mA, respectively. They design a simple circuit which is composed of a voltage source and a two-terminal VO$_2$ thin film device serially connected with a standard resistor. Room temperature electrical oscillation in vanadium dioxide has been observed and the oscillation frequency could be controlled by adjusting an external voltage and increased up to 0.5 MHz (Figure 2.5 (b)).
Figure 2.5 (a) I-V characteristics of the fabricated two-terminal devices based on the VO$_2$ thin film. The insets show the cross section and plane view of the device and the surface morphology of the VO$_2$ film used in the device. L and W in plane view indicate the length and width of the exposed VO$_2$ film, respectively. (b) Schematic diagram of the electric circuit for generating the oscillation. Measured oscillatory electrical responses of current and voltage, indicated as red circles and blue squares, respectively and one period of IO oscillation.[43]

Various ions have been used to modify the temperature dependence of VO$_2$’s electrical resistivity, such as such as niobium, molybdenum, tungsten, and fluorine. M. Soltani et al. investigated the Ti–W co-doping effects on both the electrical and optical thermochromic properties of VO$_2$ films.[2] Compared to undoped and W-doped VO$_2$, Ti–W codoping provides insulator to metal transitions with a smoother gradient and reduce optical and electrical hysteresis (Figure 2.6 a). Al$^{3+}$ was also used to reduce the transition temperature.[44] As shown in Figure 2.6 b, the electrical resistance measured upon heating and cooling of VO$_2$ films shows that the transition temperature decreases to as low as 40 °C. The magnitude of the resistance change from the insulating to metallic states also decreased
with Al$^{3+}$ doping. The hysteresis loop was narrower for the Al$^{3+}$ doped films compared to the broad hysteresis of the pure VO$_2$ film on glass.

![Figure 2.6](image_url) (a) Comparison of the temperature dependence of the electrical resistivity of VO$_2$, V$_{1-x}$W$_x$O$_2$, and V$_{1-x-y}$W$_x$Ti$_y$O$_2$ thin films. [2] (b) Temperature dependence of sheet resistance of the pure VO$_2$ films and Al$^{3+}$ doped VO$_2$ films on glass substrates. [44]

### 2.3 Optical Properties

The metal-to-insulator transition is also accompanied by an important optical transmittance and reflectance in the infrared region. The optical constants of VO$_2$ thin films below and above the transition temperature have been determined by H. Verleur et al. in 1968.[45] The optical properties of VO$_2$ were studied in the range of 0.25 to 5.0 eV and the optical constants were determined by reflection and transmission measurement on bulk single crystals and thin films. The real and imaginary parts of the dielectric constants at low temperature (300$^\circ$K) and high temperature (355$^\circ$K) were plotted in Figure 2.7. They concluded that the optical properties indicated that the electrons are responsible for the free
carrier absorption at higher temperature. But they have either become trapped in localized level or occupy two completely filled bands at temperatures below 68 °C. An energy gap of 0.6 eV was formed between the highest filled states and the next higher empty conduction band.

Figure 2.7 (a) Real part of dielectric constant for VO₂ at 300 °K, (b) Imaginary part of dielectric constant for VO₂ at 300 °K, (c) Real part of dielectric constant for VO₂ at 355 °K, (d) Imaginary part of dielectric constant for VO₂ at 355 °K. [45]

Recently, N. R. Mlyuka et al. extracted the optical constants, n and k from the measured transmittance and reflectance by fitting data calculated from Fresnel’s equations to experimental ones.[16] As shown in Figure 2.8, the data on n and k are essentially dielectric
like at $T < T_c$ and metallic-like at $T > T_c$. In particular, $k$ increases steeply toward long wavelengths for $T > T_c$.

![Figure 2.8 Optical constants, $n$ and $k$, as a function of wavelength for a 50-nm-thick VO$_2$ film at (a) 22 °C and (b) at 100 °C. [16]](image)

As a result, at the low temperature insulating state, VO$_2$ has higher infrared transmission; and at high temperature metallic state, VO$_2$ has much lower infrared transmission. Figure 2.9 shows the measured transmittance/reflectance and simulation results.
Figure 2.9 Spectral normal transmittance $T$ and near-normal reflectance $R$ for a 90-nm-thick VO$_2$ film (left) at 22 °C and (right) at 100 °C. Curves denote experimental data and symbols show fitted results. [16]

The optical and dielectric constants have also been obtained by spectroscopic ellipsometry.[46] Ellipsometry is an optical technique for surface analysis based on the polarization change of light upon reflection on a flat surface. From Figure 2.10 we can see that the switching of the optical constants $n$ and $k$ as the temperature increases is significantly larger in the near infrared region compared to the visible region.
Figure 2.10 (a) Refractive index, n and (b) extinction coefficient, k of sputtered VO$_2$ thin films at temperatures below and above the phase transition temperature of 70°C determined by UVISEL spectroscopic ellipsometry.[46]

The dielectric constants shown in Figure 2.11 obtained by ellipsometry agree well with the data measured by H. Verleru et al.[45] except the nonexistence of certain optical absorption peaks. They explained the various features in the dielectric constants of VO$_2$ thin films in the context of the Drude model. They observed a Drude-like peak below 1.5eV and a strong peak around 3.15eV from the imaginary dielectric constant of VO$_2$ at the high temperature metallic state. The Drude-like peak becomes strongly suppressed and the peak around 3.15eV shifted towards higher energy as films switched to the low temperature insulating state.
2.4 VO₂ Phase Transition Mechanism

2.4.1 Mott-Hubbard or Peierls

There is a debate about the transition mechanism of VO₂ that has gone on for decades. This debate is over which mechanism dominates, the electron-electron correlations-Mott-Hubbard[30, 31, 33, 47] or lattice instability-Peierls?[4, 12, 28, 29, 34]

The Peierls mechanism refers to instability in the normal Fermi surface of a one-dimensional metal, whereby an energy gap opens up at the Fermi surface due to periodic lattice deformations that change the periodicity of the crystal. Because of the antiferroelectric zigzag-type displacement of the vanadium atoms and the symmetry change, resulting in
lower and raise the bonding and antibonding $\pi$ and $\pi^*$ levels, as well as the $d_{//}$ states splitting. Eventually this would open the optical band gap. Electronic structure calculations, based on density functional theory within the local density approximation were carried out by Wentzcovitch et al. to support the Peierls model.[34] By using the ultrafast pump-probe spectroscopy in the range of 15-1.5fs, continuous-wave Raman and coherent phonon spectroscopy were measured. Cavalleri et al. concluded that atomic arrangement of the rutile (high-temperature) unit cell is necessary for the formation of the metallic phase of VO$_2$, suggesting significant band-like character for the semiconducting phase.[11, 41] Recently, V. Eyert provided a novel view from band theory, demonstrated that band theory as based on density functional, in combination with the recently developed hybrid functions, correctly describing the electronic properties of both the metallic and insulating phase for VO$_2$.[29]

In the Mott-Hubbard model, the transition was based on the model of an array of atomic potentials with one electron per atom and a Coulomb interaction between the electrons. For a sufficiently high electron density the ions cores will be screened and the system will be metallic. For a lattice spacing larger that a critical value, the screening will break down and the system will undergo a first order phase transition to an insulator. This model attributed the coupled metal-insulator and structural transition to the presence of strong electron-electron correlations especially in the $d_{//}$ band rather than to electron lattice interaction. Mott argued that these correlations are efficiently screened by the $\pi^*$ bands in the metallic phase. In the insulating phase, the screening of the $d_{//}$ electrons is diminished since the $\pi^*$ bands experience energetical upshift due to the antiferroelectric displacement of the V atoms. As a consequence, the narrow $d_{//}$ bands at the Fermi energy are susceptible to strong
Coulomb correlations and undergo a Mott transition. This opens the optical band gap.[30] Qazilbash et al. measured the electromagnetic response of a VO$_2$ film on a spatial scale of 20 nm, using scattering scanning near-field infrared microscopy (s-SNIM) in conjunction with far-field infrared spectroscopy.[48] They drew the conclusion that the M1 phase of VO$_2$ should be classified as a “Mott insulator with charge ordering” and that “the classic temperature-induced insulator-to-metal transition in VO$_2$ occurs from the monoclinic insulator [M1 phase] to an incipient strongly correlated metal (SCM) in the form of nanoscale puddles”. [48] J.Cao et al. measured electrical conduction of single crystal VO$_2$ microbeams across the metal-insulator transition.[49] They report a constant threshold resistivity for the insulating phase of VO$_2$ before the insulator-to-metal transition happened. The threshold resistivity is independent of the initial resistivity, transition temperature, and strain of the sample. Different lattice structures also exhibit comparable threshold resistivity. They argued that the constant threshold resistivity suggests that the transition to metallic phase occurs only when a critical free-electron concentration is reached, indicating the electronic mechanism origin of the transition.

### 2.4.2 Thermal Excitation

The simplest way to trigger the metal-to-insulator transition is by increasing the temperature of the material. Figure 2.3 shows the dependence of the resistance of VO$_2$ on temperature. As the temperature increase, the resistance decrease slowly. However, when the temperature reaches critical temperature, the resistance drops abruptly to the lowest resistance, after that there is almost no change with temperature increase. The critical
temperature is different depending on the substrates and growing conditions. It can even be controlled by doping.[2] Hysteresis on electrical resistance is observed upon the heating and the cooling of the samples. The width of the hysteresis is found to be in the range between 1-10°C along different substrate orientation. The ratios of the electrical resistance at 35 °C and 90 °C are as large as $10^5$.\[27\]

### 2.4.3 Photonic Excitation

Photonic excitation in the femtoseconds-to-picoseconds time-scale has been investigated by several groups recently because of the progress in femtosecond time-resolved techniques that enables the observation of the phase transition phenomena.[11–13] In particular, ultrafast time-resolved x-ray diffraction (XRD) and electron diffraction enables direct observation of atomic motion during the phase transition. M.F Becker et.al successfully measured the subpicosecond optical response through the metal-to-insulator transition of VO$_2$ thin films excited by a femtosecond laser.[35] Their results showed that the transition switching time to the near infrared and visible regions is less than a few picoseconds. Cavalleri et.al first directly observed the femtosecond solid-solid phase transition based on ultrafast optical and x-ray diffraction measurements of a photo induced phase transition in VO$_2$.\[11\] They measured the structural and electronic dynamics during an optical driven transition of VO$_2$ by combining the optical and X-Ray measurements. Using time-resolved x-ray diffraction measurements, Masaki Hada et.al demonstrated there was a transition state presented in the insulator to metal phase transition of VO$_2$ which was only accessible by photo excitation.[36] M. Nakajima et.al investigated the ultrafast terahertz
response to the photo excitation for VO₂ thin films using the optical-pump terahertz-probe technique.[37] The experiment was done at room temperature. They observed an ultrafast decrease of the transmittance of the terahertz radiation within 0.7ps after the metal-to-insulator transition was induced by an optical signal, providing another way to detect the phase transition of VO₂ based on the fact that the terahertz pump-probe spectroscopy is purely sensitive to the free carrier response.

Insulating to metallic transition triggered by optical excitation happening within hundreds of femtosecond has been reported. However, there are not many reports on the time scale of switching back from the metallic to insulating phase. More studies need to be carried out on if the optical excitation is reversible and if the transition is on the same time scale for insulating to metallic and metallic to insulating transitions.

2.4.4 Electrical Excitation

Electrical field control of the metal insulator transition of VO₂ is most desirable for fast and reliable electronic devices. Understanding whether electric field or thermal mechanisms are the primary cause of the phase transition is helpful for finding out the theories of the phase transition in VO₂, specifically whether VO₂ is a Mott or Peierls insulator. G Stefanovich et.al has demonstrated an electrical field driven phase transition of VO₂ at room temperature.[6] Based on their device structure, they claimed that the metal-insulator transition in their experiment was initiated by electron injection. They argued that under high electric fields, electron correlation effects contribute to the development of the insulator to metal transition which is a purely electronic Mott–Hubbard transition. B.G Chae et.al
observed the transition switching time of VO₂ as fast as 9ns by applying a voltage pulse to a two terminal device at room temperature. K. Okimura et.al measured the resistance switching during the electrical field driven phase transition of VO₂ planar devices with two terminal electrodes. They reported multiple step resistance switching during the transition and each step occurred within 100ns. The switching time depended on the device size, temperature and frequency of applied pulse voltage. Electrical field induced phase transition of nanoscale VO₂ device junctions has also been reported, which has similar I-V characteristics of macroscopic junctions. However, all those experiments were performed on two terminal devices. It inevitably provides a current flow that may heat the material over the critical temperature when apply a voltage, which makes it difficult to distinguish whether joule heating due to the current or electric field drives the phase transition in experiments on two-terminal VO₂ devices. Recently D. Ruzmetov presented three-terminal devices which are similar to a conventional field effect transistor using VO₂ as channel material. By separating VO₂ and the gate with a dielectric, they potentially overcome the current heating when the electrical field is applied on a two-terminal device. They observed reliable and reversible switching of the channel resistance upon application of a gate voltage when providing an optimal gate dielectric and its interface with VO₂. This effect might be due to the hole injection into a thin region of the VO₂ channel along the interface with the gate dielectric and highly encouraged the utilizing of the metal-to-insulator transition in future electronic devices.
Figure 2.12 Device structure from reference (a) from reference[6], (b) from reference[7], (c) from reference[8], (d) from reference[10].

Table 2.1 Electrical filed triggered devices from some publications, the thermal model calculation was based on the equation from reference[6], $t_{d,\text{min}} = c \rho \Omega_x (T_i - T_o) / VT$, $c = 690 \text{ J kg}^{-1} \text{ K}^{-1}$ and $\rho = 4340 \text{ kg m}^{-3}$, $\Omega_x$ is the volume of the VO$_2$ film per device.

<table>
<thead>
<tr>
<th>Group</th>
<th>Device Area</th>
<th>VO$_2$ thickness</th>
<th>Transition time</th>
<th>Threshold Voltage/Current</th>
<th>Thermal model calculation Transition time</th>
</tr>
</thead>
<tbody>
<tr>
<td>G Stefanovich et.al</td>
<td>0.2mm X (5-10 um)</td>
<td>0.1-1um</td>
<td>1.5ns</td>
<td>6.8v/57uA</td>
<td>900ns</td>
</tr>
<tr>
<td>B.G Chae et.al</td>
<td>3um X 30um</td>
<td>N/A</td>
<td>9ns</td>
<td>7.1V/5.4mA</td>
<td>56ns</td>
</tr>
<tr>
<td>K. Okimura et.al</td>
<td>5um X 1500um</td>
<td>220nm</td>
<td>100ns</td>
<td>2v/10mA</td>
<td>9.9us</td>
</tr>
<tr>
<td>D. Ruzmetov et.al</td>
<td>60um X 60 um</td>
<td>60nm</td>
<td>100s</td>
<td>5V/(no current)</td>
<td></td>
</tr>
</tbody>
</table>
2.5 VO₂ thin films deposition technique

The vanadium oxygen system is very complicated and has a large number of oxide phases. As we can see from Figure 2.13, there are over 20 single or mixed vanadium oxide phases. The existence of these oxides phases makes growing highly crystalline VO₂ thin films extremely challenging. Therefore researchers have been putting a great effort to grow high quality VO₂ thin films with optimal conditions.

![Figure 2.13 Phase diagram for the vanadium-oxygen system. [50]](image)

The magnitude of the resistivity change and the narrowness of the hysteresis are very sensitive to the stoichiometry and the crystalline structure of the VO₂ thin film, these parameters are good indicators of its quality. To obtain optimal quality of VO₂ thin films, various methods have been studied. S.Lu et.al prepared VO₂ thin films on different kinds of
substrates by sol-gel dip-coating method followed by heat treatment under vacuum.[25] Their films have exhibited thermally induced reversible phase transition, and the largest change of transmittance in the near infrared region was 58% with a 15-20 °C wide hysteresis. E.E. Chain has deposited VO₂ thin films onto sapphire substrates by reactive ion-beam sputtering.[26] The deposition was performed in oxygen background while an argon ion beam sputters a vanadium target. Their results showed films properties having a strong dependence on the substrate temperature. Pulsed laser deposition (PLD) has also been successfully employed for growing VO₂ thin films. Excellent electrical transition properties were observed from VO₂ thin films on (0001) and (1010) sapphire substrates.[27] The VO₂ films deposited by PLD system showed a highly oriented crystalline structure without any post annealing. Films quality would depend on the oxygen partial pressure, substrate orientation and temperature. VO₂ thin films have also been achieved by metal-organic chemical vapor deposition and evaporation.[51, 52]
Figure 2.14 (a) Electrical resistance as a function of temperature for VO₂ thin films on sapphire deposited by PLD.[27] (b) Transmittance heating curve and SEM micrograph of a vanadium oxide film deposited at 610 °C by reactive ion-beam sputtering.[26] (c) Infrared transmittance temperature hystereses of VO₂ thin films (about 440nm thick) on monocrystalline silicon (111) substrates.[25] (d) Temperature dependence of transmission for VO₂ thin films prepared by reactive evaporation.[52]
CHAPTER 3

EXPERIMENTAL TECHNIQUES

In this chapter, experimental techniques used to deposit and characterize VO$_2$ thin films, methods and tools used to fabricate VO$_2$ based devices and devices testing setups in this research are introduced. All the VO$_2$ thin films in this work were deposited by the Pulsed Laser Deposition (PLD) system in our lab. The structural characterizations of the thin film were performed by an Atomic Force Microscope. All the electrical and optical properties were measured as a function of temperature on the self-built setups with controlled heating. Devices fabrication processes including photolithography, Reactive Ion Etching (RIE), Plasma Enhanced Chemical Vapor Deposition (PECVD), and E-beam metal deposition are done in our clean room. Radio frequency devices testing was performed in Dr. Floyd's RF lab at NCSU.

