ISSN: 3067-929X
Research Article

Journal of Electronics Science and Electrical Research

Extracting Optical Parameters of Plasmonic Titanium Nitride Using Ref FIT

Maria Masood*

Germany

***Corresponding author:** Maria Masood, Germany.

Submitted: 21 May 2025 **Accepted:** 24 May 2025 **Published:** 31 May 2025

https://doi.org/10.63620/MKJESER.2025.

Citation: *Masood, MN. (2025). Extracting Optical Parameters of Plasmonic Titanium Nitride Using Ref FIT. J of Electron Sci and Electrical Res, 2(2), 01-11.*

Abstract

In this study, we investigate the optical parameters of plasmonic Titanium Nitride (TiN) thin films using the RefFIT software, employing the Drude-Lorentz model for data fitting. TiN is an emerging material for plasmonic applications due to its high melting point, wear resistance, and stability at various temperatures, positioning it as a viable alternative to traditional noble metals. Our research focuses on fabricating, characterizing and extracting optical and electrical properties of TiN thin films deposited on silicon wafers using ellipsometry and Fourier Transform Infrared (FTIR) spectroscopy.

We analyze six different samples, varying in thickness and composition, to determine key parameters such as plasma frequency and damping constants. The simultaneous fitting of reflectance and ellipsometry data in RefFIT provided results consistent with existing literature, establishing the software's reliability for such analysis. Additionally, we validated the RefFIT results by comparing them with alternative models and experimental data, demonstrating the necessity of incorporating Lorentz terms alongside Drude components for accurate optical characterization.

Our findings reveal that TiN films exhibit desirable plasmonic properties, with carrier concentration and relaxation times aligning with known trends in nitrides. The robustness of RefFIT in modeling these properties confirms its utility for future research in plasmonic materials. This study underscores the potential of TiN in advanced plasmonic devices and encourages further exploration using comprehensive modeling techniques.

Keywords: Titanium Nitride, Plasmonics, Optical Parameters, Ref FIT

Introduction

Thin films have become quite popular during the course of the last century because they play an important role in a wide variety of areas, for example, in the study of new materials and their properties [1]. In the light of obtaining the optical and electrical properties of emerging materials for use in plasmonic systems, Titanium Nitride (TiN) was studied in depth in this research. TiN has a high melting point, excellent wear resistance, high hardness, temperature resistance and is a very good alternative candidate to noble metals [2], which, in comparison, have high losses (for example, due to nano-patterning [3]) and low melting points [4-6].

The plasmonic properties of TiN films have been studied before using ellipsometry measurements and by fitting the real and imaginary part of permittivity to study the metallic optical behavior [7] and losses [8]. The credibility of using TiN thin films with changing temperatures have also been studied extensively [2, 9]. TiN has proved to be very efficient at room temperature and therefore, its ability to integrate in Complementary Metal-Oxide Semiconductor (CMOS) technology fabricated plasmonic devices which require low temperature fabrication is well recognized [10]. TiN is very robust also at high temperatures [11]. Also, the plasmonic properties of TiN have been found to be absolutely recoverable for a particular temperature [11].

Much research has been done on TiN films in the past, and all TiN films show desired plasmonic properties which are enhanced for thicker films. This is attributed to the reduced penetration depth, which is the distance electromagnetic waves penetrate into a material before being significantly attenuated.

In this research, we fabricated, characterized and extracted optical and electrical parameters by fitting the reflectance and ellipsometry data for 6 samples obtained from six different wafers for different combinations of TiN and silica or only TiN layers on a thick silicon substrate using Drude and Lorentz Model. The methodology to obtain the plasma frequency of TiN thin films, characterized using ellipsometry and FTIR spectroscopy, using the RefFIT software is a new approach with only [12] showing similar simulations. Because RefFIT has been used very rarely for obtaining plasmonic parameters of a material, in this research, we also show that the results obtained through simulations performed in RefFIT for TiN thin films are in line with the trends observed for TiN in literature and the results obtained from another method of calculation to obtain similar properties. The results obtained, thus, establish RefFIT as a reliable software for such calculations and encourage the use of RefFIT for similar insights.

Sample Description and Characterization

In this lot, there were six wafers, each with a different combination of TiN and silica layers and with thicknesses as listed in Table 1. The silica layer was deposited using Plasma Enhanced Chemical Vapor Deposition (PECVD) method, and the TiN layer was deposited using a sputtering process. These layers were grown on a 600 µm thick bare silicon wafer in a clean room. It is worth mentioning here that the type of fabrication methods of these films and their growth parameters are also known to influence their plasmonic properties. The metal-like or dielectric-like properties of TiN nitride thin films can be achieved by varying the growth parameters in magnetron sputtering fabrication processes as in [2, 13, 14].

Table 1: Six thin film wafers of different layers and thicknesses.

	1st layer	2nd layer	3rd layer
Wafer	SiO2	TiN	SiO2
1	--	100nm	--
2	200nm	100nm	--
3	--	100nm	200nm
4	--	50nm	--
5	1000nm	50nm	--
6	--	50nm	200nm

These wafers were characterized using ellipsometry to obtain the real refractive index, n and extinction coefficient, k and FTIR Spectroscopy to obtain the reflectance spectra.

Ellipsometry Specifications

A configuration was created with a combination of spectroscopic ellipsometry with three angles of incidence (59, 65 and 71°) in the wavelength range of 200-860nm and 1 angle of incidence (65°) in 900-2200nm range, and normal incidence reflectometry in the 200-860nm range. For the calculation of thickness and optical constants, the harmonic oscillator model for TiN was used. The measurements were done using KLA-Tencor Spectra Film F1.

FTIR Spectroscopy Specifications

The FTIR spectroscopy measurements were done using the Vertex 80v spectrometer from Bruker on the six samples from the wafers with an angle of incidence of 11° in the near infrared range. Before characterization of the wafers using FTIR spectroscopy, there was some sample preparation. These wafers were cut and 6 samples were taken from the wafers and polished at the back before FTIR spectroscopy characterization, and then the samples were ready to be characterized. In order to obtain mirror polished surfaces, a Struers Tegramin – 25 grinding and polishing machines was used. Polished surfaces were produced by grinding with successively finer abrasives with grain sizes of 15µm, 10µm and 5µm. Finally, suspension with 1 µm grain size was used. The spectra were recorded for all the wafer samples. Ref FIT was found to be a good software for fitting of optical spectra for data analysis. It has a user-friendly interface and, in this research, RefFIT was used to fit reflectivity and ellipsometry data simultaneously and manually, and it was easy to see on the screen precisely whatever changes were being made.

The equation below is the Drude-Lorentz model that was used in these fits:

$$\epsilon(\omega) = \epsilon_{infinite} + \sum_i \frac{\omega_{pi}}{\omega_{0i} - \omega^2 - i\gamma_i\omega}$$

Here,

- ϵinfinite is the high frequency dielectric constant.
- ωpi is the plasma frequency of the ith oscillator
- ω0i is the transverse frequency.
- γi is the scattering rate of the ith Lorentz oscillator.

