Studies of Transmission and Reflection for an Anisotropic Thin Film System

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Abstract:

Vanadium Dioxide thin films have long been a subject of study because of Vanadium Dioxide's unique properties. Vanadium Dioxide, when heated, exhibits a sharp change in conductivity; changing from an insulating medium to a conducting one. This has led to its use in a number of industries, especially in the engineering fields. A number of different types of measurements have been made to characterize this unusual change in electrical properties, including stress & strain and electrical measurements[2], as well as optical measurements. To help better understand the metal-insulator transition we have been making optical measurements with both continuous-wave and pulsed lasers of Vanadium Dioxide thin films grown on various substrates, including quartz, sapphire, and rutile[1]. Through my measurements, we found a continuous optical and electrical anisotropy for Vanadium Dioxide thin films grown on rutile (TiO_2).

Introduction:

My work initially began by taking optical measurements of Vanadium Dioxide thin films for various substrates using continuous-wave laser measurements. Kittiwatanakul et al. had reported an electrical anisotropy for two orthogonal crystal orientations for single-crystal VO_2 grown on TiO_2. Anisotropy is seen as a difference in properties for different directions, such as crystal axis or the polarization of light, and is an unusual and interesting property. As Vanadium Dioxides have been used in semiconductors and other electronics, anisotropy in these structures has potential for future engineering uses. Because optical computing is a growing field, potential uses for thin films with optical anisotropy also exist. Thus a structure which exhibits the metal-insulator transition of Vanadium Dioxide and also interesting optical properties could be extremely useful.

Another driving force for optical measurements is to develop a better understanding of the metal-insulator transition. The metal-insulator transition is extremely fast, and so it has been historically difficult to view the change as it occurs at the molecular level. Because of this, our optical measurements have been divided into two types. The first, for which I was largely responsible, were continuous-wave measurements. These are able to detect the slower optical effects of the transition as it occurs, namely changes in reflection and transmission. We observed a high reflection for the insulating stage, followed by a sharp drop-off as the thin film system was heated and passed into the metal stage. As the sample cools and reverts back to the insulator stage the reflection of the sample increases. Because of this, we are able to use reflection measurements to characterize the metal-insulator transition of Vanadium Dioxide thin films. These optical measurements also formed a baseline for the second types of experiments, which were ultrafast pulsed laser measurements. These are able to detect fast changes on the femtosecond scale which occur in the model. These results are addressed elsewhere[1], and are outside the scope of this paper. Our overall goal was to develop an understanding of the optical properties of Vanadium Dioxide thin films through the metal-insulator transition.

Experiment

(i) Optical Measurements

In order to take optical measurements through the metal-insulator transition, a specialized apparatus was required which allowed us to heat and cool the sample through the transition. This was accomplished by a Peltier cooler attached to a stand to which the sample could be attached. Transmission and reflection measurements could then be obtained in the standard way, by hitting the sample with a polarized beam and catching the reflected and transmitted beams on a photodetector.

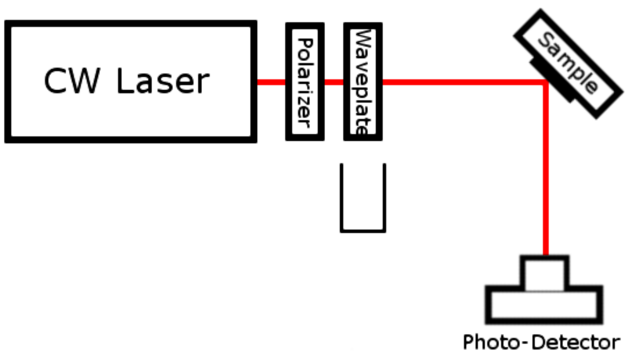

Figure 1: Optical Experimental Setup

For most substrates on which Vanadium Dioxide was grown, transmission and reflection can be measured; however, our sample grown on rutile had an unpolished back which made transmission measurements impossible. Optical measurements were taken through the metal-insulator transition for each substrate for two orthogonal polarizations of the incoming beam. Once the initial anisotropy was observed for Vanadium Dioxide on rutile, we also took measurements at intermediate polarizations. A 780nm wavelength continuous-wave laser was used for these measurements. For a comparison, we also took equivalent measurements for Vanadium Dioxide grown on quartz, which is polycrystalline.

(ii) Electrical Measurements:

In order to make a comparison to the results of Kittiwatanakul et al[1]., we also needed to take electrical measurements of the VO_2 thin film on rutile. These measurements accomplished three things. The first was to establish that our sample, which was an extended thin film medium instead of a single crystal, still exhibited electrical anisotropy. The second was to compare electrical anisotropy found in this extended medium to that found in the single crystal. The third was to observe how electrical anisotropy changed between the two orthogonal maxima. In order to do this, we used a four-point probe with a sample-holder modified so that the angle of the sample could be changed and recorded. Resistivity measurements were taken at

Figure 2: Four-Point Probe; current is measured across two points and voltage is measured across the other two, forming a simple circuit. Each contacts the surface of the thin film and the device uses Ohm's law to calculate sample resistance.

four different temperatures through the metal-insulator transition for a complete rotation of the sample. Although the single-crystal measurements were made for conductivity, resistivity is equivalent in determining changes in electrical properties.