3.1 Pulsed Laser Deposition

The synthesizing of thin films by pulsed laser deposition (PLD) is a major part of work in this research. PLD is a thin film deposition technique widely used to deposit high quality thin films of oxides. During the deposition, a high power pulsed laser beam is focused inside a vacuum chamber to vaporize the surface of the target material that is to be deposited. The short and high energy laser pulse interacts with the solid target creating highly energetic
plasma. The vaporized material from the target in the plasma plume form is deposited on the substrates. This process can occur in ultra-high vacuum or in the presence of a background gas, such as oxygen which is commonly used when depositing oxides to modify the properties of the thin films.

PLD is popular for thin films deposition because it has many advantages compared to other techniques. First, the concept is quite simple: a laser beam vaporizes a target surface, producing a film with the same composition as the target. Second many materials can be deposited, including most of the metals and oxides. Third, high quality thin films can be obtained at a fast deposition rate. In addition, multi-layered deposition of different thin films can easily be synthesized using PLD by just switching target during the deposition without breaking the vacuum.

A PLD system usually consists of three primary components: the laser source, the vacuum chamber and optical components including lens, mirrors and shutters to guide the laser beam onto the target. The schematic diagram of the PLD system using in this work is shown in Figure 3.1. Excimer lasers are most commonly used for PLD radiation since it can provide high energy density and the absorption in this wavelength range is very high for most materials. KrF was used as the laser source in this work with a wavelength of 248nm.
The process of PLD can generally be divided into four steps:

1. Laser-target interaction and plasma creation.

2. Dynamic of plasma.

3. Deposition of the ablation target material onto substrate.


During the first step, the strong electrical field generated by the laser light is used to excite free electrons in the target material. The surface of the target is heated up and evaporated due to the thermal energy generated by the free electrons oscillating within the electromagnetic field of the laser light. The whole process occurs within 10 ps of an ns laser pulse. In the second step, the plasma formed in the first step which contains charged and neutral species of atoms and molecules expands towards the substrates. The spatial distribution of
the plume is dependent on the background pressure inside the PLD chamber. The plume is very narrow and forward directed in a high vacuum chamber because almost no scattering occurs due to the background gas. Increasing the background pressure will slow down the high energy species in the expanding plasma plume as well as increasing the happening of scattering. This scattering can influence the stoichiometry and properties of the deposited film. The third step is critical to determining the quality of the deposited films. The energetic species in the plasma plume sputter some of the surface atoms of the substrates and a collision region is formed between the incident flow and the sputtered atoms. Film grows after a thermal equilibrium region is formed. Nucleation and growth of the film on the substrate surface is the fourth step. The films crystalline structure depends on many factors such as laser power, distance between substrates and target, as well as the temperature of the substrate surface and physical properties of the substrates.

In the present work, VO₂ thin films have been pulsed laser deposited using a high-vacuum PLD system from NeoCera. The system consists of an 18” diameter spherical high-vacuum chamber with a quartz laser window. The system is capable of reaching 10⁻⁸ Torr and operating between high-vacuum and up to 100-500mTorr pressure. A Lambda-Physik Compex 201 KrF (248nm) excimer laser is used to ablate polycrystalline targets of the desired composition. Laser power is typically between 150 and 300mJ per 20ns pulse, with a pulse rate of 10Hz. The power density at the target is estimated at ~3J/cm². Substrates are mechanically mounted to an inconel 600 plate that can be heated up to 950°C. The plate is rotated to promote uniform film deposition. Targets are mounted on a carousel and can be rastered and rotated to avoid pitting at the surface. The carousel can hold up to six 1” targets,
or three 2” targets, allowing users to deposit multi-layered film stacks in a single vacuum cycle.

Ablation targets are made from raw powders of different materials. In the case of VO₂, two different targets are made: V₂O₅ and V₂O₃. Both of them are made from V₂O₃ powders. Using a 1” diameter bore with two pistons, the powder is pressed into a 1” diameter disk at up to 5000 psi. After pressing, V₂O₅ target will be obtained by sintering in air at 900°C for 6 hours and V₂O₃ target will be obtained by sintering in nitrogen at 900°C for 6 hours.

3.2 Electrical Measurement

Standard four point probe electrical measurement was performed on VO₂ thin films and devices. This technique is commonly used to measure the semiconductor resistivity. The schematic is shown in Figure 3.2. A constant current is applied through the outer probes while the potential drop across the inner probes is measured. The advantage of this technique is that this system is simple and provides an accurate result for low resistivity samples. It only needs four probes, one volts meter and a current source. For probes with uniform spacing s are placed on an infinite slab material, then the resistivity, ρ is given by

\[ \rho = \frac{\pi}{\ln(2)} \frac{V}{I} = 4.532t \frac{V}{I} \]  

(3.1)

providing s>>t, where t is the thickness of the thin film.
Our setup is shown in Figure 3.3. Four probes are placed on the test sample in a linear fashion. Heaters and temperature monitor are used to control and monitor the temperature of the sample in order to measure the resistivity as a function of the temperature. A Keithley220 programmable current source was used to provide the constant current through the outer probes. A Keithley6517A electrometer was used to measure the voltage across the inner probes. The samples temperature was controlled by an electrical heater which can run up to 100 °C with a temperature monitor. A labview program was implemented to make the measurement automatically. Resistance data was collected from 20 °C to 90 °C with a 1 °C step, with two minutes waiting time between each step in order to give the samples enough time to reach the desired temperature and to be uniformly heated or cooled.
3.3 Optical Measurement

The optical properties characterization of VO₂ thin films and devices is a major part of this dissertation. The transmission and reflection data were collected by an optical configuration shown in Figure 3.4 and 3.5. For the transmission measurement, a tungsten white light was used to generate a collimated light beam. The light beam hit the mirror and reflected normally incident onto the VO₂ film. The light was focused to a very small area by a 20× objective lens in order to pass through the hole of the heater and hit the surface of the sample. The transmission light through the sample was collected by another 20× objectives and coupled into an optical fiber connecting to a spectrometer. For reflection measurement, the light beam hit a half-mirror and part of the light was reflected normally towards the
sample. The reflected light was focused onto the surface of the sample and the light reflected by the sample surface passing through the objective lens and the half-mirror coupled into an optical fiber connecting to the spectrometer. The transmission and reflection light were collected by an Ocean Optics USB 4000 spectrometer (300nm-900nm) or a BWTEK BTC261 infrared spectrometer (900nm-1600nm), while the temperature of the VO₂ film was changed between 20 °C and 90 °C. The device active area was around 1 mm² for device response collection, and the spectra show little variation for different spots on the same film.

![Figure 3.4 Schematic of transmission setup](image)

*Figure 3.4 Schematic of transmission setup*
**Figure 3.5** Schematic of reflection setup

**Figure 3.6** Photograph of the electrical and optical setups
3.4 X-Ray Diffraction

X-ray diffraction (XRD) is a traditional approach to study the crystal and orientation of thin films. It is also used to determine the phase composition of mixtures of crystalline phase materials. When an X-ray beam hits an atom, x-ray photons collide with electrons, and some of them are deflected away from the direction where they originally travel. The diffracted waves from different atoms can interfere with each other and the resulting intensity distribution is strongly modulated by this interaction. Depending on the path difference, constructive or destructive interference will happen. Constructive interference occurs only when Bragg’s law is satisfied.

\[ n\lambda = 2d \sin \theta \]  

where \( n \) is an integer, \( \lambda \) is the wavelength of the X-ray, \( d \) is the distance between atomic layers in a crystal and \( \theta \) is the incident angle of the X-ray beam.

In this study, \( \theta \)-2\( \theta \) scans were used to determine the crystalline phase and orientation of VO\(_2\) thin films. A schematic diagram for X-ray diffractometer is shown in Figure 3.7. In this technique, the thin film surface is at \( \theta \) angle and the detector is at 2\( \theta \) angle to the incident X-ray beam. The x-ray tube is stationary, the sample moves by the angle \( \theta \) and the detector simultaneously moves by the angle 2\( \theta \). In this study, data was collected using Cu-K\(_{\alpha}\) radiation at 1.5418 Å in the 0-2\( \theta \) configuration, with 0.01° steps For possible 2\( \theta \) values where we can have strong diffraction intensities, which are determined by the unit cell dimensions and what kind of atoms and where they are located in the cell. Each material produces a unique X-ray pattern which is the characteristic of its crystalline atomic structure.
By comparing the XRD pattern to the library of known pattern, we are able to identify components and phases present in a sample.

![Diagram of X-Ray diffractometer used for θ-2θ scans.](image)

**Figure 3.7** Schematic diagram of X-Ray diffractometer used for θ-2θ scans.

### 3.5 AFM

Atomic force microscopy (AFM) is a type of scanning probe microscopy with very high resolution on the order of nanometers. It is one of the most popular tools for imaging, measuring, and manipulating the surface of the specimen at the nanoscale. The AFM consists of a cantilever made of silicon or silicon nitride with a sharp tip at its end to scan the surface of the sample. During the measurement, the tip was brought to the sample surface slowly and when the tip is proximity close to the surface, forces between the tip and the surface lead to a deflection of the cantilever. The AFM reconstructs the topographic image of the sample surface by measuring this deflection which indicates local sample height. To achieve this,
most of the AFMs today measure the deflection using a laser spot reflected from the top surface of the cantilever. The reflected laser beam is then collected by an array of position sensitivity photodiodes.

AFM generally has two modes of operation: contact mode and non-contact or tapping mode. In contact mode, the tip touches the surface of the sample, the cantilever is "dragged" over the surface of the sample and the local height of the surface are measured directly using the deflection of the cantilever. In non-contact or tapping mode, the cantilever oscillates up and down at near its resonance frequency with the amplitude of a few nanometers. The oscillation frequency, phase and amplitude are modified due to the interaction of forces acting on the cantilever when the tip comes close to the surface. The characteristics of the sample surface were obtained by collecting this information and processing by the software.

In this study, AFM images of VO₂ thin films on sapphire and ITO glass substrates were taken to study the root-mean-square (RMS) surface roughness of PLD grown films different substrates and thicknesses. These measurements were carried out on a Digital Instruments AFM working in tapping mode.

**Figure 3.8** Photograph of AFM used in this work
3.6 Photolithography

Photolithography is the most commonly used technique to pattern thin films and fabricating micro scale structures. During the photolithography process, the thin films or samples were first coated with photoresist which is UV light sensitive material used to form the pattern. Then the samples with photoresist are exposed to UV light through a mask, which contains the desired patterns you would like to transfer to the samples. After the exposure process, the samples which still have the photoresist on it are submerged into a developer to selectively remove photoresist and hence create the pattern.

Positive and negative photolithography can be selected for different purpose. In a positive photolithography process, the places that have been protected by the mask pattern during exposure will stay on the sample. The photoresist in the rest of the areas will become soluble in the developer. In a negative photolithography process, the area protected by the mask pattern during the exposure will become soluble during the develop process and the rest area will stay on the sample.

In this work we use an MJB 360 mask aligner with a 365nm (i-line) UV light source which has exposure energy of 275mJ/cm². Figure 3.9. AZ5214E photoresist was used as both a positive and negative photoresist. In the positive mode the samples were exposed to the UV light for 10 seconds and developed directly in the developer for 50 seconds. In the negative mode after exposure the samples with mask for 1.5 seconds, they need to be baked at 115 °C for 90 seconds followed by a flood exposure without mask for 90 seconds before the samples were developed for 30 seconds in the developer.
Figure 3.9 Photolithography system used in this work. (a) The mask aligner and the UV light source for photolithography; (b) the spin-coating stage

3.7 Reactive Ion Etching (RIE)

After the pattern was defined by photolithography, the etching process is used to selectively remove the thin films which are not protected by the photoresist and form the desired patterns. Reactive ion etching (RIE) was used to etch VO$_2$ and silicon nitride in this work. RIE system generally consists of a vacuum chamber and a wafer platter placed in the bottom of the chamber. The wafer platter is grounded and electrically isolated from the rest of the chamber. Gas used to create the plasma enters through small inlets of the chamber, and exits to the vacuum pump system. The types and amount of gas used vary depending upon the different materials needed to be etched. CF$_3$ was used to etch silicon nitride and BCl$_3$ was used to etch VO$_2$ in the present work. During the etching process, the gas molecules were ionized by the strong RF electromagnetic field applied to the wafer platter. The negative ions were drifted toward samples which needed to be etched on the wafer platter. The etching happens due to the ions reacting chemically with the materials on the surface of the samples.
and also the ions can knock off some materials when they collide with sample surface. RIE produce very anisotropic etch profiles because of the mostly vertical delivery of reactive ions.

In this work, two RIE etch tools were used. SiN$_x$ layers were etched in an Oxford Plasmalab 80Plus parallel plate RIE system and VO$_2$ layers were etched in a Plasmatherm batchtop RIE tool. The etching rate for SiN$_x$ is 20nm/min with input RF power at 150 W, gas flow at 50 sccm and chamber pressure at 0.4 mTorr. The etching rate for VO$_2$ is 10nm/min with input RF power at 100 W, gas flow at 15 sccm and chamber pressure 35 mTorr.

**Figure 3.10** Photograph of RIE system used in this work (a) Oxford Plasmalab 80Plus parallel plate RIE system (b) Plasmatherm batchtop RIE system

### 3.8 E-beam Evaporation

E-beam evaporation is a process primarily used to deposit metals in the semiconductor fabrication process. The deposition has to occur under high vacuum which is usually in the range of 1x10$^{-5}$Torr. During the deposition process, the substrates and the material to be
deposited are placed into the chamber first. Once the chamber has been pumped down to the required high vacuum, an electron beam is focused on the crucible containing the deposition material until the material begins to evaporate. As the material in the crucible evaporates, the surface of the sample will be coated by the material. The thickness and rate of the deposition were monitored by a deposition meter which utilizes a quartz crystal inside the deposition chamber. Also, a shutter is used to block the evaporated material to be deposited on the substrates until everything is ready for the deposition.

In this study, all the metals including gold, aluminum, nickel, and chrome are deposited by E-beam evaporation. The system we used is Edwards Auto Magnetron Sputtering System which is shown in Figure 3.11.

![Figure 3.11 Edwards Auto Magnetron Sputtering System used in this work.](image)
3.9 Plasma Enhanced Chemical Vapor Deposition (PECVD)

Chemical vapor deposition (CVD) is a chemical process that is often used in the semiconductor industry to produce thin films. During the process, gases are introduced into the deposition chamber and formed the desired film on the surface of the substrate. The chemical reactions take place at the surface of the substrate while the substrates are usually kept at very high temperatures.

As a modification of CVD, Plasma enhanced chemical vapor deposition (PECVD) was developed to allow the deposition to occur at low temperature. PECVD uses a plasma source to provide energy needed for the chemical reaction to occur in addition to a thermal source during the deposition. The plasma which is highly ionized gases including ions, neutral atoms and molecules, and other highly excited species interact with the substrate to complete the chemical vapor deposition (CVD) reactions at a temperature much lower than those needed when only thermal energy is provided. In this work, an Oxford Plasmalab 80Plus parallel plate PECVD system is used to deposit SiNₓ to fabricate the SiNₓ membrane.

Figure 3.12 Oxford Plasmalab 80Plus parallel plate PECVD system used in this work
3.10 Spectroscopic Ellipsometry

Spectroscopic ellipsometry (SE) is a non-destructive measurement technique to obtain optical properties of a sample material by measuring the reflected light waves. It can be used to determine the optical and physical properties of thin-film materials through their spectral responses as well as layer thicknesses through interference phenomena. The technique measures a relative change in polarization and is therefore not dependent on absolute intensity as long as the absolute intensity is sufficient. This makes SE measurement very precise and reproducible.

In this work SE was used to obtain the dielectric constant of VO$_2$ below and above the transition temperature. The experimental setup is shown in Figure 3.13. The light source we used is a Xe lamp. The incoming light is passed through a polarizer, reflected by the sample surface, and passed through a rotating compensator and an analyzer. The reflected light was captured by a spectrometer which is equipped with a photodiode detector. In order to measure the properties of both insulating and metallic VO$_2$, the sample holder is equipped with a small heater which can be heated up to 90°C. The measurement range in our case is 1.5 – 6.0eV. After obtaining the change in the polarization state of a beam of polarized light reflected from the sample, optical model with the aid of regression analysis was used to determine the dielectric constant of the film.
Figure 3.13 Schematic of spectroscopic ellipsometry experiment setup.
CHAPTER 4

VO2 THIN FILM DEPOSITION AND CHARACTERIZATION

In this chapter, we describe how we grow VO2 thin films in our PLD system and the process in which we find the right combination of parameters to deposit highly crystalline VO2 thin films with good insulator to metal transition properties. Two different targets, V2O5 and V2O3 were made to use for pulsed laser deposition. There are many parameters that can be controlled in the PLD system. We mainly focus on substrates temperature and oxygen partial pressure. We successfully deposited high quality VO2 thin films using the V2O3 target with oxygen partial pressure at 20mTorr by keeping the substrates at 800 °C. Films were deposited on different substrates including: sapphire, ITO glass and high temperature corning 7059 glass. X-ray diffraction measurements were used to confirm the crystalline structure of the films. An atomic force microscope was used to study the surface roughness of the films on different substrates. The electrical and optical properties have been investigated. Reversible insulator to metal transition phenomena was observed. The results show the transition temperature, the width of the hysteresis loop, and the amplitude of the transition depend strongly on the substrates, which affect the strain on VO2 films. The VO2 thin films on sapphire show large amplitude transition (4 orders) and narrow hysteresis, about 8 °C. The transition temperature of heating and cooling are 70 °C and 62 °C respectively.
4.1 VO$_2$ Thin Films Deposition

VO$_2$ thin films have been successfully deposited by pulsed laser deposition (PLD) system by several groups. However, the deposition conditions are different for different systems. The work in this dissertation starts with finding the optimal deposition conditions with which we can deposit high quality VO$_2$ thin films. Two types of targets have been tried. The first one is V$_2$O$_5$ target which was made of raw powders of V$_2$O$_3$ and sintered in air at 900°C after pressing. The other one is V$_2$O$_3$ target which was made of raw powders of V$_2$O$_3$ and sintered in nitrogen at 900°C after pressing. During the deposition, the laser power was kept at 200mJ with a pulse rate of 10Hz. The oxygen partial pressure in the chamber varied from 0mT to 20mT and the substrates were kept at high temperature in the range from 750°C to 800°C.