The n and k obtained from ellipsometry measurements and the reflectance data obtained from the near infrared (NIR) range of FTIR spectroscopy measurements were simultaneously and manually fitted. One Drude and one Lorentz term was apt for making these fits. The values of the parameters of the models were varied until the model was fit to all the three datasets. These different snippets of RefFIT can be seen clearly in the results section.

Results and Discussion

FTIR Spectroscopy Results

The resulting spectra for the wafers measured using FTIR spectroscopy are shown in Fig. 1 for NIR range. The reflectance spectra for wafer 1, wafer 4, and wafer 2 are similar with different intensities. Wafer 1 and wafer 4, which have only a layer of TiN on bare silicon substrate are similar as expected, with wafer 4 having a lesser intensity than wafer 1 between 4000 cm-1 to 8000 cm-1 after which they converge. Wafer 5 spectra is different with Fabry-Perot resonances, with one peak at around 6500 cm-1 and one at around 10000 cm-1. Wafer 3 and wafer 6, again, have similar spectra with a bump at around 800 cm-1, with the intensity of wafer 3 a bit higher than that of wafer 6.

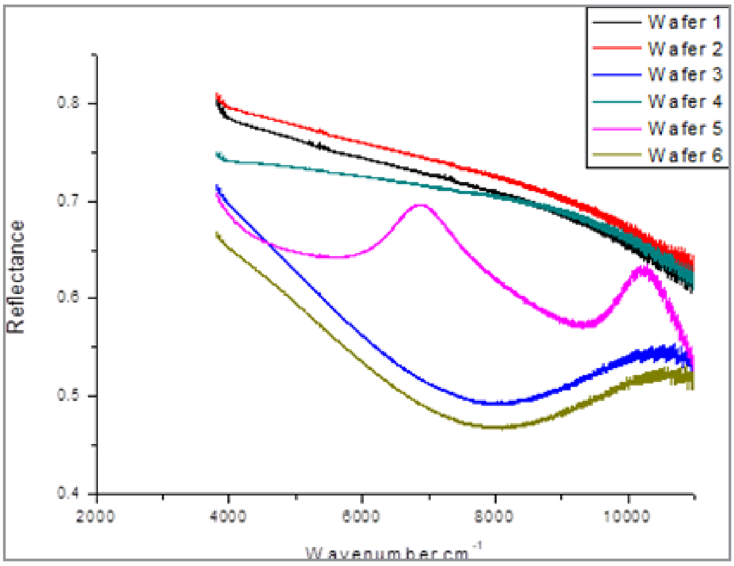

Figure 1: Reflection spectra of the six wafers in the lot

Ref FIT Results

Figs. 2-7 show, from the RefFIT software, the simultaneous fitting of different wafers.