Results:

(i) Optical Results

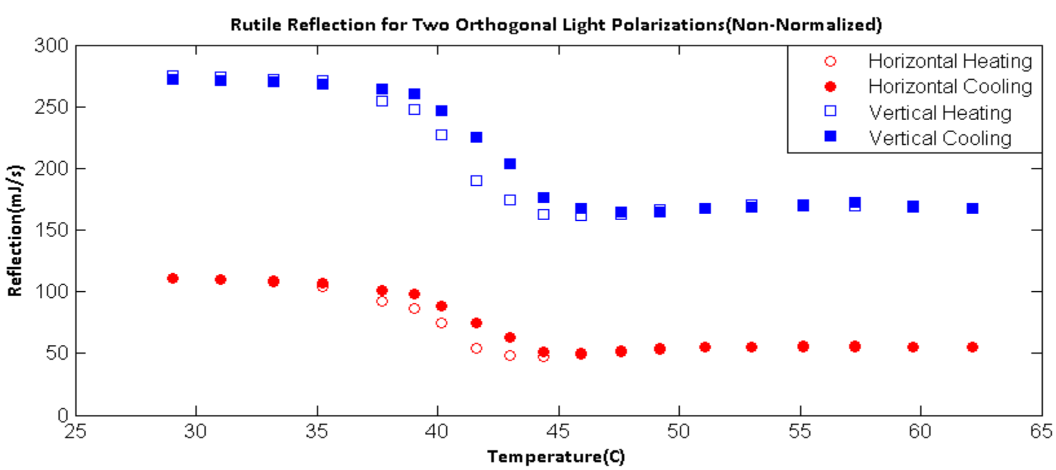

Figure 1: Hysteresis showing optical anisotropy for Vanadium Dioxide grown on Rutile

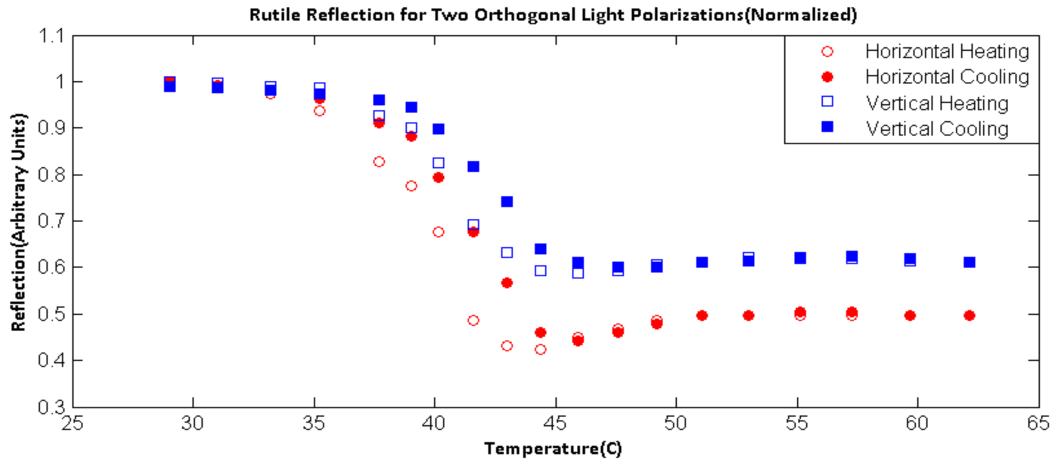

Figure 2: Hysteresis showing optical anisotropy for Vanadium Dioxide grown on Rutile (Normalized)

We observed an optical anisotropy for two orthogonal orientations of the sample for Vanadium Dioxide grown on rutile. There is a marked difference between the non-normalized reflection values we collected (Figure 1). In order to ensure that this difference was not simply due to experimental error, we normalized the values (Figure 2) and found the anisotropy to still be present, implying that the optical anisotropy is intrinsic to the film.

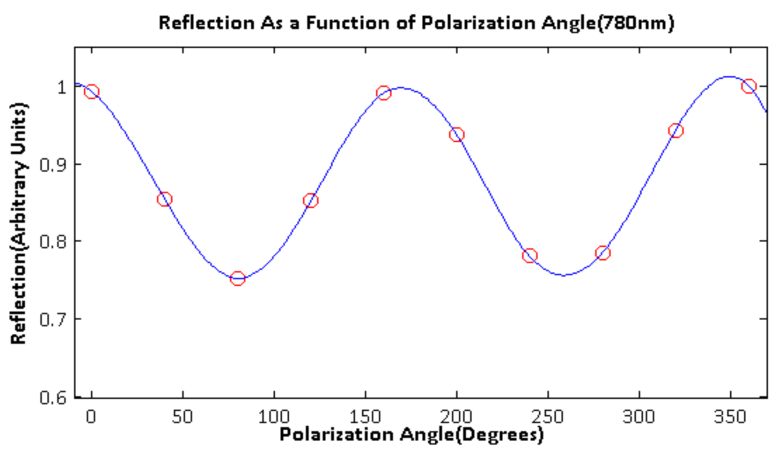

Figure 3: Continuous Anisotropy for Vanadium Dioxide Grown on Rutile

To expand upon our initial results, we also looked at differences in reflection with a change in polarization angle over an entire circular rotation at room temperature. This showed that there is a continuous change in reflection with change in polarization angle. There are no sharp changes or irregularities which we could detect in the anisotropic properties of this thin film system.