The simplest way to check the quality of VO$_2$ thin film is to examine the characteristic properties of the insulator to metal transition, including the magnitude of the change, the transition temperature and the width of the hysteresis loop. We have done the deposition using V$_2$O$_3$ and V$_2$O$_5$ targets with different oxygen partial pressures and substrate temperatures on sapphire. The results show that all the parameters will affect the quality of the film. The measured resistance versus the temperature for film deposited using V$_2$O$_3$ and V$_2$O$_5$ target at different oxygen partial pressures were plotted in Figure 4.1. According to the results, the films deposited using the V$_2$O$_5$ target at 800 °C with 20mT oxygen partial pressure gives the best insulator to metal transition. In the rest of this dissertation, all the VO$_2$ thin films were deposited with this condition. Different substrates including sapphire, ITO
glass and high temperature corning glass have been used. The deposition rate is around 1nm/300 pulses.

![Figure 4.1](image)

**Figure 4.1** Measured resistance of VO₂ thin film on sapphire as the temperature changes with different oxygen partial pressure. (a) V₂O₃ target (b) V₂O₅ target.
4.2 XRD and AFM Images of VO₂ Thin Films

The crystalline structure of the as-deposited VO₂ thin films was determined by x-ray diffraction (XRD) measurements. The result of a θ–2θ x-ray scan of VO₂ thin films on a (0001) sapphire substrate is shown at Figure 4.2. The film shows four peaks corresponding to (020), (220), (130) and (040) of monoclinic VO₂.[53]

![Figure 4.2 θ–2θ x-ray scan for a VO₂ thin film on sapphire substrate.](image)

**Figure 4.2** θ–2θ x-ray scan for a VO₂ thin film on sapphire substrate.

![Figure 4.3 AFM images of (a) VO₂/sapphire, (b) VO₂/ITO glass, (c) VO₂/SiO₂, the scan area is 2µm×2µm](image)

**Figure 4.3** AFM images of (a) VO₂/sapphire, (b) VO₂/ITO glass, (c) VO₂/SiO₂, the scan area is 2µm×2µm
4.3 Electrical Properties of VO$_2$ Thin Films

The most interesting property of VO$_2$ thin films is the abrupt resistance change around 68°C. We have successfully deposited VO$_2$ thin films with optimal insulating to metallic transition. VO$_2$ thin films were deposited by PLD under the condition mentioned previously with a thickness of 120nm on sapphire. The resistance was measured with the standard four point probe method using the setup mentioned in section 3.2. The result is shown in Figure 4.4. The resistivity has changed up to four orders through the insulating to metallic transition. The thermal hysteresis is about 8°C. The derivative of the resistivity was plotted in Figure 4.5. The transition temperature of heating and cooling are 70°C and 62°C respectively.

![Resistivity of VO$_2$ on sapphire as temperature heating up from 20°C to 90°C and cooling back.](image)

**Figure 4.4** Resistivity of VO$_2$ on sapphire as temperature heating up from 20°C to 90°C and cooling back.
Figure 4.5 Derivative of resistivity over temperature as temperature change.

The substrates effect on VO$_2$ thin films has been studied by several groups.[3, 54] Different characteristic of electronic transition have been shown on different substrates. In the high quality single crystalline form of VO$_2$, the insulating to metallic transition occurs at 68 °C and has a narrow hysteresis in the high quality single crystalline form of VO$_2$. However, the critical temperature, the width of the hysteresis loop, and the amplitude of the transition depend strongly on the film morphology and stoichiometry. Sapphire (Al$_2$O$_3$) has been approved as good candidate substrate for a VO$_2$ deposition[27, 55]. We also deposited VO$_2$ thin films on 200nm thick SiO$_2$ and ATO/ITO glass. The resistivities have been measured and are shown in Figure 4.6.
Figure 4.6 Resistivity of VO$_2$ thin films on different substrates as temperature change.

The VO$_2$ thin films on sapphire showed large amplitude transition and narrow hysteresis, which is attributed to the highly oriented columnar structure and highly stoichiometric composition of the VO$_2$ grains. But for VO$_2$ thin films on SiO$_2$ and ATO/ITO glass, the hysteresis is broader and the transition has lower amplitude. In the case of VO$_2$ on SiO$_2$, the transition temperature during heating up and cooling down are 80 °C and 50 °C respectively, resulting a 30 °C wide hysteresis. Higher resistivity in the metallic phase and lower resistivity in the insulating phase cause the lower amplitude.
Table 4.1 Transition temperature and hysteresis width of VO₂ thin films on different substrates.

<table>
<thead>
<tr>
<th>Substrate</th>
<th>Sapphire</th>
<th>ATO/ITO</th>
<th>SiO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness</td>
<td>120nm</td>
<td>120nm</td>
<td>120nm</td>
</tr>
<tr>
<td>T_c, increase</td>
<td>70°C</td>
<td>72°C</td>
<td>82°C</td>
</tr>
<tr>
<td>T_c, decrease</td>
<td>62°C</td>
<td>58°C</td>
<td>50°C</td>
</tr>
<tr>
<td>Hysteresis width</td>
<td>8°C</td>
<td>14°C</td>
<td>32°C</td>
</tr>
<tr>
<td>Amplitude</td>
<td>10³</td>
<td>10²</td>
<td>10²</td>
</tr>
</tbody>
</table>

4.4 Optical Properties of VO₂ Thin Films

Infrared transmission decrease as VO₂ goes through the insulating to metallic transition is an optical property that has a strong potential to be used in future electronic devices. We have studied the optical transmission and reflectance in the wavelength range from 400nm to 1600nm. Optical measurement setups have been mentioned in section 3.3. VO₂ on sapphire and ITO glass have been studied. The normalized transmission intensity and transmittance are shown in Figure 4.7 and Figure 4.8. For both samples, the transmittance has decreased as much as 30% in the infrared range as the temperature change from 20 °C to 90 °C. In the case of VO₂/ITO glass, the transmittance has almost no change in the visible range 550nm-650nm, but there was nearly 10% decrease for VO₂/sapphire as temperature increase from 20 °C to 90 °C.
Figure 4.7 (a) and (b): Normalized transmission intensity of VO₂/sapphire at 20 °C and 90 °C from 400nm to 1000nm; (c) and (d): Normalized transmission intensity of VO₂/ITO glass at 20 °C and 90 °C from 900nm to 1600nm.
The transmission intensity at 1200nm wavelength has been picked up and plotted as the temperature change during the phase transition. As shown in Figure 4.9, a 7 °C hysteresis has been observed for both VO₂ thin films on sapphire and ITO glass. The transition temperature of VO₂ on ITO glass is 2 °C higher than VO₂ on sapphire which might due to the strain along the ITO surface of the VO₂ films.
Figure 4.9 Transmission Light intensity changes for 1200nm wavelength during the phase transition.

The spectroscopic ellipsometry measurements were taken at 20 °C and 90 °C for VO₂ thin films on different substrates. Complex dielectric constants were extracted from the measurement results. The results are shown in Figure 4.10. All of the results show that both of the real and imaginary parts of the dielectric constant decreases as the temperature passes the transition temperature which confirms the phase change of the VO₂ below and above the critical temperature. The most significant change happens at the low energy frequency range which is consistent with the observed optical transmission change in the long wave length region.
Figure 4.10 Dielectric constant of $\text{VO}_2$ thin film on different substrates extracted from the spectroscopic ellipsometry measurements taken at 20 °C and 90 °C. (a) (b) $\text{VO}_2$/Si. (c) (d) $\text{VO}_2$/Sapphire. (d) (e) $\text{VO}_2$/ITO glass.
4.5 Summary

Highly crystalline structured VO$_2$ thin films were synthesized by pulsed laser deposition processing. With these films the resistivity changes up to 4 orders of magnitude during the insulator to metal transition which happens at 67 °C with an 8 °C wide hysteresis loop. The optical transmission decreases as the temperature increase, especially in the infrared range, the transmission decrease nearly 30%. The dielectric constant extracted from the spectroscopic ellipsometry measurement confirmed the phase change of VO$_2$ thin film below and above the transition temperature.
CHAPTER 5
THERMOCHROMIC EFFECT OF VO₂ THIN FILMS

In this chapter we have investigated metallic thin films on VO₂ and show that the magnitude of the reflected color change in that visible portion of the spectrum as VO₂ undergoes the insulating to metallic phase transition can be controlled by changing the type of metal, the thickness of the metal and by patterning the metal at the nano scale. Three device structures were fabricated with Pulsed Laser Deposition (PLD) and e-beam deposition. The reflection and transmission spectra of these devices are compared at the phase transition region of the VO₂ film. Reflectance of the VO₂ film decreases as we increase the temperature. However, we have seen opposite reflectance change after coating the VO₂ film with a layer of gold as we change the temperature from low to high. Using a chromatic diagram, we found that in comparison with VO₂ thin films that do not have the metal film, the magnitude of the color change is greatly expanded. In this investigation we consider the role of surface plasmons in the metal film and show that in the near infrared, the magnitude of the reflectivity increase for metal coated VO₂ films, but decreases for uncoated VO₂ thin films. This is explained in the context of Fresnel equations and considers the large change in the imaginary part of the dielectric constant as the VO₂ changes state from the insulating to metallic phase. The observed reflection spectra shifts has been reproduced by our calculation using thin-films multilayer models based on the optical transfer matrix method.
5.1 Introduction

Chromic phenomena are the change in color of a material because of the external influence. The most common chromic materials include photochromic material, electrochromic and thermochromic material. Most of these phenomena are reversible. Photochromic material changes color upon exposure to light due to the absorption of electromagnetic radiation. The absorption induces a reversible transformation of the material where two forms of the material have different absorption spectra. The most famous photochromic applications are the color changing lenses for sunglasses. Electrochromic materials are able to change their optical properties as a response to the application of electrical voltage. These materials were considered for application in information display and other applications in emerging technologies. Thermochromic materials are well known for the optical property of being able to change color reversibly with temperature. Thermochromic thin films whose reflectance depends on temperature can be used as coating materials for smart windows or chromic glass. The use of smart windows can save power for heating, air-conditioning and lighting by controlling the heat and light passing through. Vanadium dioxide (VO$_2$) has been one of the most interesting thermochromic materials because of its high infrared transmission in the insulating phase and high infrared reflectivity in the metallic phase. Thermochromics in infrared region have been observed from single VO$_2$ films or VO$_2$ films coated with oxide[15, 16]. In addition to continuous VO$_2$ thin film, interesting nano-structured VO$_2$ and VO$_2$ composite based thermochromic devices have been reported[56, 57].
5.2 Device Fabrication and Measurement

VO₂ thin films were deposited on ITO glass. After the deposition, the samples were cooled down at the deposition oxygen pressure to room temperature. Three devices were fabricated for comparison, as shown in Figure 5.1. The first device was simply a VO₂/ITO/Glass structure. The second device had a layer of e-beam deposited gold (180 nm) on top of the VO₂ layer to form a gold/VO₂/ITO/Glass structure. The third device was fabricated by patterning the gold layer with hexagonal array nanobump patterns for surface plasmon excitation. The 600 nm period nanobump arrays were fabricated by the nanosphere lithography method. In this process, polystyrene nanospheres were self-assembled on top of VO₂ as a template for subsequent gold deposition. The detailed procedure was described in reference.[58]

![Figure 5.1](image)

**Figure 5.1** Schematic of the three devices under test: (a) a VO₂/ITO/Glass structure, (b) a gold/VO₂/ITO/glass structure, and (c) a nanobump array patterned gold/VO₂/ITO/glass structure. A collimated tungsten light beam was normally incident from the glass side and the reflection spectra were measured. The reflected light was mostly from the VO₂/ITO interface for device (a) and from the gold/VO₂ interface for device (b) and (c).
The optical properties of these devices were measured at the temperatures between the insulating and metallic phase. A tungsten light source with 430-900 nm wavelength range was used to provide a collimated light beam normally incident onto the VO$_2$ film. The transmission and reflection light was collected by an Ocean Optics USB 4000 spectrometer, while the temperature of the VO$_2$ film was changed between 30 °C and 80 °C. The device active area was around 1 mm$^2$ for optical response collection, and the spectra show little variation for different spots on the same film. A Peltier cooler was used to control the device temperature, which was monitored by a thermocouple thermometer. The device was placed face down on the cooler, so that the VO$_2$ film was in direct contact with the cooler surface in order to guarantee accurate temperature controlling. For reflective spectra collection, the device responses were measured from the glass substrate side, as shown in Figure 5.1. The devices with gold layers on top of VO$_2$ films had two interfaces that contribute to the reflection. The reflection at the VO$_2$/ITO interface was weaker compared to the reflection at the gold/VO$_2$ interface. Thus, we consider the observed optical effects to mainly be caused by the changes that happened at the gold/VO$_2$ interface.

With only VO$_2$ on top of ITO glass, the optical reflectance is higher at the low temperature insulating state than the high temperature metallic state at wavelengths longer than 630 nm. The reflectance at wavelengths around 630 nm does not change after the temperature increases from 30 °C to 80 °C. This steady point has also been observed after coating the gold layer. Figure 5.2 (b) shows the optical transmittance in the insulating state and metallic state. As expected, the transmittance at longer wavelength beyond 700 nm...
decreases as the temperature increases. No temperature dependence was observed in the visible region.

**Figure 5.2** Spectral reflectance (a) and transmittance (b) at 30 °C and 80°C for VO₂ (120nm)/ITO (130nm) glass

After depositing a layer of gold on top of the VO₂, the reflectance at higher temperatures increased to as much as 2 times of the reflectance at low temperatures at
wavelengths longer than 630nm instead of decreasing as we have seen in Figure 5.2(a), with a steady point where the reflectance stays the same still around 630nm. (Figure 5.3)

![Figure 5.3](image)

**Figure 5.3** Spectral reflectance at 30 °C and 80°C for flat gold (180nm) /VO₂ (90nm)/ITO (130nm) glass.

By coating the VO₂ with a nano bump gold layer, we observed that, as the temperature increases from 30 °C to 80 °C, the optical reflectance at high temperature metallic state increases to nearly 2 times of the reflectance at the low temperature insulating state at wavelengths around 675nm. This is in the visible range which means that this change is more sensitive to human eyes. The steady point moves to 610nm due to the nano-gold surface plasmon tunability. Figure 5.4 (b) shows the optical transmittance at 30 °C and 80°C without significant temperature dependence observed. We have much lower transmittance in the
visible range because of the gold layer. However, due to the patterned gold surface with nano bumps, we observed enhanced transmission at wavelengths around 800nm.