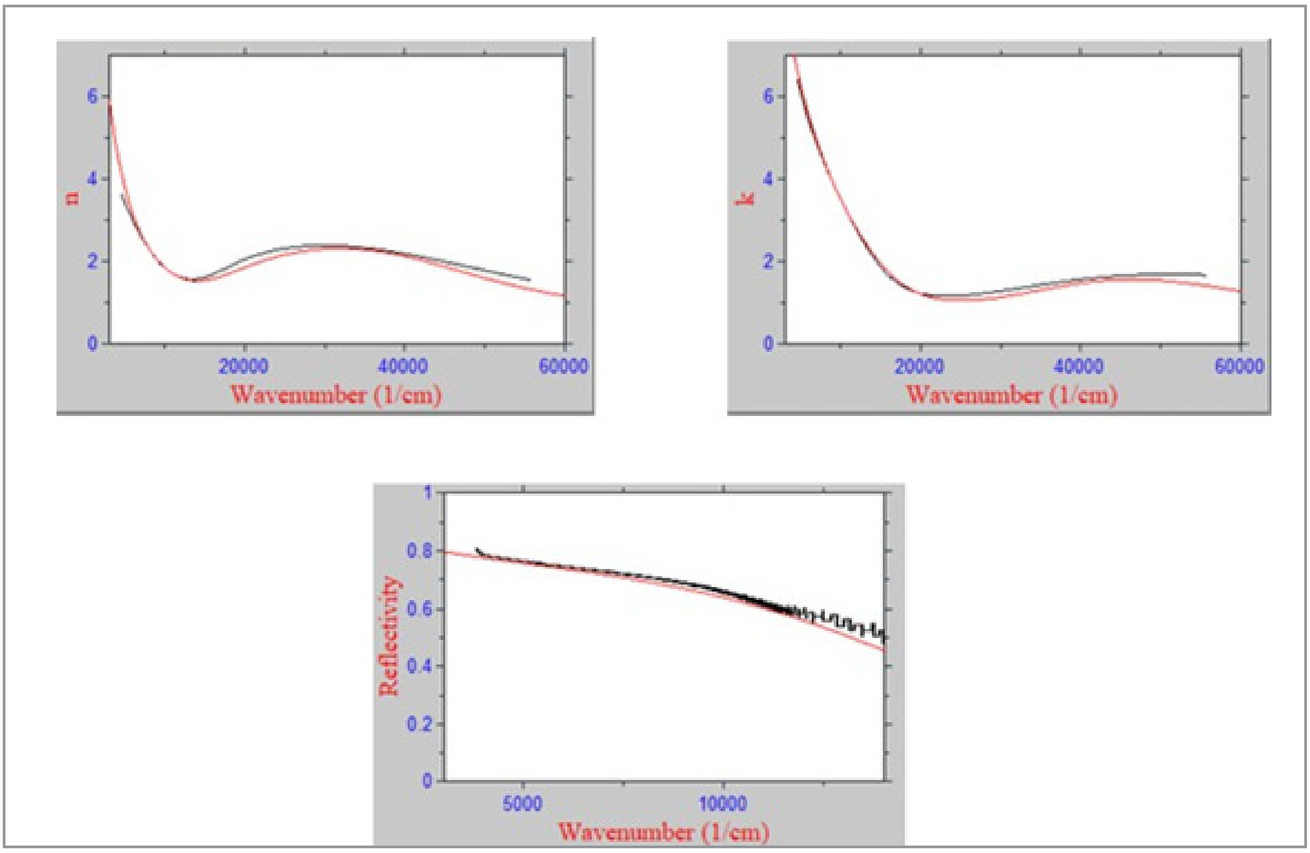

Figure 2: Simultaneous fits in RefFIT for wafer 1 using Drude-Lorentz Model

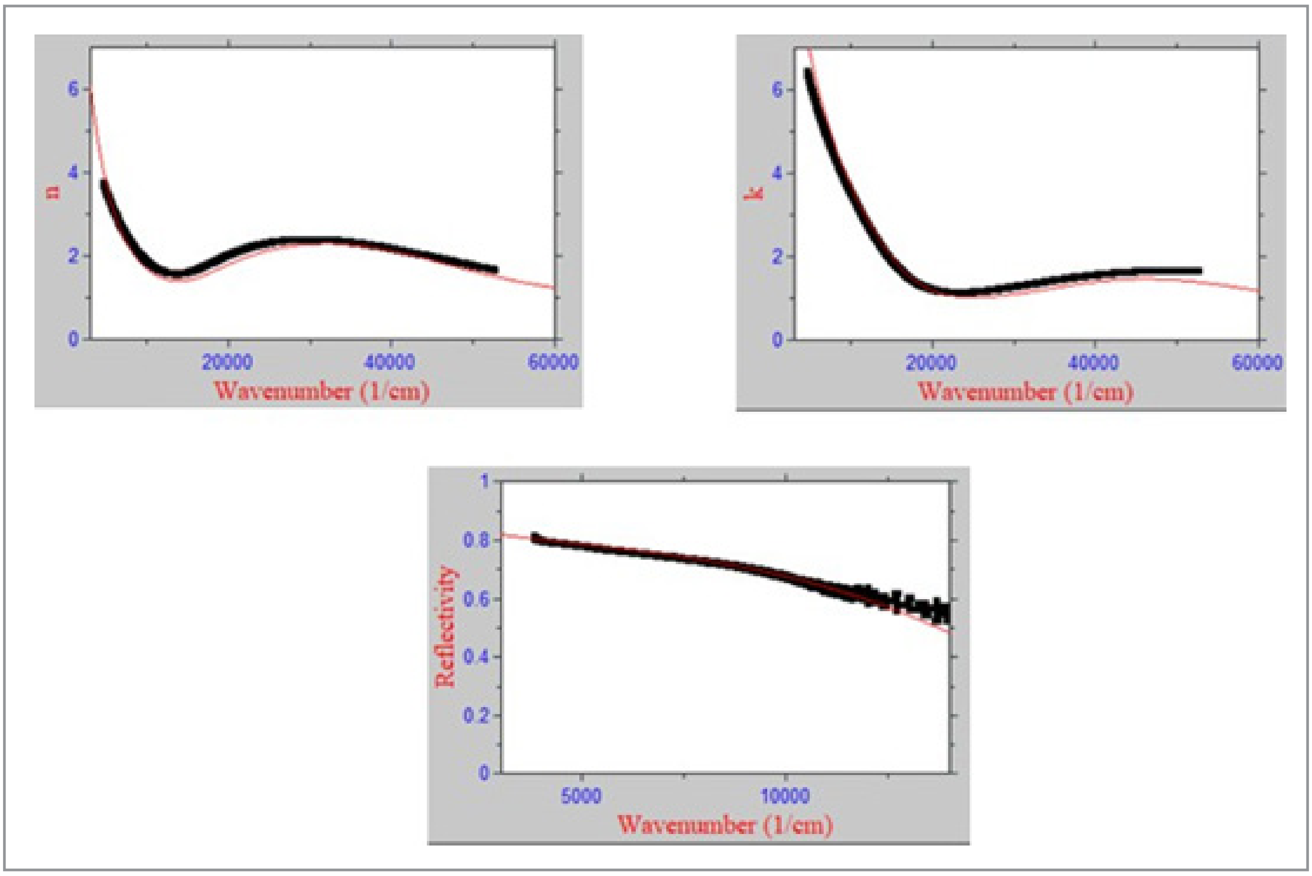

Figure 3: Simultaneous fits in RefFIT for wafer 2 using Drude-Lorentz Model

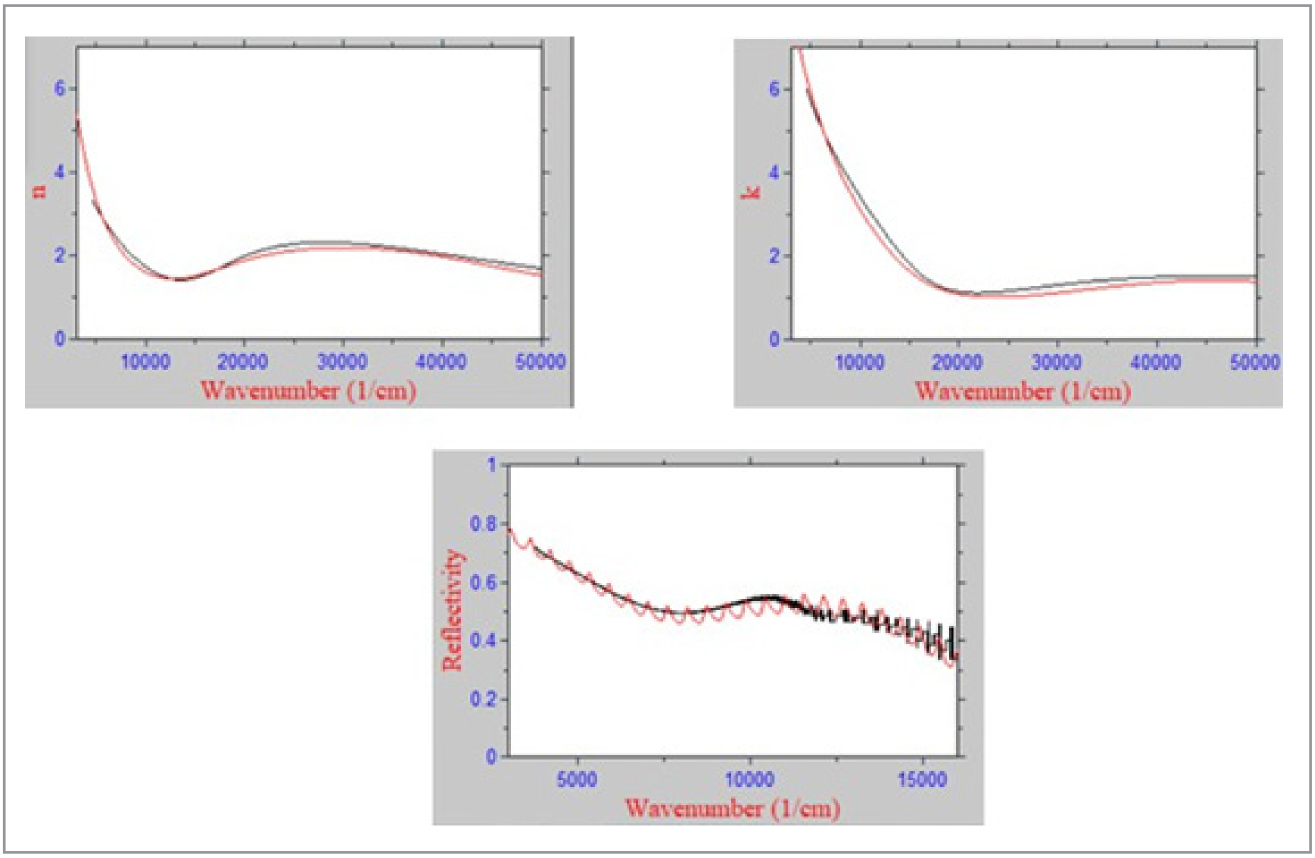

Figure 4: Simultaneous fits in RefFIT for wafer 3 using Drude-Lorentz Model

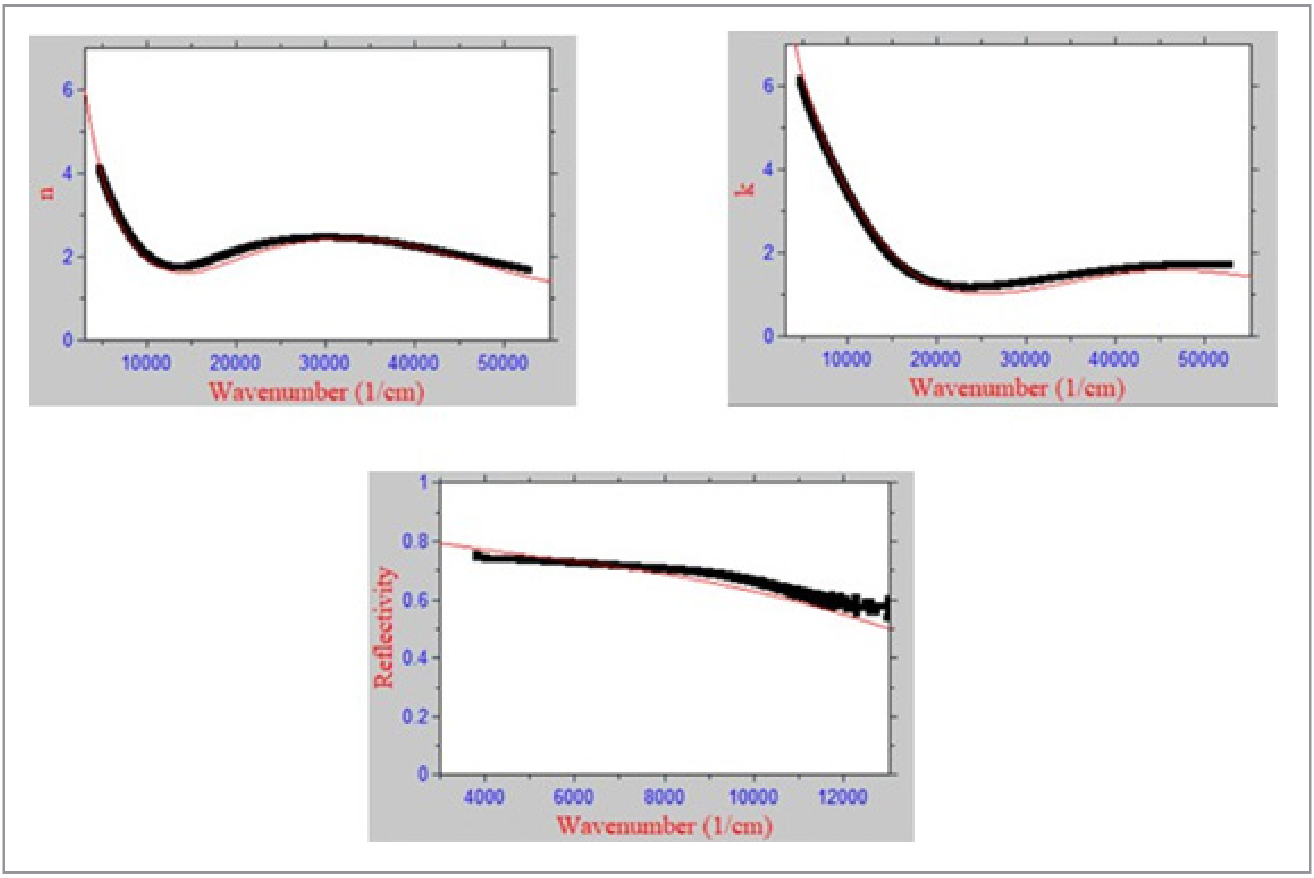

Figure 5: Simultaneous fits in RefFIT for wafer 4 using Drude-Lorentz Model

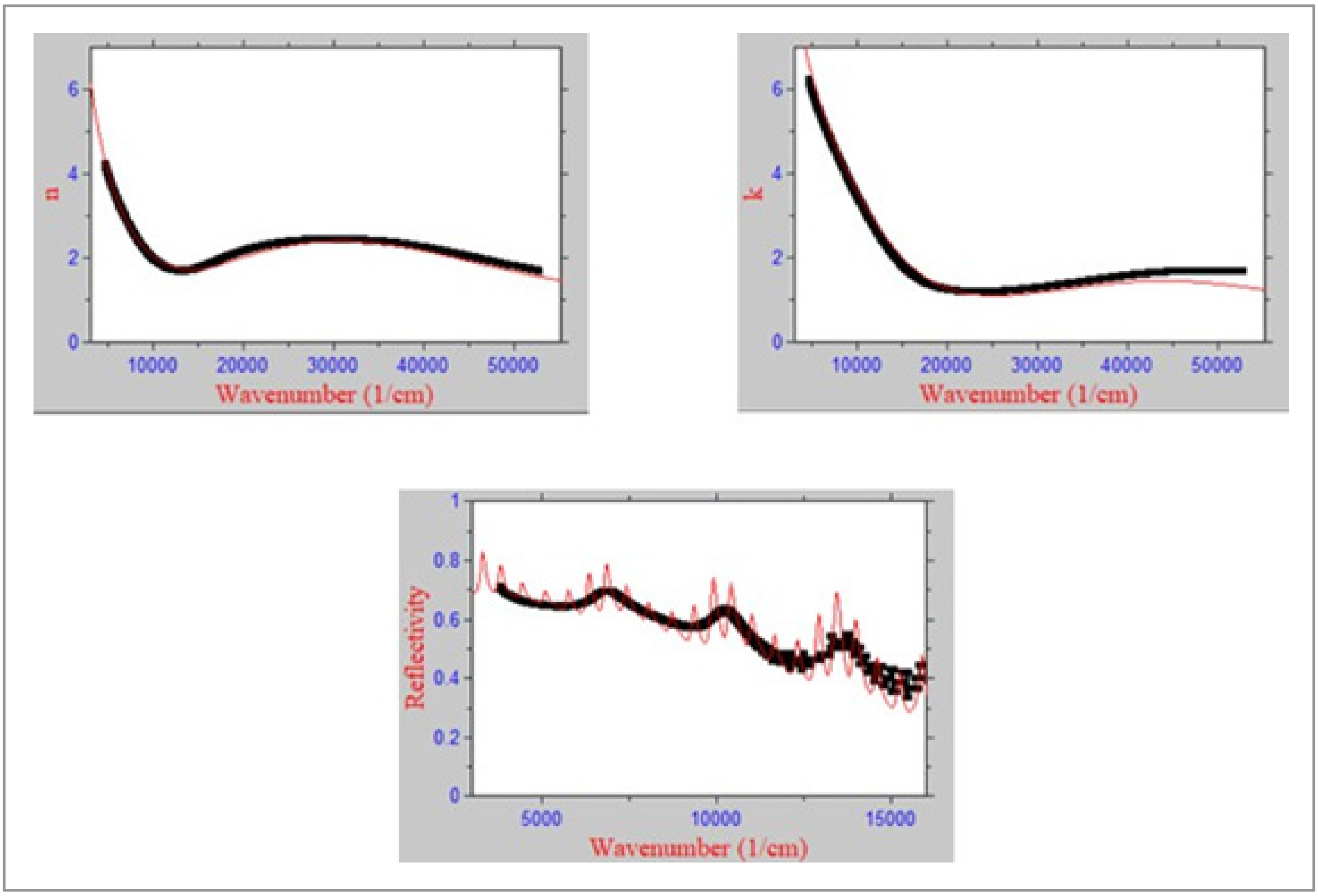

Figure 6: Simultaneous fits in RefFIT for wafer 5 using Drude-Lorentz Model

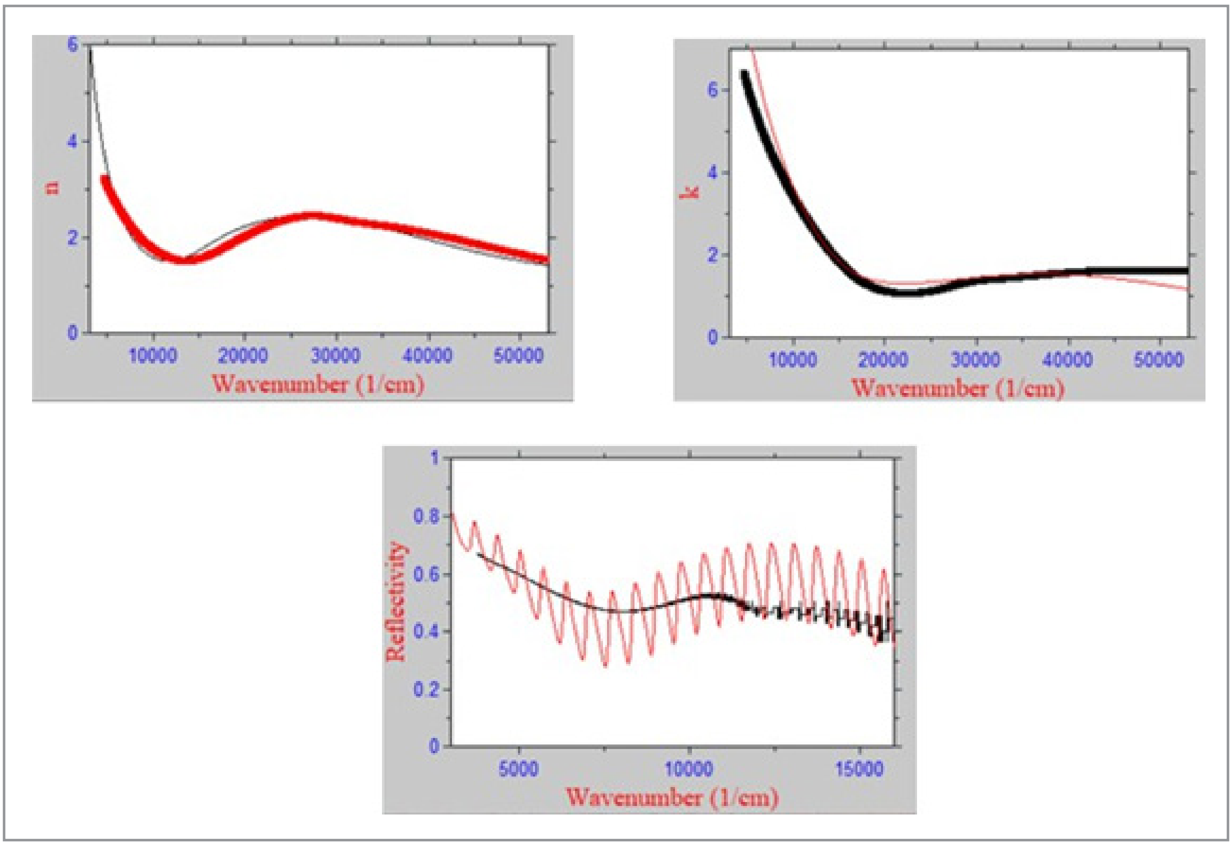

Figure 7: Simultaneous fits in RefFIT for wafer 6 using Drude-Lorentz Model