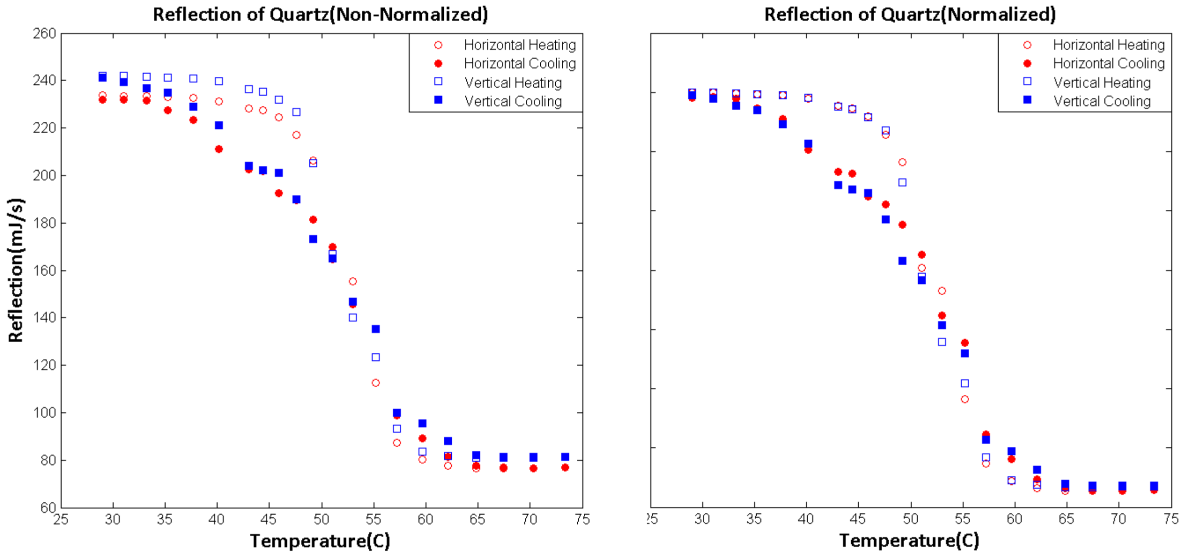

Figure 4: Hysteresis showing isotropy for Vanadium Dioxide grown on Quartz

For comparison, we found no anisotropy for Vanadium Dioxide thin films grown on Quartz (Figure 4). This difference may be due to the difference in the substrate. Quartz by itself is polycrystalline and so does not typically exhibit anisotropic behavior. Rutile, on the other hand, is monocrystalline and does normally exhibit anisotropic behavior.

(ii) Electrical Results

Our resistivity measurements also showed a strong and continuous anisotropy through the metal-insulator transition(Figures 5&6). These results are consistent with the results of Kittiwatanakul et al.; however, our results show a much lower difference in magnitude than that found for the single-crystal measurements.

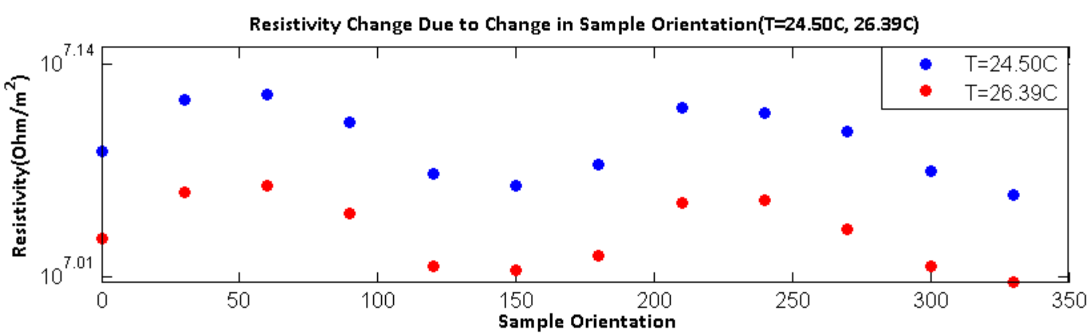

Figure 5: Electrical anisotropy through the metal-insulator transition for Vanadium Dioxide grown on Rutile

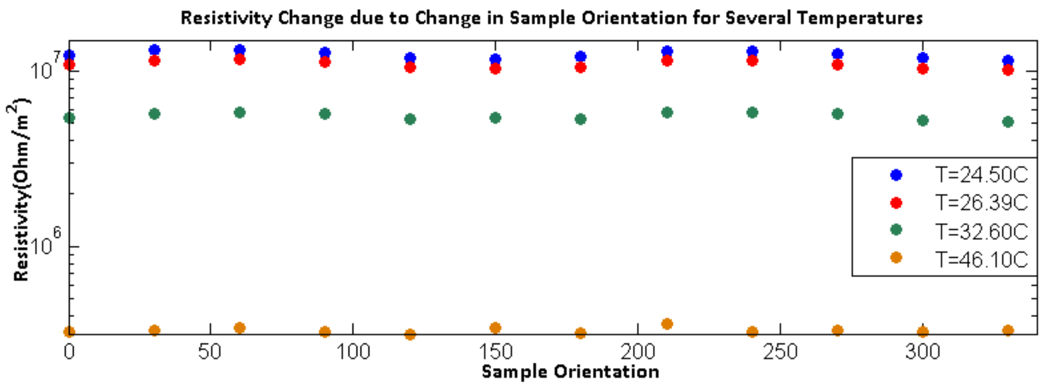

Figure 6: Electrical anisotropy for Vanadium Dioxide grown on Rutile, two temperatures highlighted to show the anisotropic behavior at each temperature

Modeling

Background

A major goal has been to develop a working computational model of thin-film transmission and reflection for our Vanadium Dioxide systems. Fortunately, Yeh[4] and Schubert[3] have a well-developed general model for anisotropic thin-film systems based on Berreman's matrix formulation for thin film systems[5]. Matlab is uniquely to converting this mathematical model to a computational one, and so our model has been developed in this system. Having a working model for our measurements will allow us to better drive further experiments and get a better understanding of the metal-insulator transition. While the existing models are suited for one temperature, modifications had to be added in order to model transmission and reflection coefficient change with temperature.