**Figure 5.4** Spectral reflectance (a) and transmittance (b) at 30 °C and 80°C for gold (90nm) with nano bumps /VO$_2$ (90nm)/ITO (130nm) glass.
The color change traces for reflection at the Gold/VO₂ and Aluminum/VO₂ interfaces during the VO₂ phase transition were plotted in the CIE 1931 color space, as shown in Figure 5.5(a). Several metal films, including 50nm and 180nm flat gold, 90nm gold with nanobump and 90nm flat aluminum, were deposited onto flat VO₂ films, respectively. The reflected light spectra were collected with a collimated tungsten light source. Compared to the reflected color of VO₂ without any metal, the reflected color of 50nm gold and 90nm aluminum on top of VO₂ has a larger tunability, which is located at the right to the edge of the color space. The trace for 90nm gold with nanobumps on top of VO₂ is at the middle of the color space with the same tunability of the flat gold/VO₂. All of the films show a yellow color at low temperature when the VO₂ is in the insulating phase, the reflection color moves to blue-green with an increasing in temperature. The traces for heating up and cooling down processes are overlapped in the CIE plot, but the correspondent color points for each temperature are not in the same location. These devices show a hysteresis effect that is commonly seen in VO₂ film during the phase transition. The reflected light intensities for the nanobump patterned gold/VO₂ interface at 675 nm are plotted for the two phase change directions, as shown in Figure 5.5(b). For the insulator to metallic transition, the transition temperature (medium) is at 75 °C and the intensity change slope is 7.9% per degree. The transition temperature for a metallic to insulator transition is at 60 °C with a slope of 6.3% per degree. The average transition temperature is 67.5 °C with a 15 °C hysteresis width.
Figure 5.5 Color change during the VO₂ insulating-metallic phase transition. (a) Reflection color traces in the CIE 1931 color space. 5 traces were plot in the diagram. Upper ends of the traces were at the metallic phase and lower ends were at the insulating phase. (b) Reflection light intensity changes of a nanobump patterned gold/VO₂/ITO structure at 675 nm wavelength during the phase transition.
The different trends of reflection spectra shifts at the NIR region can be explained by the equivalent thin film conductivity changes during the phase transition. The reflection coefficient of a thin film structure sandwiched between two dielectric materials with the refractive indices of $\tilde{n}_1$ and $\tilde{n}_2$ can be expressed as\cite{59}:

$$r_{i2} = \frac{E_{r2}}{E_{i1}} = \frac{\tilde{n}_1 \cos(\theta_i) - \tilde{n}_2 \cos(\theta_i) - y}{\tilde{n}_1 \cos(\theta_i) + \tilde{n}_2 \cos(\theta_i) + y}$$

with $y(\omega) = \sigma(\omega)d / \varepsilon_0 c$, where $\sigma(\omega)$ is the frequency dependent conductivity of the thin film with total thickness of $d$. The devices were made on an ITO/glass substrate ($n_{ITO} = 2.5-4.5$\cite{60, 61}) with air above, so that $n_1 = 3, n_2 = 1$ when light is incident from the glass side, and in the normal incident $\theta_i = \theta_r = 0$. For the VO$_2$ on ITO structure, the NIR reflectance is reduced because the conductivity of the VO$_2$ film increases from almost zero during the insulating to metallic phase transition and the reflectivity $R = r_{i2}^* r_{r2}^*$ has a negative slope this region, as shown in Figure 5.6. The Gold/VO$_2$ structure can be considered an equivalent conductive film with a thickness of $d_{VO_2} + \delta_{gold}$, where $\delta_{gold}$ is the skin depth of gold. This equivalent thin film has a relatively large conductivity due to the presence of the gold film, so that the corresponding point of $y(\omega)$ lies on the right hand side of the curve with a positive slope. During the VO$_2$ insulating to metallic transition, the equivalent conductivity of the gold/VO$_2$ layer becomes larger and thus the reflectivity is increased.
Different metals including Cr, Ti and Ni have been deposited on flat VO$_2$ thin films. The color change traces were plotted in Figure 5.7 and the reflectance of Al/VO$_2$ and Ni/VO$_2$ in the range of 450nm-950nm was shown in Fig5.8. The same changing trend has been observed as we have seen from gold on top of the VO$_2$, the reflectance at high temperature increased at wavelengths longer than a certain wavelength, which is different for different metals, instead of decreasing as without any metal on top of VO$_2$ thin films. In the case of Al/VO$_2$, the steady point is around 640nm, but it is 710nm for Ni/VO$_2$. The color change trace goes across the yellow region from light green to light red for all the metals we have investigated.
**Figure 5.7** Reflection color traces of different metals in the CIE 1931 color space. Upper ends of the traces were at the metallic phase and lower ends were at the insulating phase.

**Figure 5.8** Reflectance of (a) Al/VO$_2$ and (b) Ni/VO$_2$ in the range of 450nm-900nm.
5.3 Reflectance Calculation using Optical Matrix Method

Based on the structure of our devices, we used a double layers model to calculate the reflectance by optical transfer matrix method. The refractive index of VO$_2$ as a function of wavelength was obtained using a modified model developed by Hans Verleur et al.[45]. The refractive index of gold was from reference[62]. The double layer structure model is shown in Figure 5.9. With the light coming through the glass substrate side normally and air on top.

\[
\begin{pmatrix}
   E_{m-1}^+ \\
   E_{m-1}^-
\end{pmatrix}
= \frac{1}{t_m}
\begin{pmatrix}
   e^{i\delta_{m-1}} & r_m e^{i\delta_{m+1}} \\
   r_m e^{-i\delta_{m-1}} & e^{-i\delta_{m+1}}
\end{pmatrix}
\begin{pmatrix}
   E_m^+ \\
   E_m^-
\end{pmatrix}
\]

The $E_m^+$ and $E_m^-$ denote the positive and negative going wave in the m$^{th}$ medium.
We write the coefficients at the $m^{th}$ interface:

$$r_m = g_m + ih_m$$
$$t_m = 1 + g_m + ih_m$$

The complex dielectric constants of $(m-1)^{th}$ and the $m^{th}$ layer are $n_{m-1} - ik_{m-1}$ and $n_m - ik_m$.

For normal incidence

$$g_m = \frac{n_{m-1}^2 + k_{m-1}^2 - n_m^2 - k_m^2}{(n_{m-1} + n_m)^2 + (k_{m-1} + k_m)^2}$$

$$h_m = \frac{2(n_{m-1}k_m - n_mk_{m-1})}{(n_{m-1} + n_m)^2 + (k_{m-1} + k_m)^2}$$

The phase term $e^{i\delta_{m-1}}$ in the $m^{th}$ matrix is written

$$\exp i\delta_{m-1} = \exp \alpha_{m-1} \exp i\gamma_{m-1}$$

with $\alpha_{m-1} = \frac{2\pi}{\lambda} k_{m-1}d_{m-1}$ and $\gamma_{m-1} = \frac{2\pi}{\lambda} n_{m-1}d_{m-1}$, $d_{m-1}$ as the thickness of the $(m-1)^{th}$ layer.

In order to obtain the reflection coefficient we have to know the relation between $E_0^-$ and $E_0^+$

$$
\begin{pmatrix}
E_0^+ \\
E_0^-
\end{pmatrix}
= \begin{pmatrix} C_1 & (C_2) & \ldots & (C_{n+1}) \end{pmatrix}
\begin{pmatrix}
E_{n+1}^+ \\
E_{n+1}^-
\end{pmatrix}
= \frac{1}{t_1t_2\ldots t_{n+1}}

The matrix elements can be written as:

$$C_m = \begin{pmatrix} e^{i\delta_{m-1}} & r_m e^{i\delta_{m-1}} \\ r_m e^{-i\delta_{m-1}} & e^{-i\delta_{m-1}} \end{pmatrix} = \begin{pmatrix} p_m + iq_m & r_m + is_m \\ t_m + iu_m & v_m + i\omega_m \end{pmatrix}$$

and
\[\begin{align*}
    p_m &= e^{\alpha_{m-1}} \cos \gamma_{m-1} \\
    q_m &= e^{\alpha_{m-1}} \sin \gamma_{m-1} \\
    r_m &= e^{\alpha_{m-1}} (g_m \cos \gamma_{m-1} - h_m \sin \gamma_{m-1}) \\
    s_m &= e^{\alpha_{m-1}} (h_m \cos \gamma_{m-1} + g_m \sin \gamma_{m-1}) \\
    t_m &= e^{-\alpha_{m-1}} (g_m \cos \gamma_{m-1} + h_m \sin \gamma_{m-1}) \\
    u_m &= e^{-\alpha_{m-1}} (h_m \cos \gamma_{m-1} - g_m \sin \gamma_{m-1}) \\
    \omega_m &= e^{-\alpha_{m-1}} \cos \gamma_{m-1} \\
    \omega_m &= -e^{-\alpha_{m-1}} \sin \gamma_{m-1}
\end{align*}\]

We express \(E_{n+1}^+\) and \(E_{n+1}^-\) in terms of \(E_0^-\) and \(E_0^+\)

\[
(C_1)(C_2)......(C_{n+1}) = \begin{pmatrix} a & b \\ c & d \end{pmatrix}
\]

\[
\begin{pmatrix} E_0^+ \\ E_0^- \end{pmatrix} = \frac{1}{t_1 t_2 ...... t_{n+1}} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} E_{n+1}^+ \\ E_{n+1}^- \end{pmatrix}
\]

There is no negative-going wave in the \((n+1)\)th medium, so \(E_{n+1}^- = 0\)

We obtain \(\frac{E_0^-}{E_0^+} = \frac{c}{a}\)

The reflectance is given by

\[
R = \frac{(E_0^-)(E_0^-)^*}{(E_0^+)(E_0^+)^*} = \frac{cc^*}{aa^*}
\]
The elements of product matrices are denoted with double suffix notation. The element of \((C_1)(C_2)(C_3)\) are written as:

\[
\begin{pmatrix}
p_{13} + iq_{13} & r_{13} + is_{13} \\
t_{13} + iu_{13} & v_{13} + i\omega_{13}
\end{pmatrix}
\]

In our double layer model which has two absorbing layers on a transparent substrate, the reflectance can be obtained from:

\[
R = \frac{t_{13}^2 + u_{13}^2}{p_{13}^2 + q_{13}^2}
\]

The detailed description of the optical transfer matrix method can be found in reference[63] and Appendix A. The detailed calculation Matlab code is in Appendix B. The calculation was done in the range of 450nm-850nm and the results are shown in Figure 5.10 with comparison to the measurement results. The complex dielectric constant which is a function of the wavelength was the only different parameter between two state calculations. The dielectric constants of insulating and metallic VO\(_2\) thin film were obtained from the modified model derived in reference.[45] The calculation confirms that the observed opposite reflection phenomena is due to the dielectric change of the VO\(_2\) thin film between the insulating and metallic states.
5.4 Summary

The reflection spectrum of a Metal/VO$_2$ thin film structure was studied. The device spectrum shows modulation effect around the VO$_2$ insulating-metallic phase transition temperature and the direction of change is opposite with VO$_2$/ITO film spectrum. The experiment results matched well with the calculation results obtained from a double layer model with the optical transfer matrix method. The presence of the metal films enhances the thermochromic modulation of VO$_2$ films. Reflectivity from the interface between the nano-bump array patterned gold film and VO$_2$ shows a larger modulation effect at red and NIR wavelengths due to a surface plasmon enhanced field at the gold surface. This effect can be utilized to design temperature sensors with optically remote data collection and also for electrically controlled light modulators.
In this chapter, highly oriented crystalline VO$_2$ films were deposited on different substrates by Pulsed Laser Deposition (PLD). Optical switch devices based on the optical transmittance transition characteristics of VO$_2$ thin films have been fabricated. We switch the device from semiconductor phase, which is more transparent to light, to metal phase, which is more reflective to light, by applying a constant current. The transition happens due to the joule heating mechanism. We deposited a thickness of 100nm VO$_2$ films on top of ITO glass with a shallow mask by pulsed laser deposition. A thickness of 200nm ITO was deposited with the same method as the top transparent electrode. The result shows that for a 500um×500um device, the transition happens at 75mA, the device reaches its off state at 80mA, which causes the transmittance to decrease from 50% to 20% in the 900nm-1600nm wavelength range. The hysteresis loop was observed during the measurement. Planer structure devices, such as, two metal contacts connected by a small area of VO$_2$ thin films have also been fabricated. Constant current can be applied through the two metal contacts which causes the temperature to increase due to joule heating. To improve the performance of the optical devices, we fabricated the devices on 200nm thick silicon nitride membranes to decrease the transition time. A 300μm × 300μm area/100nm thick VO$_2$ device takes about 1000μs to reach the fully “on” state. Comparing to the devices fabricated on the normal
substrates, such as sapphire, silicon or glass, the switching speed of the devices on membranes is an order of magnitude faster. Decreasing the area and thickness of VO$_2$ on top of thinner membranes allows kHz bandwidths to be achieved.

**6.1 Introduction**

VO$_2$ has attracted much attention not only because of its famous resistivity change along with the temperature change, but also it’s interesting optical change. The transmission decreases as the temperature increases especially in the infrared wavelength range.[16] This property makes VO$_2$ an interesting material for novel optical applications, such as, optical switches, optical modulators and smart windows which can change its transmission by itself according to the environment. The insulator to metal transition and the associated optical property change can be triggered by an increase in the temperature of the material. VO$_2$ thin films have very high resistance at room temperature, when current flow through the material, it is heated up due to joule heating. Joule heating, also known as ohmic heating, is a process in which an electric current flow through a conductor generates heat. The heat produced is proportional to the square of the current multiplied by the electrical resistance of the wire.

\[ Q \propto I^2 \cdot R \]  \hspace{1cm} (6.1)

Devices based on this mechanism have been fabricated, which can be controlled “electrically” by controlling the current through the devices. The switching time depends on how much heat the whole device needs to reach the critical temperature and the thermal transportation properties.
6.2 Optical switch on sapphire and glass

6.2.1 Device Structure and Fabrication

The device structure is shown in Figure 6.1. The substrate is Corning 7059 glass substrates, 0.04 inch thick, coated with a 200 nm thick transparent conducting indium tin oxide (ITO) layer. Then 100nm VO$_2$ thin film was deposited with a shadow mask by PLD. Another 200nm thick ITO was deposited with the same method as the top transparent electrode. The whole active area of the device is 500µm × 500µm.

![Figure 6.1 Schematic of ITO/VO$_2$/ITO structure device.](image-url)
6.2.2 Device Testing Results

The transmission was measured as we change the current applied through the top and bottom ITO electrodes. A BWTEK BTC261 infrared spectrometer (900nm-1600nm) was used to collect the transmission light from the device. The results are shown in Figure 6.2. As the current increase from 0mA to 90mA, at beginning, the transmission decreases slowly. Once the current was greater than the critical current, the transmission decreases abruptly and stays at constant over 90mA.

![Normalized transmission intensity for the device under heating current of 0mA, 70mA and 90mA in the infrared range.](image)

**Figure 6.2** Normalized transmission intensity for the device under heating current of 0mA, 70mA and 90mA in the infrared range.

The transmission intensity for wavelength=1250nm has been measured as the current changes from 0mA to 100mA, which is shown in Figure 6.3. The critical current magnitude
is around 75mA, where the transmission intensity decreases abruptly as the current continues to increase. 8mA width hysteresis loop was observed as the current decrease back to 0mA from 100mA.

![Normalized transmission intensity for wavelength=1250nm as current change from 0mA to 100mA and back to 0mA.](image)

**Figure 6.3** Normalized transmission intensity for wavelength=1250nm as current change from 0mA to 100mA and back to 0mA.

Smaller joule heating devices have also been investigated. We deposited VO$_2$ films on sapphire and etched the films by RIE with photo resist as the mask. 200nm gold was deposited as contacts after etching, resulting a device with 100µm×400µm area. The structure is shown in Figure 6.4.
I-V measurement has been performed on these devices and is shown in Figure 6.5. When the voltage reaches 7V, the current abruptly jumps indicating the insulating to metallic phase transition. Hysteresis was observed during the voltage decreasing process and the devices reached its insulating phase at 5V.
We measured the transmission of these devices with voltage on and off. The results in Figure 6.6 show the transmittance decrease in the visible range from 500 nm to 800 nm as VO$_2$ changes from insulating state to metallic state.

![Figure 6.6](image)

**Figure 6.6** Normalized transmission intensity at insulating and metallic state for VO$_2$/sapphire from 450 nm to 900 nm.

The switching time has been investigated by connecting our transmission setup to a photo detector and an oscilloscope. We send out a square pulse voltage and collect the transmission response from a photo detector which converts the light signal into voltage. The photo detector is a DET10A Si detector which is from Thorlabs with a 1ns raise time. Because the detector is sensitive to the wavelength range 200nm-1100nm, what we observed is that applying voltage on the device will cause the photo detector voltage to decrease due to
the decreasing transmittance in this range. The falling time for the device to reach the fully “off” state is around 15ms and it takes about 50ms to reach the fully “on” state. The reason for the longer turn on time is that the temperature of the VO₂ thin films has to decrease by transferring the heat to the surrounding environment at room temperature which takes time. Driving voltage at different frequencies has been applied on the device. We can clearly observe the transmission intensity change corresponding to the square driving voltage. But above 30Hz, the transmittance has no response to the driving voltage because the insulating to metallic transition of VO₂ does not occur due to the short time of high voltage.

Figure 6.7 Driving voltages at different frequency and corresponding transmission changes (a) 2Hz, (b) 5Hz, (c) 20Hz, and (d) 40Hz (NCSU)
To increase the performance of the joule heating devices, we fabricated them on 200nm thick SiNₓ membranes. SiNₓ was selected because it can withstand very high temperature (1000°C) which is necessary for VO₂ thin film deposition. In addition, its high transparency makes it a good candidate for optical device application. The first step of the fabrication is to create the SiNₓ membranes. The processing flow is shown in Figure 6.8. The starting substrate is a silicon wafer with 200nm SiNₓ on both sides from the company Strataglas. Next, we do a negative photolithography to select the membrane areas where the SiNₓ will be etched away. These regions were where the silicon nitride membranes were located on the other side of the wafer. The RIE etching process is performed to etch away the selected SiNₓ areas to expose the bulk silicon underneath. An Oxford Plasmalab 80 plus parallel plate RIE system was used with an etching rate of 10nm/min. In order to etch the bulk silicon, a 40% solution of KOH was used for the bulk silicon etching process. The remaining silicon nitride layer acted as a bulk etching mask layer. The KOH bath was kept at 80°C and after 5 hours the bulk silicon area is completely etched away, leaving the SiNₓ due to the high selectivity of etching between SiNₓ and silicon. After obtaining the SiNₓ membranes, VO₂ thin films were deposited on it by PLD with the conditions mentioned in Chapter 4. Then another photolithography and RIE process were performed to etch away the VO₂ which is not on top of SiNₓ membranes. The Plasmatherm batchtop RIE tool is used here with an etching rate of 10nm/min. The last step is to deposit a metal layer by a lift-off process as the electrode contacts. The metal used for this device is gold which is deposited by E-beam deposition with a thickness around 200nm.
Figure 6.8 VO$_2$ based optical modulator on SiN$_x$ fabrication process flow: (a) silicon wafer with SiN$_x$ on both sides. (b) Negative photolithography to select the locations where we would like to have SiN$_x$ membranes. (c) RIE etches away the SiN$_x$ where we have selected. (d) Use the remaining SiN$_x$ as a mask, wet etches away the bulk silicon by KOH, leaving the SiN$_x$ membrane on the other side of the wafer. (e) VO$_2$ thin film deposited by PLD on the side with SiN$_x$ membrane. (f) Positive photolithography to protect the VO$_2$ on top of SiN$_x$ membranes. (g) RIE etches away the other VO$_2$ which is not on top of SiN$_x$ membranes. (h) Gold layer deposited by E-beam deposition as contacts by lift-off process.
The schematic of the membrane device, VO$_2$ (100nm) on 200nm SiN$_x$ membrane with gold contact, is shown in Figure 6.9. Different devices with different size were fabricated for comparison. The area of VO$_2$ on top of SiN$_x$ is 300μm×300μm and 500μm×500μm. We measured the transmission of these devices with voltage on and off. The results in Figure 6.10 show the transmittance decrease in the visible range from 500nm to 800nm as VO$_2$ change from insulating state to metallic state.