The parameters ωp (Wp in Fig. 8) and γ (G in Fig. 8) were extracted through these simultaneous fits from the Drude- term of the model parameters for which the fit was apt.

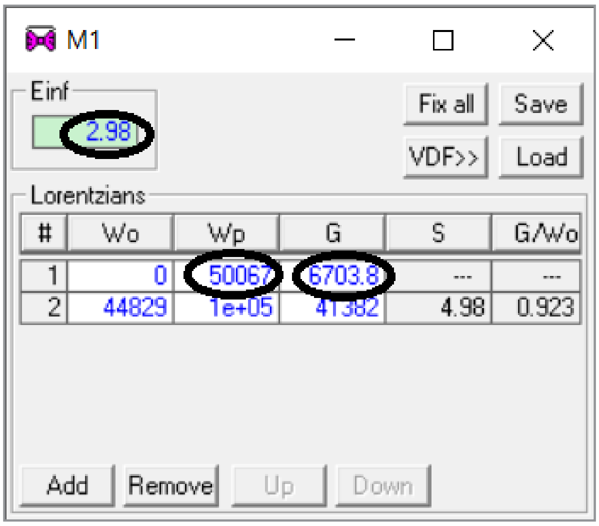

Figure 8: An example of extracted model parameters The values of the extracted parameters for each wafer are as listed in Table 2.

Table 2. List of extracted parameters for all wafers.

Wafer	ε_infinite	Plasma Frequency, ωp (cm-3)	Damping constant, γ
Wafer 1	2.37	49598	7185.9
Wafer 2	2.67	50067	6100.5
Wafer 3	2.08	43989	6128

Wafer 4	2.78	50875	7666.4
Wafer 5	3.27	52069	7748.3
Wafer 6	3.42	49763	4421.4

To find the apt thickness of each layer for wafers 3, 4 and 6, a special model with εinfinite=-2 was created in touch with a separate model for each layer. This model had parameters related to the layers. For example, for a single layer of TiN on a bare silicon substrate, the first layer is a Drude-Lorentz model as was derived with the expected thickness in the ωp column and the relative thickness as 0. The bare substrate is the second layer; for this we created a second model with constant dielectric function. So, ωp =0 and ε_infinite=n2, where n2 is the refractive index of silicon, which is 13.5 in our case. Fig. 9 is a snippet of this special model that we created to get the desired thicknesses of each layer to get the best simultaneous fits. More about this procedure can be understood from section 4.7 of the RefFIT software manual [15].