The model developed by the previously listed authors is very clever and takes advantage of Maxwell's equations and the boundary conditions between layers of the thin film system. It is an extremely interesting and very cool application of linear algebra to a physical system, and I highly recommend that the reader look into the cited papers; however, I will briefly discuss the theory relevant to the computational model I have been developing.

The heart of the model is the general transfer matrix. What this essentially accomplishes is the transfer and modification of the incoming electromagnetic wave using the boundary conditions from the wave's entry to its exit expressed as reflection, transmission, and entry coefficients. In the general matrix form this is expressed as

$$\begin{pmatrix} A_s \\ A_p \\ B_s \\ B_p \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ T_{31} & T_{32} & T_{33} & T_{34} \\ T_{41} & T_{42} & T_{43} & T_{44} \end{pmatrix} \begin{pmatrix} C_s \\ 0 \\ C_p \\ 0 \end{pmatrix}$$

Where A is the incoming field vector, B is the reflected wave vector, and C is the transmitted field vector. A useful—and fairly accurate—way of envisioning this is as a simplified cartoon instead of a matrix: the incident wave A comes in and hits the thin film system T. Part is transmitted and comes out on the other side as C, another part is reflected back from T and so stays on the same side as the incident wave.

The transfer matrix is the heart of the model; however, in our case we want to extract the reflected and transmitted vectors so we can calculate the reflection and transmission coefficients. Their components can be calculated from the matrix elements of T, as demonstrated by Yeh[4]:

$$r_{ss} = \left(\frac{B_s}{A_s}\right) = \frac{T_{21}T_{33} - T_{23}T_{31}}{T_{11}T_{33} - T_{13}T_{31}}$$

$$r_{pp} = \left(\frac{B_p}{A_p}\right) = \frac{T_{11}T_{43} - T_{41}T_{13}}{T_{11}T_{33} - T_{13}T_{31}}$$

$$t_{ss} = \left(\frac{C_s}{A_s}\right) = \frac{T_{33}}{T_{11}T_{33} - T_{13}T_{31}}$$

$$t_{pp} = \left(\frac{C_s}{A_s}\right) = \frac{T_{11}}{T_{11}T_{33} - T_{13}T_{31}}$$

These can then be used to calculate the reflection and transmission coefficients as usual:

$$\rho = |r^2|$$

$$\tau = \frac{n_2}{n_1}|t^2|$$

where ρ is the reflection coefficient and τ is the transmission coefficient.

While this approach is fairly straightforward on the surface, under the hood it gets much more complicated. Schubert[3] defines the transfer matrix as

$$\mathbf{T} = \mathbf{L}_{\mathrm{a}}^{-1} \prod_{\mathrm{i}=1}^{\mathrm{N}} \mathbf{T}_{\mathrm{ip}}(-d_i)\mathbf{L}_{\mathrm{f}}$$

There are a few different approaches used to calculate these components depending on the situation[3,4,5]; we selected the method devised by Schubert which was general enough for anisotropic media and allowed us to use the inputs from our experimental data. In this case the components are devised as follows:

$$\mathbf{L}_{\mathrm{a}}^{-1} = \frac{1}{2}\begin{pmatrix} 0 & 1 & -\frac{1}{\mathrm{n_a}\cos\Phi_{\mathrm{a}}} & 0 \\ 0 & 1 & \frac{1}{\mathrm{n_a}\cos\Phi_{\mathrm{a}}} & 0 \\ -\frac{1}{\cos\Phi_{\mathrm{a}}} & 0 & 0 & \frac{1}{\mathrm{n_a}} \\ -\frac{1}{\cos\Phi_{\mathrm{a}}} & 0 & 0 & \frac{1}{\mathrm{n_a}} \end{pmatrix}$$

$$\mathbf{L}_{\mathrm{f}} = \frac{1}{2}\begin{pmatrix} 0 & 0 & \sqrt{1-[\mathrm{n_a}/\mathrm{n_f}\sin\Phi_{\mathrm{a}}]^2} & 0 \\ 0 & 1 & \frac{1}{\mathrm{n_a}\cos\Phi_{\mathrm{a}}} & 0 \\ -\mathrm{n_f}\sqrt{1-[\mathrm{n_a}/\mathrm{n_f}\sin\Phi_{\mathrm{a}}]^2} & 0 & 0 & 0 \\ 0 & 0 & \mathrm{n_f} & 0 \end{pmatrix}$$

where Φ_a is the incident angle of the incoming wave, n_a is the index of refraction of