![Figure 6.9](image)

**Figure 6.9** Schematic of VO$_2$ based optical modulator on SiN$_x$ membrane. (A) Cross sections view. (b) Top view.

![Figure 6.10](image)

**Figure 6.10** Normalized transmission intensity at insulating and metallic state for VO$_2$/SiN$_x$ from 450nm to 900nm.
The optical properties of these devices were measured at the temperatures between the insulating and metallic phase. A tungsten light source with a 430-900nm wavelength range was used to provide a collimated light beam normally incident onto the VO$_2$ film. The transmission light was collected by an Ocean Optics USB 4000 spectrometer and a BWTEK BTC261 infrared spectrometer. The switching time has been investigated by connecting our transmission setup to a photo detector and an oscilloscope. We send out the square pulse voltage and collect the transmission response from a photo detector which converts the light signal into voltage. The photo detector is a DET10A Si detector which is from Thorlabs with 1ns raise time.

For the devices with an area of $500\mu m \times 500\mu m$, it takes 5ms to switch from insulating state to metallic state. As shown in Figure 6.11 (b) (c). The results also show that for a $300\mu m \times 300\mu m$ device, the transition time is about 3ms. Comparing to the devices fabricated on sapphire, the switching speed is an order of magnitude faster. These devices were fabricated based on the joule heating mechanism. With $500\mu m$ thick sapphire substrates underneath the VO$_2$ films, more heat is needed to heat up the films to its transition temperature, leading to longer switching time. However, same thickness of VO$_2$ films on 200nm thick SiNx membrane requires much less heat to reach the critical temperature, which increase the transition speed of the devices.
Figure 6.11 Transmission changes for different devices at different voltage pulse period, (a) devices on sapphire at 5Hz, (b) devices on SiN$_x$(500µm×500µm), 10ms voltage pulse, (c) devices on SiN$_x$(500µm×500µm), 5ms voltage pulse, (d) devices on SiN$_x$(300µm×300µm), 5ms voltage pulse, (e) devices on SiN$_x$(300µm×300µm), 3ms voltage pulse, (f) devices on SiN$_x$(300µm×300µm), 2ms voltage pulse.
6.4 Summary

The switching activity of VO\(_2\) was studied by fabricating joule heating optical modulators. The switches were controlled by the current flowing through the VO\(_2\) thin film. Temperature increases due to the heat from the current and trigger the phase transition of VO\(_2\). The switching time from insulating to metallic state of the devices can be controlled by changing the area and the thickness of VO\(_2\) thin films. The switching speed of the devices on membrane has been improved an order of magnitude faster comparing to the devices fabricated on the normal substrates.
CHAPTER 7
RADIO FREQUENCY SWITCHES AND RECONFIGURABLE ANTENNAS BASED ON VO₂ THIN FILMS

In this chapter, we discuss the investigation of radio frequency (RF) applications utilizing the reversible insulator to metal transition of VO₂. RF switches which are designed based on a microwave coplanar waveguide (CPW) were fabricated on two types of substrates (C-plane sapphire and high temperature corning 7059 glass), and in both series and shunt configurations. The switches are controlled by thermally triggering the phase transition of VO₂. Both of the simulation and measurement results show that the switches integrated with VO₂ thin films can achieve an average insertion loss as low as 0.7dB and an average isolation over 20-40dB in the frequency of 1GHz – 10GHz.

Reconfigurable dipole antennas were also fabricated on the two types of substrates. Two VO₂ switches are placed on small gaps in both dipole arms. When the temperature overpasses the transition temperature of VO₂, the effective dipole length increases due to the metallic VO₂ bridging the gaps and hence lowers the resonance frequency of the antenna. The measured return losses are presented, showing a frequency shift of up to 50%, which matched well with the simulated results. A small modulation effect was also achieved by adding a short length of VO₂ at the ends of each dipole arm.
The work in this chapter demonstrates that VO₂ has the ability to control the propagation of RF and microwave signals because of its insulator to metal transition and is a very promising candidate for future telecommunication applications.

7.1 Introduction

With the increase in demand for multiband antennas, the realization of reconfigurable antennas has attracted a lot attention in recent years. Reconfigurable antennas which can switch to different working frequencies simplify the design for systems that require complicated wideband and multiband antennas. For a traditional antenna, once the design is finalized, the operational characteristics cannot change during operation. It can be viewed as a device with static and constant characteristics. However, the development of reconfigurable antennas provides the designer more freedom to meet the requirements of modern technology. This can be viewed as a traditional antenna with dynamic radiating structures that can be reconfigured during operation. The most popular method to implement reconfigurable antenna is using high performance RF switches. The RF switch operates simply as either connecting or breaking a conduction path to enable or block the RF signal propagate through. Different switches, including microelectromechanical system (MEMS) switches[64–66], mechanical switches[67], PIN diodes[68] and FET switches[69, 70], have been investigated by many groups. However, most of those RF switches in an antenna design induce additional electrical conduction lines which will affect the performance of the antenna such as resistance, capacitance and inductance which make reconfigurable antenna design more complex. The reversible insulating to metallic phase transition makes VO₂ a potential
material for RF switches. We can use this property to switch on and off an incoming electromagnetic field propagating in a microwave planar waveguide. The VO₂ switches can be activated by controlling the temperature or laser excitation to avoid putting metallic lines around it. We can avoid interfering with radiation patterns when implementing the switches on antennas.

7.2 Introduction to S-Parameters

S-Parameters refer to scattering parameters, which describe the input-output relationship between different ports of electrical networks. S-parameters are represented in matrix form and refer to how the RF signal in a transmission line is affected during the process of propagating. For an RF signal incident on one port, part of the signal reflects back out of that port, some of it scatters and is transmitted out from other ports, and some of it is lost in the form of heat or electromagnetic radiation. S-parameters are complex because both the magnitude and phase of the input signal are changed during the transmission, but the magnitude is of the most interest and is often referred to as the S-Parameters alone. An S-matrix for an N-port system contains N² coefficients. Those coefficients are referred as S-parameters and each one representing a possible input-output path.

The 2-port network S-parameter matrix is the most common used for studying RF devices and electrical networks. As shown in Figure 7.1, for each port, “a” denotes the signal coming into the device or system and “b” denotes the signal going out from the device or system.
In this case the relationship between the incident and reflected signal and the S-parameter matrix is given by:

\[
\begin{pmatrix}
  b_1 \\ b_2
\end{pmatrix} =
\begin{pmatrix}
  S_{11} & S_{12} \\ S_{21} & S_{22}
\end{pmatrix}
\begin{pmatrix}
  a_1 \\ a_2
\end{pmatrix}
\]

(7.1)

S\(_{12}\) represents the power transferred from Port 2 to Port 1. S\(_{21}\) represents the power transferred from Port 1 to Port 2. S\(_{11}\) measures the power reflected from Port 1 when the signal is injected into Port 1. S\(_{22}\) measures the power reflected from Port 2 when the signal is injected into Port 2.

In practice, the most commonly quoted S-Parameters in regards to an RF switch is S\(_{21}\). It measures the transmission efficiency for the on state of the switch and is referred to as insertion loss. Isolation is defined for the off state of the switch and it represents how well the switch blocks the output from the input points. Small insertion loss, which increases the transmission efficiency during the on state and high level of isolation, which blocks RF energy from propagating through during the off state are the most important requirements for
a high quality RF switch. The performance of the switch can be obtained by measuring the contrast between the insertion loss and isolation.

On the other hand, $S_{11}$ is the most useful S-Parameter for an antenna. It represents how much power is reflected from the antenna which is known as the reflection coefficient or return loss. $S_{11}$ is a measure of how much power the antenna "accepts". For instance, if $S_{11}$ is -10 dB, then 10% of the energy a receiver sends is reflected by the antenna. The remainder 90% of the power was accepted by or delivered to the antenna. This accepted power is either radiated or absorbed as losses within the antenna. Because S-Parameters vary as a function of frequency, $S_{11}$ can be used to identify the resonant frequency of the antenna, at which the antenna radiates best.

### 7.3 Coplanar Waveguide Switch

The RF switches in this research were designed based on the coplanar waveguide (CPW) structure. Coplanar waveguide was invented by Cheng P. Wen in 1969.[71] A traditional CPW consists of a strip of thin metallic film deposited on the surface of a dielectric slab with two ground electrodes running adjacent and parallel to the strip on the same surface, as shown in Figure 7.2. One of the most important advantages of CPW is that all the conductors lie on the single side of the same plane. This makes it possible to be fabricated by thin film deposition techniques and other classic semiconductor processes. In addition, it also makes it easier to test with an RF probe station. Another important characteristic of the CPW is that we can control the characteristic impedance $Z_0$ by modifying the ratio of slot width/center conductor width.[72]
The design equations for the coplanar waveguide are[72]:

\[
Z_0 = \frac{30.0\pi K(k')}{\sqrt{\varepsilon_{\text{eff},1} K(k')}} \tag{7.2}
\]

\[
\varepsilon_{\text{eff},1} = \varepsilon_{\text{eff}} - \frac{\varepsilon_{\text{eff}} - 1.0}{(b - a)/2 K(k) + 0.7t K'(k) + 1.0} \tag{7.3}
\]

\[
\varepsilon_{\text{eff}} = 1.0 + \frac{\varepsilon_r - 1.0}{2.0} \frac{K(k')K(k_1)}{K(k)K(k_1)} \tag{7.4}
\]

\[
k_i = \frac{a_i}{b_i} \quad \text{and} \quad k = \frac{a}{b} \tag{7.5}
\]

\[
k_i' = \sqrt{1.0 - k_i^2} \quad \text{and} \quad k' = \sqrt{1.0 - k} \tag{7.6}
\]

\[
k_1 = \frac{\sinh\left(\frac{\pi a_1}{4.0h}\right)}{\sinh\left(\frac{\pi b_1}{4.0h}\right)} \tag{7.7}
\]
\[ k_i' = \sqrt{1.0 - k_i^2} \quad (7.8) \]
\[ a_i = a + \frac{1.25t}{\pi} \left[ 1.0 + \ln\left(\frac{4.0\pi a}{t}\right) \right] \quad (7.9) \]
\[ b_i = b - \frac{1.25t}{\pi} \left[ 1.0 + \ln\left(\frac{4.0\pi a}{t}\right) \right] \quad (7.10) \]

It has been reported that coplanar waveguides have lower loss and dispersion for impedances near 50\(\Omega\).\cite{73} Most of the source impedance of the test equipment is 50\(\Omega\) as well. So based on the equations 7.2-7.10, we design our VO\(_2\) RF switches with dimensions as shown in Figure 7.3. Two configurations of devices, including series and shunt, are fabricated on sapphire (450\(\mu\)m) or high temperature corning 7059 glass (1000\(\mu\)m). The ground electrodes metal stripes are made of aluminum or copper with thicknesses from 0.5\(\mu\)m to 1\(\mu\)m. The width is 400\(\mu\)m and length is 4000\(\mu\)m. The signal line in the center is 100\(\mu\)m wide. The probes which will be used to test these switches have ground-signal-ground structure. The distance between signal and ground is 150\(\mu\)m each. So the parameter “a” and “b” in Figure 7.2 are limited and we finally have the characteristic impedance 68 \(\Omega\). This number is acceptable and will not affect the testing results too much due to the mismatch. For the series configuration, the center metal line was broke into two parts and connected by VO\(_2\) thin films. At room temperature, the switch is in an “off” state. The signal will be blocked by the VO\(_2\) which is at insulating state. After the VO\(_2\) changes to its metallic state, the signal will propagate through it and the switch is in the “on” state. For shunt configuration, the continuous center metal line was connected to the ground electrodes by
VO₂ thin films. At room temperature, the switch is in the “on” state because the signal can propagate through the center signal line without any blocking. However, after the VO₂ changes to its metallic state, the center signal line is grounded by the VO₂ thin films and the RF signal will be lost to ground. No signal will be received by the other end of the switch which will be considered as “off” state. For both configurations, the insulator to metal transition of VO₂ was triggered by heating up the whole device to the critical temperature which is around 68°C.
Figure 7.3 Schematic of VO₂ thin films based RF switch (a) series (b) shunt

- Substrate: Sapphire(450μm) or Glass(1000μm)
- Metal lines(Al:0.5μm, Cu:1μm)
- VO₂(250nm)
7.4 Reconfigurable Dipole Antenna

The basic behavior of all classical electromagnetic phenomena can be fully described in differential form by the Maxwell equations[74]:

\[
\begin{align*}
\nabla \cdot \vec{D} &= \rho \\
\nabla \times \vec{H} &= \vec{J} + \frac{\partial \vec{D}}{\partial t} \\
\n\nabla \cdot \vec{B} &= 0 \\
\n\nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} &= 0
\end{align*}
\]

(7.11)

The conservation of energy, often called Poynting’s theorem states that “the time rate of change of electromagnetic energy within a certain volume, plus the energy flowing out through the boundary surfaces of the volume per unit time, is equal to the negative of the total work done by the fields on the sources within the volume.”[74] The equation representation is:

\[
\frac{\partial \vec{u}}{\partial t} + \nabla \cdot \vec{S} = -\vec{J} \cdot \vec{E}
\]

(7.12)

Where vector \( \vec{S} \) representing energy flow, is called the Poynting vector.

\[
\vec{S} = \vec{E} \times \vec{H}
\]

(7.13)

The total power radiated from a source can be found using Poynting’s theorem as:

\[
P_{\text{rad}} = \oint_{\Delta s} \vec{E} \times \vec{H} \cdot ds
\]

(7.14)

A dipole antenna is the most elementary and commonly used type of antenna. It usually consists of a conductive rod which has been split in the center and fed from a balanced
transmission line that carries equal and oppositely flowing current. As shown in Figure 7.4. The dipole length determines most of the characteristics of the antenna. The electromagnetic field of a dipole can be described by these equations[75]:

\[
E_r = \frac{1}{2\pi \varepsilon} \left( \frac{1}{r^2} + \frac{jk}{r^2} \right) \cos \theta p_0 e^{j(\omega t - kr)} \\
E_\theta = \frac{1}{4\pi \varepsilon} \left( \frac{1}{r^2} \right) \sin \theta p_0 e^{j(\omega t - kr)} \\
H_\phi = \frac{1}{4\pi} \left( \frac{1}{r^2} + \frac{jk}{r} \right) \sin \theta p_0 e^{j(\omega t - kr)} \\
E_\phi = 0 \quad H_r = 0 \quad H_\theta = 0
\] (7.15)

where \( l \) is the length of the conductor carrying charge \( q = q_0 e^{j\omega t} \), \( p_0 = q_0 l \), \( r \) is the distance from the doublet to the point where the fields are evaluated, \( k = 2\pi/\lambda \) is the wavenumber.

\[
\lambda
\]

Figure 7.4 Schematic of dipole antenna

A special case of the dipole antenna, which is called half-wave dipole antenna, has its length equal to a half-wavelength of the frequency of operation. \( l = \lambda/2 \). This makes it possible to modify the antenna’s operating frequency by adjusting the arm length of the dipole. In this research, the design of the reconfigurable antenna is based on this idea. VO₂
thin films have been integrated into the antenna structure. As shown in Figure 7.5 (a), for each of the dipole arm, the discontinuous metal lines which are made of aluminum (500nm) are linked together through a VO₂ (250nm) thin film (1mm × 300µm). At room temperature, VO₂ is in the insulating state so the effective dipole length is L₁ with the corresponding operation frequency f₁. After the temperature reaches over the transition temperature, the metal lines will be connected together through the metallic state VO₂ and the effective dipole length will increase to L₂ with an operation frequency f₂ (f₂<f₁). VO₂ thin films of length 550µm have also been put at the ends of the normal dipole antenna to study the small modulation effect of the operation frequency as shown in Figure 7.5 (b). The effective dipole length in this design is within 20mm to 50mm considering the size of the substrates and the interesting frequency range, which is 1GHz to 10GHz. The testing of the antennas will be performed on a station which can heat up in order to trigger the insulator to metal transition of VO₂.