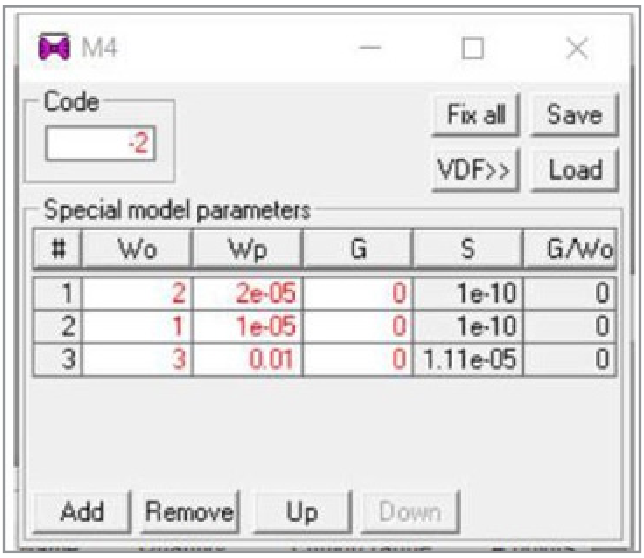

Figure 9: A special model created to get the desired thickness of each layer to get the best simultaneous fits

The values of the plasma frequency of TiN obtained through these measurements and fits are in line with the typical plasma frequencies of TiN in literature which is between 4.8 x 104 Hz to 1.45 x 1015 Hz, which roughly calculates to between 6120 cm-1 to 48360 cm-1 of wavenumber [16, 17]. These plasma frequencies obtained in Table 2 reinforce the use of the methodology employed in this part of our research about plasmonic materials to obtain the plasma frequency of TiN.

Carrier Concentration and Relaxation Time

The carrier concentration determines the plasma frequency. The sample possessing higher plasma frequency accompanies a higher carrier concentration. Our calculations of carrier density from the extracted parameters from RefFIT are in line with this trend as seen in Table 3. Normally, nitrides have carrier concentration in the range of 1022 cm-3 or 1028 m-3.

Table 3. Calculated carrier density, relaxation time and thickness of each wafer using the parameters extracted by RefFIT.

Wafer 1	6.31	4.64 x 10-15		
Wafer 2	6.423	5.43 x 10-15		
Wafer 3	5.5251	5.43 x 10-15	SiO2	200
			TiN	100
			Si	1.00E+05
Wafer 4	6.639	4.33 x 10-15	TiN	50
Wafer 5	6.954	4.303 x 10-15	SiO2	1000
			Si	1.00E+05
Wafer 6	6.352	6.31 x 10-15	SiO2	168
			TiN	50
			Si	1.00E+05

Metallicity of TiN depends also on the carrier relaxation time. More defects reduce the carrier relaxation time, and hence result in low metallicity. Thin films resistivity also depends on the relaxation time of the free electrons. Increased grain size means longer electron relaxation time. The relaxation times reported in this research are of the same order compared to [9] (orders of 10-15).

Further Validation of the Ref FIT Simulations

To verify the credibility of the results obtained through Ref FIT by fitting the optical constants with a model, wafer 2 was studied further in depth. The parameters obtained using these fits were used to calculate the permittivity and refractive index using the following two equations:

Drude Model

$$\varepsilon(\omega) = \frac{\omega_p^2}{\omega(\omega+\frac{i}{\gamma})}$$

Drude-Lorentz Model

$$\varepsilon(\omega) = \varepsilon_{infinite} + \frac{\omega_{p1}^2}{\omega^2 - i\omega\gamma_1} + \frac{\omega_{p2}^2}{\omega_{02}^2 - \omega^2 - i\omega\gamma_2}$$

The following plots were obtained (Fig. 10 and Fig. 11)

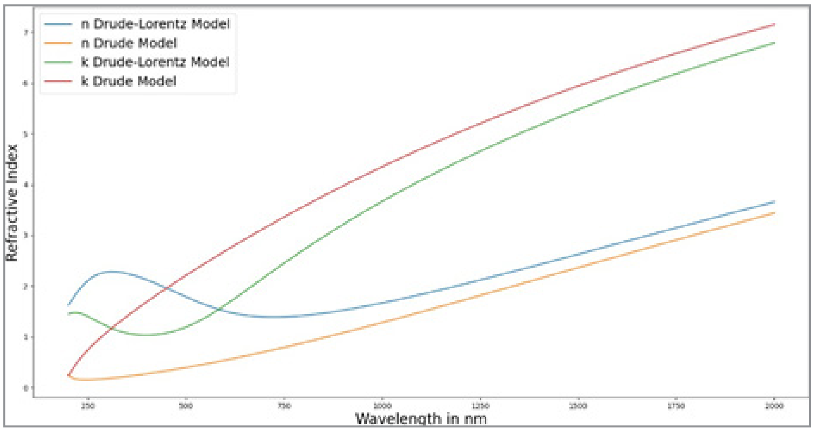

Figure 10: A comparison of n and k of TiN calculated using equations 2 and 3

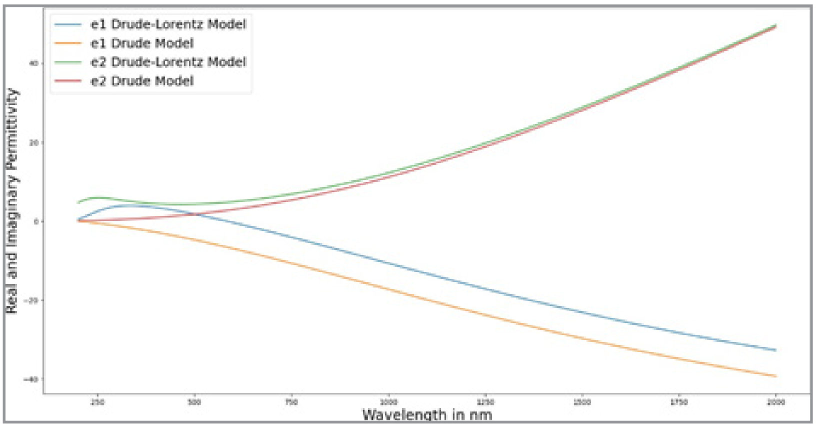

Figure 11: A comparison of real and imaginary permittivity of TiN calculated using equations 2 and 3

To understand which model between the Drude and the Drude-Lorentz terms are best for the calculations of permittivity and refractive index of TiN, a new sample with the parameters as listed in Table 4, sample B, of 100nm TiN thickness was studied and compared to the permittivity and refractive index of wafer 2.

Table 4: Parameters for Sample B of 100nm TiN layer for equation 4.

(eV)	(eV)
E infinite	0.7839
E_{pl}	6.0808
Y_D	0.9426
E_1	2.9655

F_1	0.0469
Y_1	0.9934
E_2	4
F_2	0.4458
Y_2	2
E_3	6.6355
F_3	6
Y_3	5.1801

The model used to calculate the n, k and permittivity of sample B is as follows. It has 3 Lorentz terms.

$$\varepsilon(E) = \varepsilon_{infinite} + \frac{E_{pl}^2}{-E^2 - iE\gamma_D} + \sum_j \frac{f_i E_{pl}^2}{E_j^2 - E^2 - iE\gamma_j}$$

The following results were obtained for sample B. The n and k obtained for TiN from ellipsometry measurements for wafer 2 is also plotted. It is noted that the refractive index, n and extinction coefficient, k of wafer 2 (obtained experimentally by ellipsometry) and calculated for Sample B using Equation 4 (one Drude and three Lorentz terms) are similar.