$$\mathbf{T}_p = \exp\{i\frac{\omega}{c}d\Delta\}$$

where

$$\boldsymbol{\Delta} = \begin{pmatrix} -k_x\frac{\varepsilon_{31}}{\varepsilon_{33}} & -k_x\frac{\varepsilon_{32}}{\varepsilon_{33}} & 0 & 1-\frac{k_x^2}{\varepsilon_{33}} \\ 0 & 0 & -1 & 0 \\ \varepsilon_{23}\frac{\varepsilon_{31}}{\varepsilon_{33}}-\varepsilon_{21} & k_x^2-\varepsilon_{22}+\varepsilon_{23}\frac{\varepsilon_{32}}{\varepsilon_{33}} & 0 & k_x\frac{\varepsilon_{23}}{\varepsilon_{33}} \\ \varepsilon_{11}-\varepsilon_{13}\frac{\varepsilon_{31}}{\varepsilon_{33}} & \varepsilon_{12}-\varepsilon_{13}\frac{\varepsilon_{32}}{\varepsilon_{33}} & 0 & k_x\frac{\varepsilon_{13}}{\varepsilon_{33}} \end{pmatrix}$$

where ε_{mn} are components of the dielectric tensor and $k_x = n_a\sin\Phi$ is the x component of the wave vector.

Upon seeing the multitude of matrices it should become apparent as to why we used Matlab, a programming language designed to handle large matrix operations. Our Vanadium Dioxide samples were composed of two layers: a substrate layer and the VO_2 layer. Therefore our general transfer matrix for our systems is given as

$$T = L_a^{-1}T_{substrate}T_{VO_2}L_f$$

Results

Early results for the modeling are promising, and replicating our data for our examples is largely limited by the availability of the proper parameters. We first began with the simplest model: modeling the transmission of light through a film of glass. This yielded the expected results, with approximately 4% reflection and 96% transmission. Additionally, around the Brewster angle we saw reflection drop off, also as we would expect. These results indicated that our model was working as expected for simple systems, allowing us to delve into models of interest, beginning with modeling our results for quartz.

There is a great deal of variation in the dielectric constant of Vanadium Dioxide with temperature, which is further complicated by variation due to deposition technique, crystal structure and so on. These have made measurements difficult[7]; however, Swan and De Smet were able to use ellipsometry to find the refractive indices of a Vanadium Dioxide thin film at room temperature and at 84 C, in other words, before and after the transition[6]. For room temperature they found a refractive index of 2.82-0.317*i* and for 84 C they reported a refractive index of 2.24-0.456*i*. We were therefore able to use these values to compare our model to the experiment results we had before and after the transition.

We first looked at our simpler, isotropic quartz model. Using the standard value for the refractive index of quartz of 1.5387, along with the Vanadium Dioxide layer thickness of 70nm and quartz layer thickness of .5mm, we were able to calculate the reflection of our 780nm beam for room temperature and high temperature. For these calculations we used an initial angle value of 0 for simplicity. For room temperature R_{RT} was calculated as 0.5752 and for high temperature R_{HT} was calculated to be .2035. This corresponds to a decrease in reflection from the insulator to metal stage of 35.5%. In our experiment, from 29.05 C to 84.95 C we saw a 33.9% decrease in reflection power. As the reflection and reflection power are proportional, we can meaningfully compare the percent reduction in both. This comparison shows that our model is accurately able to replicate our experimental results. The difference between the two can likely be accounted for by the fact that our temperatures do not exactly match up with those used to calculate refractive indices and changes in thin film thickness due to changes in temperature.

For our Vanadium Dioxide grown on Rutile the procedure was slightly different. Because the back of the sample was unpolished and opaque, we instead used a single-layer model with the exit medium as rutile. From Palik, Ghosh, and Gorachand[1]'s *Handbook of Optical Constants of Solids*, we obtained a refractive index of 2.484 for one polarization and 2.826 for the other at room temperature. This gave a reflection coefficient in one direction of .6646 and .7779 for the other. The second polarization gives a reflection increase of 1.17 times over the first. From our experimental values we would expect 275 in one direction and 111 in the other, which would give a 2.48 times increase. While we see anisotropy, it is not as great as we might expect; however, there are a number of confounding variables here. For one, the *Handbook* only offers values for the rutile index of refraction for certain wavelengths. While our experiments used a wavelength of 780nm, the closest available index of refraction was for a wavelength of 708.2nm. Additionally, these values were for a temperature of 25 C, whereas our experimental measurements started at 29.05 C. Adjusting the wavelength and temperature can cause fairly large perturbations the reflection and transmission coefficients with our model.

In addition to these sources of error, structural differences in the Vanadium Dioxide grown on Rutile may also have contributed to this difference. While the index of refraction we used for Vanadium Dioxide gave good modeling results for quartz, this does not mean they are good for use in modeling our Rutile data. Vanadium Dioxide grown on rutile exhibits a metal-insulator transition at a lower temperature than Vanadium Dioxide grown on quartz[1], and the factors which cause this difference may also mean that the optical parameters are also different. The difference between the monocrystalline structure of Vanadium Dioxide grown on rutile and the polycrystalline structure of Vanadium Dioxide grown on quartz may result in differences in the optical parameters. It is also possible that differences in deposition technique and thin film growth also play a role in this discrepancy.

Overall these data indicate that our current assumptions do not give the full story behind the optical anisotropy we find in Vanadium Dioxide thin films grown on rutile. While our model works well for matching our isotropic results with the quartz substrate, it performs less well for the anisotropic results on the rutile substrate. This suggests that there are significant differences in the parameters for the anisotropic thin film system which bear further experimental investigation.