![Figure 7.5 Schematic of reconfigurable dipole antennas](image)
7.5 Device Fabrication

The RF switches and reconfigurable dipole antennas in this research are all fabricated on sapphire or high temperature corning glass. One reason for this is that VO$_2$ needs to be deposited at 800°C as described in Chapter 4, so the substrates have to be able to stand the high temperature. We also need to consider the films quality due to the lattice mismatch between VO$_2$ and the substrates which will affect the performance of the devices. Another reason is that the dielectric constants of these two substrates are suitable for RF applications. The device fabrication flow is shown in Figure 7.6. First 250nm VO$_2$ thin films are deposited on the substrates. Thicker films are needed to get better signal transmission. Because the substrates are kept at a high temperature, we cannot use photo resist and lift-off processes to make the pattern. The second step is that we do the positive photolithography to protect where we want the VO$_2$ to be left with 1.5 µm photo resist. Then we etch away the other VO$_2$ by Reactive Ion Etching (RIE). We use the Plasmatherm batchtop RIE tool with input RF power at 100 W, BCl$_3$ gas flow at 15 sccm and a chamber pressure of 35 mTorr. The etching rate for VO$_2$ and photo resist is 10nm/min and 45nm/min respectively at this condition. Another negative photolithography step is performed after the VO$_2$ has been etched away. All the metal lines are deposited by E-beam deposition. Aluminum and copper, which are the most commonly used metals in RF applications because of their higher conductivity, are used in this work.
**Figure 7.6** Device fabrication flow (a) VO\textsubscript{2} deposited on substrate by PLD, (b) positive photolithography, (c) RIE etching away VO\textsubscript{2}, (d) negative photolithography, (e) metal deposition by E-beam.

### 7.6 Simulation and Experiment Testing Results

The simulation results of all the devices have been obtained using Sonnet Suites, which is a software development for precise RF models for planar circuits and antennas. It requires a physical description of your circuit, such as the arbitrary layout and material properties for metal and dielectrics, and employs a rigorous Method-of-Moments EM analysis based on Maxwell's equations that includes all parasitic, cross-coupling, enclosure and package resonance effects. The dimensions of the switches and dipole antennas simulated in the software are exactly the same as the devices we fabricated for testing. The insulator to metal transition of VO\textsubscript{2} has been realized by changing the conductivity of the VO\textsubscript{2} thin films, which is obtained from the measurements on the films deposited by our PLD system. The parameters of all the materials used in the simulation are shown in Table 7.1. The simulation structures, which are the same as the device mask layout, are shown in Figure 7.7.
Table 7.1 Materials parameters used in the simulation

<table>
<thead>
<tr>
<th>Materials</th>
<th>Thickness</th>
<th>Conductivity (S/m)</th>
<th>Dielectric Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>VO₂ (Insulating)</td>
<td>250nm</td>
<td>250</td>
<td>NA</td>
</tr>
<tr>
<td>VO₂ (Metallic)</td>
<td>250nm</td>
<td>$5 \times 10^5$</td>
<td>NA</td>
</tr>
<tr>
<td>Aluminum (Al)</td>
<td>0.5μm</td>
<td>$3.72 \times 10^7$</td>
<td>NA</td>
</tr>
<tr>
<td>Copper (Cu)</td>
<td>1μm</td>
<td>$5.98 \times 10^7$</td>
<td>NA</td>
</tr>
<tr>
<td>Sapphire</td>
<td>450μm</td>
<td>NA</td>
<td>9.3</td>
</tr>
<tr>
<td>Glass</td>
<td>1000μm</td>
<td>NA</td>
<td>5.84</td>
</tr>
</tbody>
</table>
Figure 7.7 (a) Schematic of dipole antennas and probe pads for simulation (b) schematic of RF switches for simulation (c) Simulation structure

Figure 7.8 shows the simulation results for the RF switches of both configurations. The substrates are sapphire and the metal lines are aluminum (500nm) with VO$_2$ (250nm) thin films in the center (100µm x 100µm). The transmission signals $S_{21}$ are plotted from 1GHz to 10GHz for the switches with VO$_2$ at the insulating and metallic state respectively. For series configuration, as shown in Figure 7.8 (a), the switch is off when the VO$_2$ is at the insulating state because the RF signal is blocked by the insulating VO$_2$ thin films. The
isolation is about 35dB on average in the range from 1GHz to 10GHz. The insertion loss is within 1dB when the switch is on after the VO₂ change to metallic with the signal propagating through it to the output end. For the shunt configuration, Figure 7.8 (b), the switch is on when the VO₂ is in the insulating state because the continuous center metal line provides a channel for the RF signal to transmit. The insertion loss is within 1.3dB which is larger than the series configuration due to the additional VO₂ thin films. When the VO₂ changes to a metallic state, the signal transmission line is shorted to the ground by the metallic VO₂. The switch will shut off with isolation to about 23dB on average. Simulation results show that VO₂ is a very good candidate for controlling RF signal propagation and the device structure and dimensions would also give us decent experimental results.

Figure 7.8 Simulation results of the transmission signal when VO₂ is at insulating and metallic state (a) series configuration switch, (b) shunt configurations switch.

Reconfigurable dipole antennas have also been simulated. The simulated return loss S₁₁ for the dipole antenna with insulating and metallic VO₂ is plotted in Figure 7.9, (a) is on corning 7059 glass (b) is on sapphire. The VO₂ thin films connecting the two parts of the
dipole are effectively RF switches. When the VO₂ is at an insulating state, which indicates that both of the switches are off, the dipole length is 16mm. When the VO₂ is in the metallic state, the dipole length increases to 36mm because the metallic VO₂ links the two parts of the dipole on each arm together and hence reduces the resonance frequency. For the dipole on glass, the resonance frequency switches from 3.6GHz to 2.0GHz as the VO₂ change from insulating state to metallic state. The resonance frequency switches from 3.2GHz to 1.8GHz for the dipole on sapphire with different VO₂ state. The size of the gap where is VO₂ thin films is chosen as 300µm. Smaller distance will not provide the reconfigurable effects and return loss will decrease with larger distance due to the lower conductivity of metallic VO₂ compared to aluminum or copper. Simulation results show that VO₂ thin films based reconfigurable dipole antennas present very good application potential.

Figure 7.9 Simulated changes in return loss S₁₁ for dipole antenna with insulating and metallic state VO₂ (a) glass substrate (b) sapphire substrate
The measurement of the RF switches and reconfigurable dipole antennas were performed using a RF probe station from Cascade Microtech (Figure 7.10 a) with an E8361C PNA Microwave Network Analyzer from Agilent Technologies (Figure 7.10 b). The wafer stage of the probe station can be heated up to several hundred degrees which makes it possible to test the devices with VO$_2$ at insulating and metallic states. Before taking the S-Parameters of all the devices, calibration is required to eliminate the effect of the cable and other system noise.

**Figure 7.10** (a) RF probe station from Cascade Microtech. (b) E8361C PNA Microwave Network Analyzer from Agilent Technologies.
The measured $S_{21}$ parameter, which is the transmission of the RF signal over the switch, is plotted with the simulation results for comparison. Figure 7.11 shows the results for switches fabricated on sapphire with (a) 1µm thick copper line and (b) 0.5µm thick aluminum line, as the temperature is changed from 20°C to 90°C. For the series configuration (Figure 7.11 a), during the off state when VO$_2$ is insulating, the isolation is about 18dB which mean that less than 2% of the signal has transmitted. When the temperature overpasses the transition temperature, the signal will be able to propagate through the metallic VO$_2$. The average insertion loss is about 1dB when the switch is on. The same measurements have been under taken for the shunt configuration switch. As shown in Figure 7.11 (b), at room temperature, when the switch is on, the average insertion loss is around 0.7dB, which has not been affected too much by the additional insulating VO$_2$. At high temperature, the metallic VO$_2$ shorts the signal line to the ground. The switch is off with an average isolation around 21dB. The same investigations have been made on switches fabricated on high temperature corning 7059 glass in both configurations (Figure 7.12). The insertion loss is 4dB and 0.9dB for the series and shunt configurations respectively when the switch is on. The corresponding isolation is 41dB and 15.8dB when the switch is off. Both of the measurement and simulation results confirm the potential of using the reversible insulator to metal transition of VO$_2$ in the area of RF applications.
Figure 7.11 Measurement and simulation $S_{21}$ results for switch fabricated on sapphire (a) series configuration with 1µm thick copper line (b) shunt with 0.5µm aluminum line
Figure 7.12 Measurement and simulation $S_{21}$ results for switch fabricated on high temperature corning 7059 glass with 0.5µm aluminum line (a) series (b) shunt
The measured return loss $S_{11}$ signal which indicates the resonance frequency of the antenna is plotted as the temperature changes from 20°C to 90°C. Figure 7.13 shows the results for the VO$_2$ based reconfigurable dipole antenna fabricated on high temperature Corning 7059 glass ($L_1$=16mm, $L_2$=36mm). Compared to the simulation results, the measured resonant frequency is at the same position for both insulating and metallic VO$_2$ states with a 44% shift from 3.6GHz to 2.0GHz. Similar results were obtained from the dipole antennas fabricated on sapphire ($L_1$=12mm, $L_2$=28mm). The measured resonance frequency shifts from 3.5GHz to 1.9GHZ. The resonance frequency shifts to low frequency for both insulating and metallic VO$_2$ states compared to the simulation results which shifts from 3.8GHz to 2.2GHz. But the change of the frequency between the two states is the same, which is 1.8GHz.

We have taken further studies to find the reason why the bandwidth of the measurement results is larger than that of simulation results. The bandwidth of the antenna can be characterized by the $Q$ factor called the quality factor. The relationship between the bandwidth and $Q$ factor is:

$$\Delta f = \frac{f_c}{Q}$$

(7.16)

where $f_c$ is the resonance frequency, $\Delta f$ is the bandwidth.

$Q$ is defined in terms of the ratio of the energy stored in the reactive field to the energy lost and radiated.

$$Q = 2\pi f_c \frac{\text{Energy Stored}}{\text{Energy Lost}}$$

(7.17)
The stored energy is the sum of energies stored in the equivalent inductors and capacitors of the circuit. The lost energy is the energy lost due to the resistance which includes the loss resistance and radiation resistance. During the simulation, the conductivity of aluminum we used is $3.72 \times 10^7$ S/m, which is normally used in most of the simulation software. However, the aluminum in this study is a 500nm think film. The effective conductivity is smaller than that used in the simulation. It is $2.24 \times 10^6$ S/m in our case. The lower conductivity of the E-beam deposited aluminum increases the lost energy and hence decreases the Q factor which leads to a wider bandwidth.

To improve the performance of the reconfigurable dipole antenna, we fabricated another sets of devices with 1µm thick nickel as the metal lines. The band width decreased as expected because of the thicker metal lines and larger conductivity of nickel decrease the lost energy. The results are shown in Figure 7.15 and Figure 7.16. Compared to the antennas fabricated on glasses, the resonant frequency of the antenna fabricated on sapphire shifted to a lower frequency. The reason is that the devices were placed on a sample stage which is made of metal. During the measurement, the metal lines on the antenna, the substrate and the sample stage construct a capacitor which will affect the performance of the antenna. The dielectric constant of sapphire is larger than that of glass and the thickness is smaller which make the effective capacitance greater and hence the effect on the performance is more obvious during the measurement. By putting a layer of metal underneath the sapphire substrate during the simulation, we obtained the results with the same resonant frequency as the experimental results (Figure 7.17).
Figure 7.13 Measurement and simulation return loss results for dipole antennas on high temperature corning 7059 glass with a 0.5µm aluminum line (a) low temperature insulating state (b) high temperature metallic state
Figure 7.14 Measurement and simulation return loss results for dipole antennas on sapphire with a 0.5µm aluminum line (a) low temperature insulating state (b) high temperature metallic state
Figure 7.15 Measurement and simulation return loss results for dipole antennas on high temperature corning 7059 glass with a 1µm nickel line (a) low temperature insulating state (b) high temperature metallic state
Figure 7.16 Measurement and simulation return loss results for dipole antennas on sapphire with a 1µm nickel line (a) low temperature insulating state (b) high temperature metallic state
Figure 7.17 Measurement and improved simulation return loss results for dipole antennas on sapphire with a 1µm nickel line (a) low temperature insulating state (b) high temperature metallic state
Small modulation effect has also been investigated. The dipole antenna with 550µm VO$_2$ on each end of the dipole arm was fabricated on high temperature corning 7059 glass. The measured return loss $S_{11}$ is plotted with simulation results as the temperature changes from 20°C to 90°C in Figure 7.17. Although the bandwidth is larger due to the resistance loss compared to the simulation results, the change of the measured frequency is the same as the simulation results between insulating and metallic VO$_2$ states, which is 60MHz. For measurement, the resonance frequency shifts from 2.31GHz to 2.25GHz and it shifts from 2.43GHz to 2.37GHz in the simulation.

The results of this work highly suggest that VO$_2$ thin films based devices can be used in more complex RF designs. Utilizing the reversible insulating to metallic transition of VO$_2$, these devices demonstrate very good potential for future microwave and radio frequency research and applications.

![Figure 7.18](image.png)

**Figure 7.18** Measurement and simulation return loss results for dipole antennas on glass with 550µm VO$_2$ at each end of the dipole arm.
7.7 Summary

Radio frequency (RF) switches and reconfigurable dipole antennas integrated with VO₂ thin films were designed, fabricated and tested. Both of the series and shunt configuration switches provided low insertion loss and high isolation. The reconfigurable antenna was realized by utilizing the insulator to metal transition of VO₂. The resonance frequency of the antenna shifted due to the phase change of the VO₂ which changed the effective dipole length. The results in this work demonstrated the promising application potential of VO₂ in a more complex and advanced RF system.
CHAPTER 8
CONCLUSION AND SUGGESTIONS FOR FUTURE WORK

8.1 Conclusion

The focus of the research presented in this dissertation is to deposit vanadium dioxide (VO₂) thin film by the pulsed laser deposition processes for thin film electrical and optical devices applications and to demonstrate the fast switching ability of the VO₂ by presenting the performances of various devices integrated with VO₂ thin films, which utilizes its insulator to metal transition.

VO₂ thin films with larger magnitude resistivity and narrow hysteresis were synthesized by a pulsed laser deposition process. Films were characterized by different techniques. X-ray diffraction results and the measured electrical and optical properties show the highly crystalline structure of VO₂. The change of the dielectric constant extracted from spectroscopic ellipsometry measurements confirmed VO₂ that undergoes a phase change from insulator to metal transition as the temperature overpasses the transition temperature.

Thermochromic effect of VO₂ was also studied in this work. We expanded the thermochromic color change by putting metal layers on top of the VO₂ film. We showed that the magnitude of the reflectivity increases for metal coated VO₂ films, but decreases for uncoated VO₂ thin films in the near infrared. The measured opposite optical reflectance change matches well with our calculation results from a double layer model using the optical
transfer matrix method. We also demonstrated that the magnitude of the reflected color change due to the insulator to metal transition of VO$_2$ can be controlled by changing the type of metal, the thickness of the metal and by patterning the metal at the nano scale.

We improved the switching response of VO$_2$ thin films by depositing the film on silicon nitride membranes. Joule heating devices which switch from semiconductor phase to metal phase by applying a constant voltage across two metal contacts were fabricated on different substrates. The switching speed of the devices on the membranes is an order of magnitude faster compared to the devices fabricated on the normal substrates, such as sapphire, silicon or glass.

We designed and fabricated radio frequency (RF) switches and reconfigurable dipole antennas using the insulator to metal transition of VO$_2$. We presented the high contrast between the insertion loss and isolation for both series and shunt configuration switches. We also demonstrated the shift of the resonant frequency by measuring the return loss of the dipole antenna during the phase transition of VO$_2$. 


8.2 Suggestions for Future Work

1. Room Temperature VO₂ Thin Films Deposition

Having investigated VO₂ thin film based applications, it will be helpful and interesting to find a condition for growing VO₂ thin films at room temperature. High temperature deposition has several limitations such as the fact that we cannot use photo resist to pattern the feature and only substrates that can stand high temperature can be used. It is necessary to find a condition that we can deposit optimal VO₂ thin films at room temperature with or without post processing. The PLD system has several variables to control, oxygen partial pressure, substrate temperature, laser power and target combination. By varying these parameters, we end up with different thin films. Experiments should start with different targets, such as V₂O₅ and V₂O₃, by varying oxygen partial pressure at room temperature or annealing films in oxygen or nitrogen at different temperatures.

Unfortunately in experiment we performed with this type of structure we did not see conclusive results.

2. Electrical Field Triggered Devices

Electrical field triggered VO₂ based devices are a promising application. To eliminate the current heating effect, VO₂ thin films should be put between two dielectrics and voltage should be applied through the top and bottom contacts. One of the candidate device structures is shown in Figure 8.1
The devices will be based on high temperature deposition of VO₂ thin films. The proposed process includes photolithography, RIE, PECVD and E-beam deposition. As mentioned in reference[10], the dielectric and its interface with VO₂ will largely affect the performance of the devices. Different dielectric including SiO₂, Si₃N₄ and Al₂O₃ could be deposited on devices with varied sizes. As a high voltage is applied to the devices, one can measure the resistance of the VO₂ film to confirm if the transition happens.

3. **VO₂ based Memory Devices**

Because of the different transition temperature for heating and cooling through the transition, hysteresis could make VO₂ a proper candidate for memory device applications. Memory resistors or optical switches based on VO₂ thin films are proposed for fabrication. VO₂ will become metallic with low infrared transmission.
above the transition temperature or the turn on current. Because of the hysteresis it will stay at the metallic state even after the excitation condition is removed.