Finally, a comparison was made for n, k, real and imaginary permittivity for:

- **Wafer 2:** parameters obtained from RefFIT fit and calculated using Drude and Drude-Lorentz Model (Equations 2 and 3)
- **Wafer 2:** n and k obtained from ellipsometry measurements
- **Sample B:** calculated from parameters in Table 4.

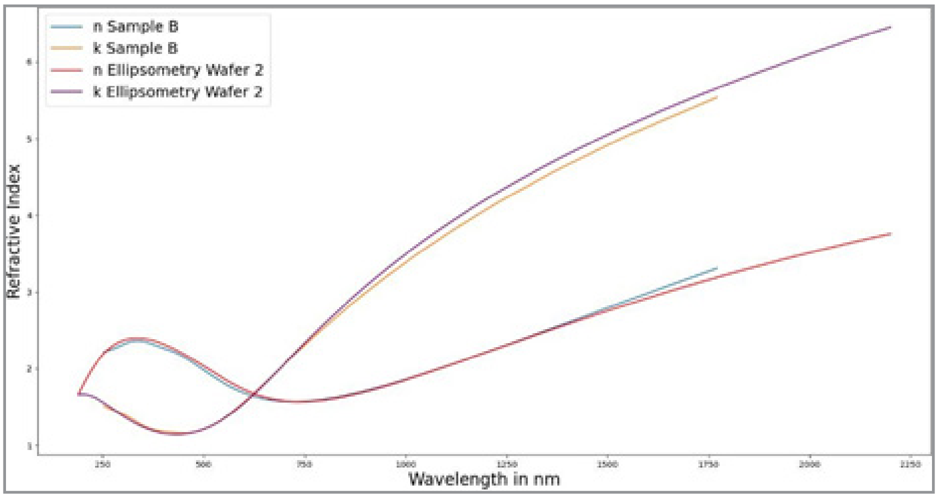

Figure 12: comparison of calculated n and k of sample B and from ellipsometry of wafer 2

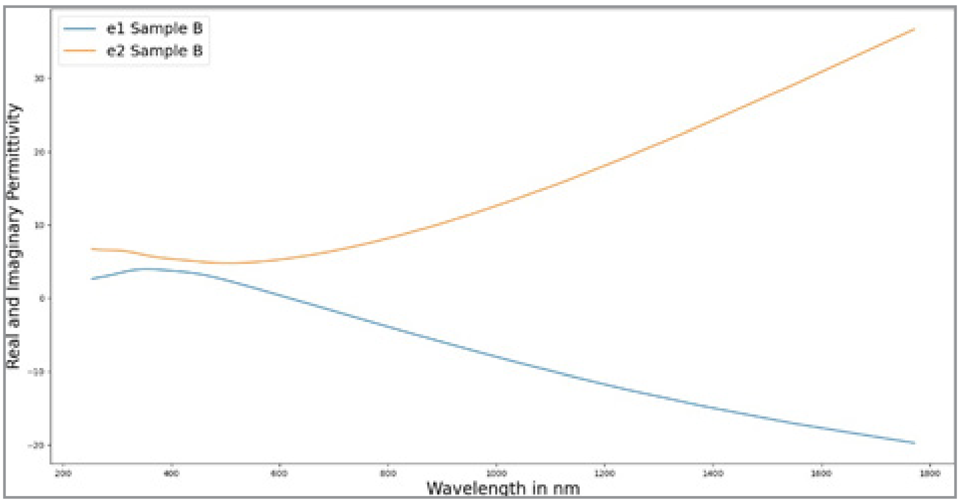

Figure 13: A comparison of calculated real and imaginary permittivity of sample B and from ellipsometry of wafer 2

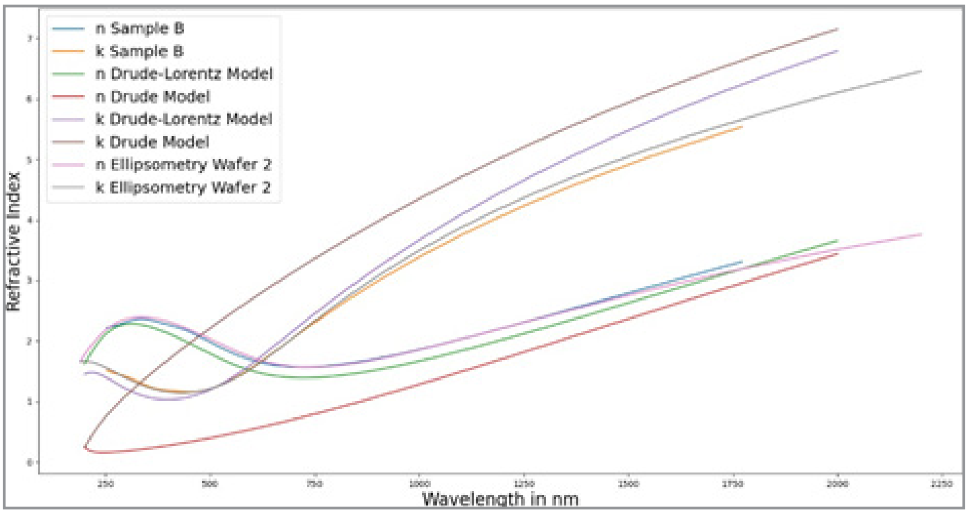

Figure 14: A comparison of all the calculated and measured n and k

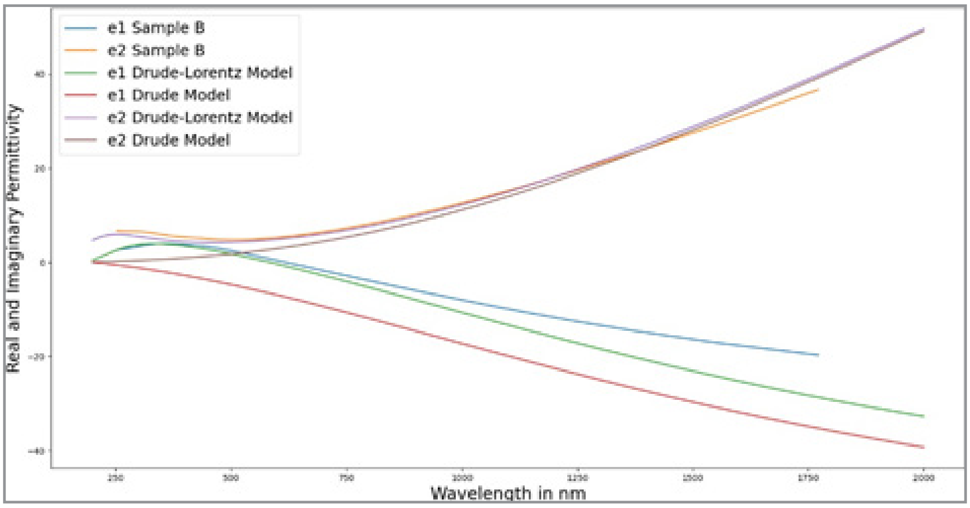

Figure 15: A comparison of all the calculated and measured real and imaginary permittivities

From these plots of Fig. 12, Fig. 13, Fig. 14 and Fig. 15, the n, k, real and imaginary permittivity (e1 and e2) plots for TiN obtained through only one Drude term are not similar. We derived that calculations using the parameters obtained from the RefFIT simulations are very similar to the n, k, e1, e2 for a totally different sample of the same thickness of the TiN layer obtained through calculations using formulae. Hence, the RefFIT simulations have been validated.