Conclusion:

We have found both electrical and optical anisotropies for Vanadium Dioxide thin films grown on Titanium Dioxide (rutile) for an extended thin film system. The electrical results match what has already been reported[2], although the magnitude of the anisotropy is greatly reduced from that found for the single crystal. Additionally, we showed that the change in resistivity is continuous and periodic with changing orientation of the sample. We also found an equivalent optical anisotropy for reflection intensity through the metal-insulator transition with a dramatic difference in intensity for two orthogonal sample orientations. Changing the polarization of the incoming beam gave a continuous and periodic change in optical properties, similar to the electrical properties. We were able to successfully model changes in reflection for Vanadium Dioxide grown on quartz using known parameters; however, attempts to model Vanadium Dioxide grown on rutile were met with less success. This suggests that further experiments are necessary to characterize the dielectric parameters for Vanadium Dioxide grown on rutile, which may shed more light on the cause of the optical anisotropy seen in these samples. Altogether Vanadium Dioxide grown on rutile exhibits anisotropy in optical and electrical properties, which promise to have great potential in both gaining a better understanding of the metal-insulator transition and as a material for use in electronics applications.

Works Cited

1. Radue, Crisman, Wang, Kittiwatanakul, Lu, Wolf, Lukasew, Novikova "Substrate Effect on Optical Properties of Insulator-Metal Transition in VO_2 Thin Films" arXiv:1210.7746
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7. Tobar, Ghosh, Gorachand. *Handbook of Optical Constants of Solids.* Academic Press, San Diego. 1998.

Appendix: Listings for Matlab Reflection and Transmission Model

Listing 1: RTCoefficientsIsotropicTransferMatrix.m

```
function [Tp] = RTCoefficientsIsotropicTransferMatrix(eps0,n,lambda,d,phi)
% Evan Crisman 2012
% Creates the transfer matrix for a layer in an anisotropic thin film system.
% eps0x,eps0y,eps0z are the x,y,z portions of the dielectric tensor.
% lambda is the wavelength of the incoming wave
% omega is the angular frequency of the incoming initial beam.
% d is the thickness of the layer in meters.
% n is the refractive index
%% Creating the Dielectric Tensor:
%(Assumes the orientation of the Cartesian Crystal Coordinate system is the
% same as the laboratory system.)
    function DielectricTensor=DielectricTensorFn(eps0layer)
        DielectricTensor=zeros(3,3);
        DielectricTensor(1,1)=eps0layer;
        DielectricTensor(2,2)=eps0layer;
        DielectricTensor(3,3)=eps0layer;
    end

%% Creating the Delta Matrix
kx=n*sin(phi);
% The x component of the wave vector is necessary for the delta matrix.
%Phi is the angle of the incoming beam from incident.
%For incident light, phi is zero, and so kx=0 in this case.
c=3e8; % Speed of light
omega=2*pi*c/lambda;
    function DeltaMatrix=DeltaMatrixFn(DielectricTensor)
        DeltaMatrix=zeros(4,4);
        DeltaMatrix(1,1)=(-kx*DielectricTensor (3,1)./DielectricTensor(3,3));
        DeltaMatrix(1,2)=(-kx*DielectricTensor (3,2)./DielectricTensor(3,3));
        DeltaMatrix(1,4)=1-((kx^2)/DielectricTensor(3,3));
        DeltaMatrix(2,3)=-1;
        DeltaMatrix(3,1)=DielectricTensor(2,3)*(DielectricTensor
(3,1)./DielectricTensor(3,3))-DielectricTensor(2,1);
        DeltaMatrix(3,2)=kx^2-
DielectricTensor(2,2)+(DielectricTensor(2,3)*(DielectricTensor
(3,2)./DielectricTensor(3,3)));
        DeltaMatrix(3,4)=kx*DielectricTensor (2,3)./DielectricTensor(3,3);
        DeltaMatrix(4,1)=DielectricTensor(1,1)-
(DielectricTensor(1,3)*DielectricTensor (3,1)./DielectricTensor(3,3));
        DeltaMatrix(4,2)=DielectricTensor(1,2)-
(DielectricTensor(1,3)*DielectricTensor (3,2)./DielectricTensor(3,3));
        DeltaMatrix(4,4)=-kx*DielectricTensor (1,3)./DielectricTensor(3,3);
    end
%% Calculating the Transfer Matrix
DielectricTensor=DielectricTensorFn(eps0);
DeltaMatrix=DeltaMatrixFn(DielectricTensor);
Tp=expm(1i*(omega/c)*DeltaMatrix*d);
end
```