Memory device based on an indium gallium zinc oxide (IGZO) thin film transistor has been developed by incorporating platinum nanoparticles in the gate dielectric stack[76]. VO₂ thin films could be used instead of platinum nanoparticles between the gate dielectric and channel layer. The proposed device structure is shown in Figure 8.2. One would expect to observe a corresponding hysteresis between the transistor’s on and off state because of the transition hysteresis of VO₂.

![Proposed VO₂/IGZO based memory device structure](image)

Figure 8.2 Proposed VO₂/IGZO based memory device structure

4. **Terahertz Transmission Switches**

The thickness of the VO₂ thin films typical is much smaller than the effective Terahertz (THz) frequency’s skin depth, which makes the films still very transparent at these wavelengths even as the VO₂ film is in a metallic state. However, by
combining sub-wavelength apertures or nano-slot structures, the THz wave switching capability of VO$_2$ thin films has been highly improved. One could add those patterns, which are also name nanoresonators, in a gold layer on top of the VO$_2$ thin film. The resonance frequency is determined by the resonator length, periodicities of the pattern arrays, and the refractive index of substrates. When the VO$_2$ film is in an insulating state, it is transparent to the incoming terahertz waves at resonance because of the nanoresonators. But when the film undergoes phase transition to metallic state, the nanoresonator structures no longer work and therefore simple reflection occurs throughout the metallic part of the sample, resulting in a very small transmittance. The proposed structures are shown in Figure 8.3

![Figure 8.3 Proposed THz wave transmission switches with subwavelength apertures (a) and nano-slots (b) in a gold layer on top of VO$_2$ thin films](image)
5. **Reconfigurable patch antenna and advanced RF system**

Reconfigurable patch antennas can be fabricated with VO$_2$ to construct different radiation patterns utilizing in the insulator to metal transition of VO$_2$. The patched antenna, as shown in Figure 8.4, would have multiple RF switches and those switches would be activated by a laser to avoid putting metallic lines around it and one would not interfere with radiation patterns when implementing the switches on antennas. By turning on and off the switches at different positions, we are expecting different radiation patterns.

![Figure 8.4 Schematic of reconfigurable patch antennas](image-url)
REFERENCES


APPENDICES
Appendix A: Matrix Method for Evaluating Reflectance

This section introduces the matrix method for reflectance calculation used in Chapter 5. The notation, calculation equations and the derived steps are all from O.S.Heavens’s Optical Properties of Solid Films.[63]

Consider a layer of thin film with index of \( n_1 \) between media of indices \( n_0 \) and \( n_2 \). The amplitude of the incident wave vector is \( E_0^+ \) and the reflected wave is \( E_0^- \). Inside the film, all the positive-going waves, including the multiple times reflections, sum to \( E_1^+ \) and those of the negative-going to \( E_1^- \). In the third medium, the negative-going wave is zero and we only have \( E_2^+ \). In the following calculations, the z-axis is chosen normal to the plane of the film and the xz plane is chosen as the plane of the incidence. The origin of the co-ordinates is set to the point of the incidence in the \( n_0/n_1 \) surface.

The phase factors of the waves in the three media are given:

\[
\exp i(\omega t - \frac{2\pi n_{0,x} \sin \varphi_0}{\lambda} \pm \frac{2\pi n_{0,z} \cos \varphi_0}{\lambda}) \quad (\text{medium } n_0)
\]

\[
\exp i(\omega t - \frac{2\pi n_{1,x} \sin \varphi_1}{\lambda} \pm \frac{2\pi n_{1,z} \cos \varphi_1}{\lambda}) \quad (\text{medium } n_1)
\]

\[
\exp i(\omega t - \frac{2\pi n_{2,x} \sin \varphi_2}{\lambda} - \frac{2\pi n_{2,z} \cos \varphi_2}{\lambda}) \quad (\text{medium } n_2)
\]

After applying the boundary conditions at each of the interfaces, the z-dependent parts of the x- and y- components of the electric and magnetic vectors can be written with as:
\[ E_{0x} = (E_{0p}^+ e^{-i\chi_0} + E_{0p}^- e^{+i\chi_0}) \cos \varphi_0 \]
\[ E_{0y} = E_{0s}^+ e^{-i\chi_0} + E_{0s}^- e^{+i\chi_0} \]
\[ H_{0x} = (-E_{0s}^+ e^{-i\chi_0} + E_{0s}^- e^{+i\chi_0}) n_0 \cos \varphi_0 \]
\[ H_{0y} = E_{0p}^+ e^{-i\chi_0} - E_{0p}^- e^{+i\chi_0}) n_0 \]
\[ E_{1x} = (E_{1p}^+ e^{-i\chi_1} + E_{1p}^- e^{+i\chi_1}) \cos \varphi_1 \]
\[ E_{1y} = E_{1s}^+ e^{-i\chi_1} + E_{1s}^- e^{+i\chi_1} \]
\[ H_{1x} = (-E_{1s}^+ e^{-i\chi_1} + E_{1s}^- e^{+i\chi_1}) n_1 \cos \varphi_1 \]
\[ H_{1y} = E_{1p}^+ e^{-i\chi_1} - E_{1p}^- e^{+i\chi_1}) n_1 \]
\[ E_{2x} = E_{2p}^+ e^{-i\chi_2} \cos \varphi_2 \]
\[ E_{2y} = E_{2s}^+ e^{-i\chi_2} \]
\[ H_{2x} = -E_{2s}^+ e^{-i\chi_2} n_2 \cos \varphi_2 \]
\[ H_{2y} = E_{2p}^+ e^{-i\chi_2} n_2 \]

Where \( \chi_m = \frac{(2\pi n_m \cos \varphi_m)}{\lambda} \)

For the \( m^{th} \) layer in an \( n \) layers system, the \( x \) and \( y \) components are \( E \) and \( H \):

\[ E_{0x} = (E_{0p}^+ e^{-i\chi_0} + E_{0p}^- e^{+i\chi_0}) \cos \varphi_0 \]
\[ E_{0y} = E_{0s}^+ e^{-i\chi_0} + E_{0s}^- e^{+i\chi_0} \]
\[ H_{0x} = (-E_{0s}^+ e^{-i\chi_0} + E_{0s}^- e^{+i\chi_0}) n_0 \cos \varphi_0 \]
\[ H_{0y} = E_{0p}^+ e^{-i\chi_0} - E_{0p}^- e^{+i\chi_0}) n_0 \]

If the thickness of the \( i^{th} \) layer is \( d_i \), then writing \( c_m = \sum_{i=1}^{m-1} d_i \), for the \( m^{th} \) surface,

separating the \( (m-1)^{th} \) and the \( m^{th} \) layers.
For $p$ component:

\[
\left( E_{m-1,p}^+ e^{-i\chi_{m-1}c_m} + E_{m-1,p}^- e^{+i\chi_{m-1}c_m} \right) \cos \varphi_{m-1} = \left( E_{m,p}^+ e^{-i\chi_m c_m} + E_{m,p}^- e^{+i\chi_m c_m} \right) \cos \varphi_m
\]

\[
n_{m-1}(E_{m-1,p}^+ e^{-i\chi_{m-1}c_m} + E_{m-1,p}^- e^{+i\chi_{m-1}c_m}) \cos \varphi_{m-1} = n_m(E_{m,p}^+ e^{-i\chi_m c_m} + E_{m,p}^- e^{+i\chi_m c_m}) \cos \varphi_m
\]

For $s$ component:

\[
E_{m-1,s}^+ e^{-i\chi_{m-1}c_m} + E_{m-1,s}^- e^{+i\chi_{m-1}c_m} = E_{m,s}^+ e^{-i\chi_m c_m} + E_{m,s}^- e^{+i\chi_m c_m}
\]

\[
n_{m-1}(-E_{m-1,s}^+ e^{-i\chi_{m-1}c_m} + E_{m-1,s}^- e^{+i\chi_{m-1}c_m}) \cos \varphi_{m-1} = n_m(-E_{m,s}^+ e^{-i\chi_m c_m} + E_{m,s}^- e^{+i\chi_m c_m}) \cos \varphi_m
\]

Given

\[
\frac{E_{m-1,p}^-}{E_{m-1,p}^+} = r_{m,p} \quad \quad \quad \frac{E_{m-1,s}^-}{E_{m-1,s}^+} = r_{m,s}
\]

\[
\frac{E_{m,p}^+}{E_{m-1,p}^+} = t_{m,p} \quad \quad \quad \frac{E_{m,s}^+}{E_{m-1,s}^+} = t_{m,s}
\]

We obtain

\[
E_{m-1}^+ e^{-i\chi_{m-1}c_m} = (E_{m}^+ e^{-i\chi_m c_m} + r_m E_{m}^- e^{+i\chi_m c_m}) / t_m
\]

\[
E_{m-1}^- e^{+i\chi_{m-1}c_m} = (r_m E_{m}^+ e^{-i\chi_m c_m} + E_{m}^- e^{+i\chi_m c_m}) / t_m
\]

By writing $\delta_m = \chi_m c_m$, then

\[
E_{m-1}^+ = (e^{i\delta_{m-1}} E_{m}^+ + r_m e^{i\delta_{m-1}} E_{m}^-) / t_m
\]

\[
E_{m-1}^- e^{+i\chi_{m-1}c_m} = (r_m e^{-i\delta_{m-1}} E_{m}^+ + e^{-i\delta_{m-1}} E_{m}^-) / t_m
\]
This relation can be written in matrix form:

\[
\begin{pmatrix}
E_{m-1}^+ \\
E_{m-1}^-
\end{pmatrix} = \frac{1}{t_m} \begin{pmatrix}
e^{i\delta_{m-1}} & r_m e^{i\delta_{m-1}} \\
r_m e^{-i\delta_{m-1}} & e^{-i\delta_{m-1}}
\end{pmatrix} \begin{pmatrix}
E_m^+ \\
E_m^-
\end{pmatrix}
\]

In order to obtain the reflection and transmission coefficient we have to know the relation between \(E_0^-\) and \(E_0^+, E_{n+1}^+\) and \(E_0^-\)

\[
\begin{pmatrix}
E_0^+ \\
E_0^-
\end{pmatrix} = \frac{(C_1)(C_2)\ldots(C_{n+1})}{t_1 t_2 \ldots t_{n+1}} \begin{pmatrix}
E_{n+1}^+ \\
E_{n+1}^-
\end{pmatrix}
\]

Where

\[
C_m = \begin{pmatrix}
e^{i\delta_{m-1}} & r_m e^{i\delta_{m-1}} \\
r_m e^{-i\delta_{m-1}} & e^{-i\delta_{m-1}}
\end{pmatrix}
\]

We express \(E_{n+1}^+\) and \(E_{n+1}^-\) in terms of \(E_0^-\) and \(E_0^+\)

\[
(C_1)(C_2)\ldots(C_{n+1}) = \begin{pmatrix}
a & b \\
c & d
\end{pmatrix}
\]

\[
\begin{pmatrix}
E_0^+ \\
E_0^-
\end{pmatrix} = \frac{1}{t_1 t_2 \ldots t_{n+1}} \begin{pmatrix}
a & b \\
c & d
\end{pmatrix} \begin{pmatrix}
E_{n+1}^+ \\
E_{n+1}^-
\end{pmatrix}
\]

There is no negative-going wave in the \((n+1)\)th medium, so \(E_{n+1}^- = 0\)

We obtain

\[
\frac{E_0^-}{E_0^+} = \frac{c}{a} \quad \frac{E_{n+1}^+}{E_0^+} = \frac{t_1 t_2 \ldots t_{n+1}}{a}
\]
The reflectance and transmittance are given by

\[
R = \frac{(E_0^-)(E_0^0)^*}{(E_0^0)(E_0^+)^*} = \frac{c^c}{a^a^*}
\]

\[
T = \frac{n_{n+1}^{-1}(E_{n+1}^+)(E_{n+1}^0)^*}{n_0^{-1}(E_0^+)(E_0^0)^*} = \frac{(t_1 t_2 \ldots t_{n+1})(t_1^* t_2^* \ldots t_{n+1}^*)}{a^a^*}
\]

To use this treatment in a succinct and convenient form, a notation for the matrix elements was introduced. We write the coefficients at the m\textsuperscript{th} interface:

\[
r_m = g_m + ih_m
\]

\[
t_m = 1 + g_m + ih_m
\]

The complex dielectric constants of (m-1)\textsuperscript{th} and the m\textsuperscript{th} layer are $n_{m-1} - i k_{m-1}$ and $n_m - i k_m$. For normal incidence

\[
g_m = \frac{n_{m-1}^2 + k_{m-1}^2 - n_m^2 - k_m^2}{(n_{m-1} + n_m)^2 + (k_m + k_m)^2}
\]

\[
h_m = \frac{2(n_{m-1} k_m - n_m k_{m-1})}{(n_{m-1} + n_m)^2 + (k_m + k_m)^2}
\]

The phase term $e^{i \delta_{m-1}}$ in the m\textsuperscript{th} matrix is written

\[
\exp i \delta_{m-1} = \exp \alpha_{m-1} \exp i \gamma_{m-1}
\]

with $\alpha_{m-1} = \frac{2 \pi}{\lambda} k_{m-1} d_{m-1}$ and $\gamma_{m-1} = \frac{2 \pi}{\lambda} n_{m-1} d_{m-1}$, $d_{m-1}$ is the thickness of the (m-1)\textsuperscript{th} layer.

Because all the elements of the matrices are complex, we write the m\textsuperscript{th} matrix as

\[
C_m = \begin{pmatrix}
p_m + iq_m & r_m + is_m \\
t_m + iq_m & v_m + i \omega_m
\end{pmatrix}
\]

and
\[
\begin{align*}
p_m &= e^{\alpha_{m-1}} \cos \gamma_{m-1} \\
q_m &= e^{\alpha_{m-1}} \sin \gamma_{m-1} \\
r_m &= e^{\alpha_{m-1}} (g_m \cos \gamma_{m-1} - h_m \sin \gamma_{m-1}) \\
s_m &= e^{\alpha_{m-1}} (h_m \cos \gamma_{m-1} + g_m \sin \gamma_{m-1}) \\
t_m &= e^{-\alpha_{m-1}} (g_m \cos \gamma_{m-1} + h_m \sin \gamma_{m-1}) \\
u_m &= e^{-\alpha_{m-1}} (h_m \cos \gamma_{m-1} - g_m \sin \gamma_{m-1}) \\
\omega_m &= -e^{-\alpha_{m-1}} \sin \gamma_{m-1}
\end{align*}
\]

The elements of product matrices are denoted with double suffix notation. The element of \((C_1) (C_2)\) are written as:

\[
\begin{pmatrix}
p_{12} + i q_{12} & r_{12} + i s_{12} \\
t_{12} + i u_{12} & v_{12} + i \omega_{12}
\end{pmatrix}
\]

The element of \((C_1) (C_2) (C_3)\) are written as:

\[
\begin{pmatrix}
p_{13} + i q_{13} & r_{13} + i s_{13} \\
t_{13} + i u_{13} & v_{13} + i \omega_{13}
\end{pmatrix}
\]
The elements of \((C_1) (C_2) \ldots \ldots (C_{n-1})\) can be obtained from the following recurrence relation:

\[
\begin{align*}
p_{1,n+1} &= p_{1n}p_n - q_{1n}q_n + r_{1n}t_n - s_{1n}u_n \\
q_{1,n+1} &= q_{1n}p_n + p_{1n}q_n + s_{1n}t_n + r_{1n}u_n \\
r_{1,n+1} &= p_{1n}r_n - q_{1n}s_n + r_{1n}v_n - s_{1n}\omega_n \\
s_{1,n+1} &= s_{1n}r_n + p_{1n}s_n + s_{1n}v_n + r_{1n}\omega_n \\
t_{1,n+1} &= t_{1n}p_n - u_{1n}q_n + u_{1n}t_n - \omega_{1n}u_n \\
u_{1,n+1} &= u_{1n}p_n + u_{1n}q_n + \omega_{1n}t_n + v_{1n}u_n \\
v_{1,n+1} &= t_{1n}r_n - u_{1n}s_n + v_{1n}v_n - \omega_{1n}\omega_n \\
\omega_{1,n+1} &= u_{1n}r_n + t_{1n}s_n + \omega_{1n}v_n + v_{1n}\omega_n
\end{align*}
\]

Then the reflectance can be obtained:

\[
R = \frac{(E_0^-)(E_0^-)^*}{(E_0^+)(E_0^+)^*} = \frac{cc^*}{aa^*} = \frac{(t_{1n} + iu_{1n})(t_{1n} - iu_{1n})}{(p_{1n} + iq_{1n})(p_{1n} - iq_{1n})} = \frac{t_{1n}^2 + u_{1n}^2}{p_{1n}^2 + q_{1n}^2}
\]
Appendix B: MATLAB Implementation

This section contains the MATLAB code used to implement optical transfer matrix method described previously.