Conclusion

In this paper, we undertook a comprehensive analysis of optical data using the RefFIT software. This sophisticated tool proved highly effective for fitting data according to the Drude-Lorentz model, a framework well-regarded for its precision in modeling the optical properties of materials. Through meticulous simultaneous fitting of optical data, we successfully derived a plethora of parameters, for six distinct samples, that are critical for understanding the behavior of materials, particularly nitrides, for plasmonic applications. The parameters obtained directly from the fits were the plasma frequency and the damping constant essential in calculating also the carrier density and relaxation times for each sample. These calculations are pivotal as they provide insights into the electronic properties of the materials, such as how quickly charge carriers can move through the material and how frequently they scatter. The trends observed in our calculated plasma frequency, carrier concentrations and relaxation times were consistent with established trends in nitrides, reinforcing the reliability of our fitting process and the validity of our results.

To ensure the accuracy and validity of our findings, we extended our analysis to another sample – a 100 nm thick TiN film with different intrinsic parameters – which was not part of the lot. The results from this sample were in strong agreement with those obtained from the initial analysis, thus providing further validation of our approach and the robustness of the RefFIT software in handling diverse material parameters.

Another significant observation from our study was the inadequacy of using a model with only one Drude term without any Lorentz terms for the RefFIT simulations. The Drude model, while useful for describing the free electron response in materials, was insufficient on its own to accurately capture the complex optical behavior of the samples. The inclusion of Lorentz terms, which account for bound electron oscillations, was crucial for achieving a precise fit. This finding underscores the necessity of employing a comprehensive Drude-Lorentz model to accurately describe the optical properties of TiN.

In summary, this paper successfully highlights the efficacy of the RefFIT software in fitting optical data using the Drude-Lorentz model, facilitating the extraction of critical plasmonic parameters of TiN.

Statements and Declarations

Funding

The author declares that no fund or grants were received during the preparation of this manuscript. However, the author would personally like to thank Mr. S. G. Masood for his kind contribution.

Competing Interests

The authors have no relevant financial or non-financial interests to disclose.

Data Availability

The datasets generated during and/or analysed during the current study are not publicly available but are available from the author on reasonable request.

References

1. Ramesh, R., & Spaldin, N. A. (2007). Multiferroics: progress and prospects in thin films. Nat Mater 6, 21-29.
2. Reddy, H., Guler, U., Kudyshev, Z., Kildishev, A. V., Shalaev, V. M., Boltasseva, A. (2017). Temperature-dependent optical properties of plasmonic titanium nitride thin films. ACS Photonics 4, 1413-1420.
3. Khurgin, J. B., & Boltasseva, A. (2012). Reflecting upon the losses in plasmonics and metamaterials. MRS Bulletin, 37(8), 768-779.
4. Asoro, M., Damiano, J., & Ferreira, P. (2009). Size effects on the melting temperature of silver nanoparticles. Microscopy and Microanalysis, 15(2), 706-707.
5. Chernyshev, A. P. (2009). Effect of nanoparticle size on the onset temperature of surface melting. Materials Letters, 63, 1525-1527.
6. Alarifi, H. A., Atiş, M., Özdoğan, C., Hu, A., Yavuz, M., Zhou, Y. (2013). Determination of complete melting and surface premelting points of silver nanoparticles by molecular dynamics simulation. Journal of Physical Chemistry C, 117, 12289-12298.
7. Bower, R., Loch, D. A. L., Ware, E., Berenov, A., Zou, B., Hovsepian, P. E., Ehiasarian, A. P., & Petrov, P. K. (2020). Complementary metal-oxide-semiconductor compatible deposition of nanoscale transition-metal nitride thin films for plasmonic applications. ACS Appl Mater Interfaces 12, 45444-45452.
8. Maurya, K. C., Shalaev, V. M., Boltasseva, A., Saha, B. (2020). Reduced optical losses in refractory plasmonic titanium nitride thin films deposited with molecular beam epitaxy. Opt Mater Express 10, 2679-2692.
9. Sundari, S. T., Ramaseshan, R., Jose, F., Dash, S., Tyagi, A. K. (2014). Investigation of temperature dependent dielectric constant of a sputtered TiN thin film by spectroscopic ellipsometry. J Appl Phys 115, 033516.
10. Briggs, J. A., Naik, G. V., Petach, T. A., Baum, B. K., Goldhaber-Gordon, D., & Dionne, J. A. (2016). Fully CMOS-compatible titanium nitride nanoantennas. Appl Phys Lett 108, 051110.
11. Briggs, J. A., Naik, G. V., Zhao, Y., Petach, T. A., Sahasrabuddhe, K., Goldhaber-Gordon, D., Melosh, N. A., ……. & Dionne, J. A. (2017). Temperature-dependent optical properties of titanium nitride. Appl Phys Lett 110, 101901.
12. Vertchenko, L., Leandro, L., Shkondin, E., Takayama, O., Bondarev, I. V., Akopian, N., ……. & Lavrinenko, A. V. (2019). Cryogenic characterization of titanium nitride thin films. Opt Mater Express 9, 2117-2127.
13. Ringdalen, E., Tangstad, M. (2016). Softening and melting of SiO2, an important parameter for reactions with Quartz in Si production. In R. G. Reddy, P. Chaubal, P. C. Pistorius, & U. Pal (Eds.), Advances in molten slags, fluxes, and salts: proceedings of the 10th international conference on molten slags, fluxes and salts, 43-51.
14. Kuzmenko, A. B. (2005). Kramers–Kronig constrained variational analysis of optical spectra. Rev Sci Instrum 76, 083108.
15. Kuzmenko, A. (2018). Guide to Ref FIT software to fit optical spectra. https://reffit.ch/wp- content/uploads/2018/10/Manual.pdf.
16. Ferry, V. E., Sweatlock, L. A., Pacifici, D., Atwater, H. A. (2008). Plasmonic nanostructure design for efficient light coupling into solar cells. Nano Lett 8, 4391-4397.
17. Yu, P. Y., & Cardona, M. (2010). Fundamentals of semiconductors: Physics and materials properties. Springer, New York.

Copyright: ©2025 Maria Masood. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.