Listing 2: RTCoefficientsAnisotropicTransferMatrix.m

```
function [Tp] =
RTCoefficientsAnisotropicTransferMatrix(eps0x,eps0y,eps0z,n,lambda,d,phi)
% Evan Crisman 2012
% Creates the transfer matrix for a layer in an anisotropic thin film system.
% eps0x,eps0y,eps0z are the x,y,z portions of the dielectric tensor.
% lambda is the wavelength of the incoming wave
% omega is the angular frequency of the incoming initial beam.
% d is the thickness of the layer in meters.
% n is the refractive index
%% Creating the Dielectric Tensor:
%(Assumes the orientation of the Cartesian Crystal Coordinate system is the
% same as the laboratory system.)
    function
DielectricTensor=DielectricTensorFn(eps0xlayer,eps0ylayer,eps0zlayer)
        DielectricTensor=zeros(3,3);
        DielectricTensor(1,1)=eps0xlayer;
        DielectricTensor(2,2)=eps0ylayer;
        DielectricTensor(3,3)=eps0zlayer;
    end

%% Creating the Delta Matrix
kx=n*sin(phi);
% The x component of the wave vector is necessary for the delta matrix.
%Phi is the angle of the incoming beam from incident.
%For incident light, phi is zero, and so kx=0 in this case.
c=3e8; % Speed of light
omega=2*pi*c/lambda;
    function DeltaMatrix=DeltaMatrixFn(DielectricTensor)
        DeltaMatrix=zeros(4,4);
        DeltaMatrix(1,1)=(-kx*DielectricTensor (3,1)./DielectricTensor(3,3));
        DeltaMatrix(1,2)=(-kx*DielectricTensor (3,2)./DielectricTensor(3,3));
        DeltaMatrix(1,4)=1-((kx^2)/DielectricTensor(3,3));
        DeltaMatrix(2,3)=-1;
        DeltaMatrix(3,1)=DielectricTensor(2,3)*(DielectricTensor
(3,1)./DielectricTensor(3,3))-DielectricTensor(2,1);
        DeltaMatrix(3,2)=kx^2-
DielectricTensor(2,2)+(DielectricTensor(2,3)*(DielectricTensor
(3,2)./DielectricTensor(3,3)));
        DeltaMatrix(3,4)=kx*DielectricTensor (2,3)./DielectricTensor(3,3);
        DeltaMatrix(4,1)=DielectricTensor(1,1)-
(DielectricTensor(1,3)*DielectricTensor (3,1)./DielectricTensor(3,3));
        DeltaMatrix(4,2)=DielectricTensor(1,2)-
(DielectricTensor(1,3)*DielectricTensor (3,2)./DielectricTensor(3,3));
        DeltaMatrix(4,4)=-kx*DielectricTensor (1,3)./DielectricTensor(3,3);
    end
%% Calculating the Transfer Matrix
DielectricTensor=DielectricTensorFn(eps0x,eps0y,eps0z);
DeltaMatrix=DeltaMatrixFn(DielectricTensor);
Tp=expm(1i*(omega/c)*DeltaMatrix*d);
end
```

Listing 3: RTCoefficientsTwoLayerIA.m

```
function [Rss,Rpp,Tss,Tpp] =
RTCoefficientsTwoLayerIA(eps0isotropic,eps0x,eps0y,eps0z,lambda,d1,d2,na,nf,p
hi)
%IA stands for ISOTROPIC Layer followed by ANISOTROPIC Layer.
%Calculates the transmission and reflection coefficients t and r for the s
%and p polarizations.
%eps0isotropic is the dielectric constant for the isotropic substrate
%eps0x,eps0y,eps0z are the dielectric coefficients in each direction for
%the anisotropic layer.
%lambda is the wavelength of the incoming wave in meters
%d is the thickness of the thin film layer.
%rss is the s polarized reflection coefficient for an s-polarized incoming
% wave.
%rpp is the p polarized reflection coefficient for a p-polarized incoming
% wave.
%tss is the s polarized transmission coefficient for an s-polarized
% incoming wave.
%tpp is the p polarized transmission coefficient for a p-polarized incoming
% wave.
%n is the index of refraction of the first layer, and is the same at each
%boundary.
%na is the index of refraction of the entrance medium
% nf is the index of refraction of the exit medium

%% Creation of the T Matrix
% This matrix is used for calculating the Reflection and Transmission
% coefficients.
y=real(eps0isotropic);
n=sqrt(y);
% (i) Entry Matrix
InvLa=RTCoefficientsIncidentIncidentMatrix(na);
% (ii) Transfer Matrix(Layer 1)
d1=-d1;
TransferMatrix1=RTCoefficientsIsotropicTransferMatrix(eps0isotropic,n,lambda,
d1,phi);
% (iii Transfer Matrix(Layer 2)
d2=-d2;
TransferMatrix2=RTCoefficientsAnisotropicTransferMatrix(eps0x,eps0y,eps0z,n,l
ambda,d2,phi);
% (iii) Exit Matrix
Lf=RTCoefficientsIncidentExitMatrix(na,nf);
% (iv) General Transfer Matrix T
T=InvLa*TransferMatrix1*TransferMatrix2*Lf;

%% Calculation of transmission and reflection coefficients
rss=((T(2,1)*T(3,3))-(T(2,3)*T(3,1)))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
rpp=((T(1,1)*T(4,3))-(T(4,1)*T(1,3)))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
tss=(T(3,3))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
tpp=(T(1,1))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
Rss=Real(rss)^2;
Tss=(nf/na)*Real (tss)^2;
Rpp=Real(rpp)^2;
Tpp=(nf/na)*Real(tpp)^2;
end
```

Listing 4: RTCoefficientsIncidentIncidentMatrix.m

```
function [ InvLa ] = RTCoefficientsIncidentIncidentMatrix(na)
%Evan Crisman 2012
%Creates the Inverse Incident Matrix(La^-1) for an isotropic entry medium,
%which calculates the entry of the beam at an incident angle. This is used to
%solve for the RT coefficients of the system. Generally this medium is air.
%For the incident case phia is 0,where phia is the angle of the incoming
beam,
%and so cos(phia)=1.
%na is the index of refraction of the initial medium.

%% Creating the Inverse Incident Matrix, InvLa
    function InvLa=InvLaFn(na)
        phia=0;
        InvLa=zeros(4,4);
        InvLa(1,2)=1;
        InvLa(1,3)=-1/(na*cos(phia));
        InvLa(2,2)=1;
        InvLa(2,3)=1/(na*cos(phia));
        InvLa(3,1)=1/(cos(phia));
        InvLa(3,4)=1/na;
        InvLa(4,1)=-1/cos(phia);
        InvLa(4,4)=1/na;
    end

%% Calculating the Inverse Incident Matrix, InvLa
InvLa=1/2*InvLaFn(na);
end
```