Formula from reference [62] for gold:

Complex dielectric function $\varepsilon_r(\omega) = \varepsilon_r^{(f)}(\omega) + \varepsilon_r^{(b)}(\omega)$

Intraband part $\varepsilon_r^{(f)}(\omega) = 1 - \frac{\Omega_p^2}{\omega(\omega - i\Gamma_0)}$

Interband part $\varepsilon_r^{(b)}(\omega) = \sum_{i=1}^{k} \frac{f_i \omega_p^2}{(\omega_i^2 - \omega^2) + i\omega\Gamma_i}$

Final parameters:

<table>
<thead>
<tr>
<th>Thickness</th>
<th>$f_0$</th>
<th>$\Gamma_0$</th>
<th>$f_1$</th>
<th>$\Gamma_1$</th>
<th>$\omega_1$</th>
<th>$f_2$</th>
<th>$\Gamma_2$</th>
<th>$\omega_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>180nm</td>
<td>0.760</td>
<td>0.053</td>
<td>0.024</td>
<td>0.241</td>
<td>0.415</td>
<td>0.010</td>
<td>0.345</td>
<td>0.830</td>
</tr>
<tr>
<td>$f_3$</td>
<td>$\Gamma_3$</td>
<td>$\omega_3$</td>
<td>$f_4$</td>
<td>$\Gamma_4$</td>
<td>$\omega_4$</td>
<td>$f_5$</td>
<td>$\Gamma_5$</td>
<td>$\omega_5$</td>
</tr>
<tr>
<td>0.071</td>
<td>0.870</td>
<td>2.969</td>
<td>0.601</td>
<td>2.494</td>
<td>4.304</td>
<td>4.384</td>
<td>2.214</td>
<td>13.32</td>
</tr>
</tbody>
</table>

Formula from reference [45] for VO₂:

Complex dielectric function $\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_n^2}{\omega^2 + i\omega\omega} + \sum_{i=1}^{n} \frac{s_i}{1 - \omega^2 / \omega_i^2 - i\Gamma_i \omega / \omega_i}$
Final parameters used for insulating VO₂:

<table>
<thead>
<tr>
<th>Thickness</th>
<th>$\varepsilon_\infty$</th>
<th>$\omega_1$</th>
<th>$\omega_2$</th>
<th>$\omega_3$</th>
<th>$\omega_4$</th>
<th>$\omega_5$</th>
<th>$\omega_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>90nm</td>
<td>4.26</td>
<td>1.02</td>
<td>1.30</td>
<td>1.50</td>
<td>2.9</td>
<td>8.49</td>
<td>3.76</td>
</tr>
<tr>
<td>$\omega_7$</td>
<td>$s_1$</td>
<td>$s_2$</td>
<td>$s_3$</td>
<td>$s_4$</td>
<td>$s_5$</td>
<td>$s_6$</td>
<td>$s_7$</td>
</tr>
<tr>
<td>5.1</td>
<td>0.79</td>
<td>0.474</td>
<td>0.583</td>
<td>0.136</td>
<td>1.316</td>
<td>1.060</td>
<td>0.99</td>
</tr>
<tr>
<td>$\Gamma_1$</td>
<td>$\Gamma_2$</td>
<td>$\Gamma_3$</td>
<td>$\Gamma_4$</td>
<td>$\Gamma_5$</td>
<td>$\Gamma_6$</td>
<td>$\Gamma_7$</td>
<td></td>
</tr>
<tr>
<td>0.55</td>
<td>0.55</td>
<td>0.75</td>
<td>0.07</td>
<td>0.25</td>
<td>0.26</td>
<td>0.395</td>
<td></td>
</tr>
</tbody>
</table>

Final parameters used for metallic VO₂:

<table>
<thead>
<tr>
<th>Thickness</th>
<th>$\varepsilon_\infty$</th>
<th>$\omega_c$</th>
<th>$\omega_n$</th>
<th>$\omega_1$</th>
<th>$\omega_2$</th>
<th>$\omega_3$</th>
<th>$\omega_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>90nm</td>
<td>3.95</td>
<td>3.33</td>
<td>0.66</td>
<td>0.46</td>
<td>4</td>
<td>3.48</td>
<td>2.87</td>
</tr>
<tr>
<td>$s_1$</td>
<td>$s_2$</td>
<td>$s_3$</td>
<td>$s_4$</td>
<td>$\Gamma_1$</td>
<td>$\Gamma_2$</td>
<td>$\Gamma_3$</td>
<td>$\Gamma_4$</td>
</tr>
<tr>
<td>1.816</td>
<td>2.35</td>
<td>0.34</td>
<td>0.45</td>
<td>0.01</td>
<td>0.05</td>
<td>0.28</td>
<td>0.08</td>
</tr>
</tbody>
</table>

VO₂ insulating state:

```
LL=450:1:850;  % wavelength range in nm
L= LL.*(10^(-9));  % convert wavelength to m
h=6.63*10^(-34);  % Planck’s constant
c=3*10^8;        % speed of light
w=(h*c./L)./(1.6*10^(-19));  % frequency range
```

%%%%%%dielectric constant model for gold, [62]%%%%%%%


```
ff0=0.760;     % parameters for gold dielectric constant model
ff1=0.024;
ff2=0.010;
```
ff3=0.071;
ff4=0.601;
ff5=4.384;
ww1=0.415;
ww2=0.830;
ww3=2.969;
ww4=4.304;
ww5=13.32;
TT0=0.053;
TT1=0.241;
TT2=0.345;
TT3=0.870;
TT4=2.494;
TT5=2.214;
wp=9.01;
wwp=sqrt(ff0)*wp;

erw=1-(wwp^2./(w.*(w-i*TT0)))+((ff1*wp^2)./(ww1^2-
w.^2)+i*TT1.*w)+((ff2*wp^2)./(ww2^2-w.^2)+i*TT2.*w)+((ff3*wp^2)./(ww3^2-
w.^2)+i*TT3.*w)+((ff4*wp^2)./(ww4^2-w.^2)+i*TT4.*w)+((ff5*wp^2)./(ww5^2-
w.^2)+i*TT5.*w));
n2 = sqrt((sqrt(real(erw).^2 + imag(erw).^2) + real(erw))./2);  % refractive index of gold as a function of frequency
k2 = sqrt((sqrt(real(erw).^2 + imag(erw).^2) - real(erw))./2);  % refractive index of gold as a function of frequency

%%%%%%dielectric constant model for VO2 insulating state, [45]%%%%%%
Properties of VO2 between 0.25 and 5 eV,” Physical Review, vol. 172, no. 3,
p. 788, 1968. %%%%%

s1=0.79;                  % parameters for gold dielectric constant model
ss2=0.474;
s3=0.583;
s4=0.136;
s5=1.316;
s6=1.060;
s7=0.99;
w1=1.02;
w2=1.30;
w3=1.50;
w4=2.9;
w5=8.49;
w6=3.76;
w7=5.1;
T1=0.55;
T2=0.55;
T3=0.75;
T4=0.07;
T5=0.25;
T6=0.26;
T7=0.395;
\[ E_0 = 4.26; \]
\[ E = E_0 + s_1/(1-w^2) + s_2/(1-w^2) + s_3/(1-w^2) + s_4/(1-w^2) + s_5/(1-w^2) + s_6/(1-w^2) + s_7/(1-w^2); \]
\[ n_1 = \sqrt{(\sqrt{\text{real}(E)^2 + \text{imag}(E)^2) + \text{real}(E))}/2; \quad \text{refractive index of VO2 insulating as a function of frequency} \]
\[ k_1 = \sqrt{(\sqrt{\text{real}(E)^2 + \text{imag}(E)^2) - \text{real}(E))}/2; \quad \text{refractive index of VO2 insulating as a function of frequency} \]
\[ n_0 = 4.5; \quad \% \text{refractive index of ITO glass} \]
\[ k_0 = 0; \quad \% \text{refractive index of ITO glass} \]
\[ n_3 = 1; \quad \% \text{refractive index of air} \]
\[ k_3 = 0; \quad \% \text{refractive index of air} \]
\[ d_1 = 90 \times 10^{-9}; \quad \% \text{thickness of VO2} \]
\[ d_2 = 180 \times 10^{-9}; \quad \% \text{thickness of gold} \]

\text{% optical transfer matrix method for reflectance calculation%}
\[ g_1 = (n_0^2 - n_1^2 - k_1^2)/(n_0 + n_1)^2 + k_1^2; \]
\[ h_1 = (2n_0^2k_1)/(n_0 + n_1)^2 + k_1^2; \]
\[ g_2 = (n_1^2 - n_2^2 + k_2^2)/(n_1 + n_2)^2 + (k_1 + k_2)^2; \]
\[ h_2 = (2(n_1 + k_2))/(n_1 + n_2)^2 + (k_1 + k_2)^2; \]
\[ g_3 = (n_2^2 - n_3^2 + k_3^2)/(n_2 + n_3)^2 + (k_3 + k_2)^2; \]
\[ h_3 = (2(n_2 - n_3))/(n_2 + n_3)^2 + (k_3 + k_2)^2; \]
\[ a_1 = (2\pi^2k_1)/(n_0 + n_1)^2 + k_1^2; \]
\[ r_1 = (2\pi^2k_2)/(n_0 + n_1)^2 + k_1^2; \]
\[ a_2 = (2\pi^2k_2)/(n_0 + n_1)^2 + k_1^2; \]
\[ r_2 = (2\pi^2k_2)/(n_0 + n_1)^2 + k_1^2; \]
\[ p_1 = \exp(a_1) \cdot \cos(r_1); \]
\[ q_1 = \exp(a_1) \cdot \sin(r_1); \]
\[ p_2 = \exp(a_2) \cdot \cos(r_2); \]
\[ q_2 = \exp(a_2) \cdot \sin(r_2); \]
\[ v_2 = \exp(-a_2) \cdot \cos(r_2); \]
\[ w_2 = -\exp(-a_2) \cdot \sin(r_2); \]
\[ t_2 = \exp(-a_2) \cdot (g_2 \cdot \cos(r_1) + h_2 \cdot \sin(r_1)); \]
\[ u_2 = \exp(-a_2) \cdot (h_2 \cdot \cos(r_1) - g_2 \cdot \sin(r_1)); \]
\[ t_3 = \exp(-a_3) \cdot (g_3 \cdot \cos(r_2) + h_3 \cdot \sin(r_2)); \]
\[ u_3 = \exp(-a_3) \cdot (h_3 \cdot \cos(r_2) - g_3 \cdot \sin(r_2)); \]
\[ R_2 = \exp(a_1) \cdot (g_2 \cdot \cos(r_1) - h_2 \cdot \sin(r_1)); \]
\[ s_2 = \exp(a_1) \cdot (h_2 \cdot \cos(r_1) + g_2 \cdot \sin(r_1)); \]
\[ p_12 = p_2 + g_1 \cdot t_2 - h_1 \cdot u_2; \]
\[ q_12 = q_2 + h_1 \cdot t_2 + g_1 \cdot u_2; \]
\[ t_12 = t_2 + g_1 \cdot p_2 - h_1 \cdot u_2; \]
\[ u_12 = u_2 + h_1 \cdot p_2 + g_1 \cdot u_2; \]
\[ r_12 = R_2 + g_1 \cdot v_2 - h_1 \cdot w_2; \]
s12 = s2 + h1.*v2 + g1.*w2;
v12 = v2 + g1.*R2 - h1.*s2;
w12 = w2 + h1.*R2 + g1.*s2;
p13 = p12.*p3 - q12.*q3 + r12.*t3 - s12.*u3;
q13 = q12.*p3 + p12.*q3 + s12.*t3 + r12.*u3;
t13 = t12.*p3 - u12.*q3 + v12.*t3 - w12.*u3;
u13 = u12.*p3 + t12.*q3 + w12.*t3 + v12.*u3;

l13 = (l+g1).*(l+g2).*(l+g3)-h2.*h3.*(l+g2)-h1.*h2.*(l+g3);
m13 = h1.*(l+g2).*(l+g3)+h2.*h3.*(l+g2)+h3.*(l+g1).*(l+g2)-h1.*h2.*h3;

T_insulating = (n3./n0).*(l13.^2 + m13.^2)/(p13.^2 + q13.^2);

R_insulating = (t13.^2 + u13.^2)/(p13.^2 + q13.^2);

plot(LL,R_insulating);
VO₂ metallic state:

LL=450:1:850; % wavelength range in nm
L= LL.*(10^(-9)); % convert wavelength to m
h=6.63*10^(-34); % planck's constant
c=3*10^8; % speed of light
w=(h*c./L)./(1.6*10^(-19)); % frequency range

%%%%%%dielectric constant model for gold [62]%%%%%%%
%%%%%%[62] D. Rakic, a B. Djurisic, J. M. Elazar, and M. L. Majewski,
“Optical properties of metallic films for vertical-cavity optoelectronic

ff0=0.760; % parameters for gold dielectric constant model
ff1=0.024;
ff2=0.010;
ff3=0.071;
ff4=0.601;
ff5=4.384;
ww1=0.415;
ww2=0.830;
ww3=2.969;
ww4=4.304;
ww5=13.32;
TT0=0.053;
TT1=0.241;
TT2=0.345;
TT3=0.870;
TT4=2.494;
TT5=2.214;
wp=9.01;
wwp=sqrt(ff0)*wp;

erw=1-(wwp^2./(w.^2-i.*TT0)).+((ff1*wp^2)./(ww1^2-w.^2+i.*TT1.*w)+
(ff2*wp^2)./(ww2^2-w.^2+i.*TT2.*w)+
(ff3*wp^2)./(ww3^2-w.^2+i.*TT3.*w)+
(ff4*wp^2)./(ww4^2-w.^2+i.*TT4.*w)+
(ff5*wp^2)./(ww5^2-w.^2+i.*TT5.*w));
n2 = sqrt((sqrt(real(erw).^2 + imag(erw).^2) +
real(erw))./2); % refractive index of gold as a function of frequency
k2 = sqrt((sqrt(real(erw).^2 + imag(erw).^2) -
real(erw))./2); % refractive index of gold as a function of frequency
% dielectric constant model for VO2 insulating state, [45]


s1=1.816;                 % parameters for gold dielectric constant model
s2=2.35;
s3=0.34;
s4=0.45;
w1=0.46;
w2=4;
w3=3.48;
w4=2.87;
T1=0.01;
T2=0.05;
T3=0.28;
T4=0.08;
E0=3.95;
wn=3.33;
w=0.66;

E=E0-wn^2./(w.^2+i*wc.*w)+s1./(1-w.^2./w1^2-i*T1.*w./w1)+ss2./(1-w.^2./w2^2-i*T2.*w./w2)+s3./(1-w.^2./w3^2-i*T3.*w./w3)+s4./(1-w.^2./w4^2-i*T4.*w./w4);

n1 = sqrt((sqrt(real(E).^2 + imag(E).^2) + real(E))./2);        %
refractive index of VO2 metallic as a function of frequency
k1 = sqrt((sqrt(real(E).^2 + imag(E).^2) - real(E))./2);        %
refractive index of VO2 metallic as a function of frequency

n0 = 4.5;       %refractive index of ITO glass
k0 = 0;         %refractive index of ITO glass

n3 = 1;         %refractive index of air
k3 = 0;         %refractive index of air

d1 = 90*10^-9;  %thickness of VO2
d2 = 180*10^-9; %thickness of gold

% optical transfer matrix method for reflectance calculation

h1 = 2*(n0.*k1)/((n0 + n1).^2 + k1.^2);  

h2 = (2.*(n1.*k2 - n2.*k1))/((n2 + n1).^2 + (k1 + k2).^2);  
g3 = (n2.*n3 + k2.^2 - k3.^2)/((n2 + n3).^2 + (k3 + k2).^2);  
h3 = (2*(n2.*k3 - n3.*k2))/((n2 + n3).^2 + (k3 + k2).^2);  

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a1 = (2*pi.*k1.*d1)./L;
r1 = (2*pi.*n1.*d1)./L;
a2 = (2*pi.*k2.*d2)./L;
r2 = (2*pi.*n2.*d2)./L;
p2 = exp(a1).*cos(r1);
q2 = exp(a1).*sin(r1);
p3 = exp(a2).*cos(r2);
q3 = exp(a2).*sin(r2);
v2 = exp(-a1).*cos(r1);
w2 = -exp(-a1).*sin(r1);

t2 = exp(-a1).*(g2.*cos(r1) + h2.*sin(r1));
u2 = exp(-a1).*(h2.*cos(r1) - g2.*sin(r1));
t3 = exp(-a2).*(g3.*cos(r2) + h3.*sin(r2));
u3 = exp(-a2).*(h3.*cos(r2) - g3.*sin(r2));
R2 = exp(a1).*(g2.*cos(r1) - h2.*sin(r1));
s2 = exp(a1).*(h2.*cos(r1) + g2.*sin(r1));
p12 = p2 + g1.*t2 - h1.*u2;
q12 = q2 + h1.*t2 + g1.*u2;
t12 = t2 + g1.*p2 - h1.*q2;
u12 = u2 + h1.*p2 + g1.*q2;
r12 = R2 + g1.*v2 - h1.*w2;
s12 = s2 + h1.*v2 + g1.*w2;
v12 = v2 + g1.*R2 - h1.*s2;
w12 = w2 + h1.*R2 + g1.*s2;
p13 = p12.*p3 - q12.*q3 + r12.*t3 - s12.*u3;
q13 = q12.*p3 + p12.*q3 + s12.*t3 + r12.*u3;
t13 = t12.*p3 - u12.*q3 + v12.*t3 - w12.*u3;
u13 = u12.*p3 + t12.*q3 + w12.*t3 + v12.*u3;

l13 = (1+g1).*(1+g2).*h2.*h3.*(1+g3) - h1.*h2.*(1+g3);
m13 = h1.*(1+g2).*h2.*h3.*(1+g3) + h1.*h3.*(1+g1).*h2.*h3;
T_metallic = (n3./n0).*(l13.^2 + m13.^2)./(p13.^2 + q13.^2);

R_metallic = (t13.^2 + u13.^2)./(p13.^2 + q13.^2); %%%% Reflectane %%%%
plot(LL,R_metallic,'r');
hold on;