Listing 5: RTCoefficientsIncidentExitMatrix.m

```
function [Lf] = RTCoefficientsIncidentExitMatrix(na,nf)
%Evan Crisman 2012
%Creates the exit matrix Lf for an isotropic exit medium, which calculates
%the exit from an anisotropic medium due to an initial incident beam. The
%angle phif of the exit beam is calculated using Snell's law. in this case
%phia, the angle of the incoming beam, is 0.
%% Calculating cos(phif), a component of Lf
phia=0;
cosphif=sqrt(1-((na/nf)*sin(phia))^2);

%% Creating the exit matrix, Lf
    function Lf=LfFn(cosphif,nf)
        Lf=zeros(4,4);
        Lf(2,1)=1;
        Lf(3,1)=-nf*cosphif;
        Lf(1,3)=cosphif;
        Lf(4,3)=nf;
    end

%% Calculating the exit matrix, Lf
Lf=LfFn(cosphif,nf);
```

```
end
```

Listing 5: RTCoefficientsIncidentSingleLayer.m

```
function [Rss,Rpp,Tss,Tpp] =
RTCoefficientsIncidentSingleLayer(eps0x,eps0y,eps0z,lambda,d,na,nf)
% Calculates the transmission and reflection coefficients t and r for the s
% and p polarizations.
%eps0x,eps0y,eps0z are the dielectric coefficients in each direction.
%omega is the angular frequency of the incoming wave.
%d is the thickness of the thin film layer.
%rss is the s polarized reflection coefficient for an s-polarized incoming
% wave.
%rpp is the p polarized reflection coefficient for a p-polarized incoming
% wave.
%tss is the s polarized transmission coefficient for an s-polarized
% incoming wave.
%tpp is the p polarized transmission coefficient for a p-polarized incoming
% wave.
%na is the index of refraction of the entrance medium
% nf is the index of refraction of the exit medium

%% Creation of the T Matrix
% This matrix is used for calculating the Reflection and Transmission
% coefficients.

% (i) Entry Matrix
InvLa=RTCoefficientsIncidentIncidentMatrix(na);
% (ii) Transfer Matrix(Layer)
d=-d;
TransferMatrix=RTCoefficientsIncidentTransferMatrix(eps0x,eps0y,eps0z,lambda,
d);
% (iii) Exit Matrix
Lf=RTCoefficientsIncidentExitMatrix(na,nf);
% (iv) General Transfer Matrix T
T=InvLa*TransferMatrix*Lf;

%% Calculation of transmission and reflection coefficients
rss=((T(2,1)*T(3,3))-(T(2,3)*T(3,1)))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
rpp=((T(1,1)*T(4,3))-(T(4,1)*T(1,3)))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
tss=(T(3,3))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
tpp=(T(1,1))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
Rss=real(rss)^2;
Tss=(nf/na)*real(tss)^2;
Rpp=real(rpp)^2;
Tpp=(nf/na)*real(tpp)^2;
end
```

Listing 7: RTCoefficientsIncidentTwoLayersII.m

```
function [Rss,Rpp,Tss,Tpp] =
RTCoefficientsTwoLayerSystemII(eps1,eps2,lambda,d1,d2,na,nf,phi)
%IA stands for ISOTROPIC Layer followed by ISOTROPIC Layer.
%Calculates the transmission and reflection coefficients t and r for the
%two layer system.
```

```
%
%n is the index of refraction of the first layer, and is the same at each
%boundary.
%na is the index of refraction of the entrance medium
% nf is the index of refraction of the exit medium

%% Creation of the T Matrix
% This matrix is used for calculating the Reflection and Transmission
% coefficients.
n1=sqrt(eps1);
n2=sqrt(eps2);
n1=real(n1);
n2=real(n2);
% (i) Entry Matrix
InvLa=RTCoefficientsIncidentIncidentMatrix(na);
% (ii) Transfer Matrix(Layer 1)
d1=-d1;
TransferMatrix1=RTCoefficientsIsotropicTransferMatrix(eps1,n1,lambda,d1,phi);
% (iii Transfer Matrix(Layer 2)
d2=-d2;
TransferMatrix2=RTCoefficientsIsotropicTransferMatrix(eps2,n2,lambda,d2,phi);
% (iii) Exit Matrix
Lf=RTCoefficientsIncidentExitMatrix(na,nf);
% (iv) General Transfer Matrix T
T=InvLa*TransferMatrix1*TransferMatrix2*Lf;

%% Calculation of transmission and reflection coefficients
rss=((T(2,1)*T(3,3))-(T(2,3)*T(3,1)))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
rpp=((T(1,1)*T(4,3))-(T(4,1)*T(1,3)))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
tss=(T(3,3))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
tpp=(T(1,1))./((T(1,1)*T(3,3))-(T(1,3)*T(3,1)));
Rss=real(rss)^2;
Tss=(nf/na)*real(tss)^2;
Rpp=real(rpp)^2;
Tpp=(nf/na)*real(tpp)^2;
end
```