Novel Quantum Materials for Low Power Electronics

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Abstract

Global energy consumption is increasing rapidly due to the proliferation of electronic devices, causing sustainability concerns, thereby requiring the use of new semiconductor materials. The quantum material Vanadium Dioxide (VO_2) is a prime candidate, as it undergoes a sharp insulator-to-metal phase transition (IMT) near room temperature (67ºC) and can act as a switch. The IMT can be optimized by electron doping using tungsten (W 6+). Currently, there are few models for determining the properties of this alloy material, given its complex electronic properties. Further, characterization of materials containing low dopant concentrations is challenging. In this study, linear models were developed based on experimental data collected from literature review to define the relationships between composition (dopant atom-percent concentration, ionic radius) and IMT properties (transition temperature, threshold voltage, activation energy). The linear models demonstrate that transition temperature and threshold voltage reduce as W concentration increases (~21K/at. % and ~19.6V/at. % respectively). These models were compared with impurity conduction theory and were found to agree at doping concentrations <1.8 at. %. Threshold voltage for IMT displays a similar trend as IMT temperature, suggesting that their mechanisms are related. Rutherford Backscattering Spectroscopy (RBS) was simulated using SimNRA and was determined to be a powerful method for characterizing the concentration of tungsten doped VO_2 thin films. The models predict that power consumption per device could reduce as much as 76%. The results from this study have established a quantitative relationship between impurity doping, transition temperature, and threshold voltage reduction to design low power electronics.

Novel Quantum Materials for Low Power Electronics

The need for low power electronics

ChatGPT, a generative artificial intelligence (AI) tool, has become widely known since its introduction. As new versions are released, interest and excitement only grow, with more and more companies entering the AI sector and creating their own products. However, as global usage of AI and electronic devices increases, with the increased accessibility of mobile phones and computers, power consumption also dramatically grows, causing concerns about the sustainability of future computing technologies. In January 2023, ChatGPT consumed around the same amount of electricity as 175,000 people (Ludvigsen, 2023). It is predicted that by 2027, AI servers will consume upwards of 85 terawatt-hours of electricity per year, which is more than some small countries (de Vries, 2023).

As a result, scientists are currently looking for ways to build computers that require less energy. One source of inspiration for these new computers is the human brain, given that it can perform complex tasks rapidly while using an extremely limited amount of energy (around 20 W). These brain-inspired, or neuromorphic, computers have an architecture emulating the brain, with devices made from materials acting as artificial neurons and synapses. Scientists are currently facing challenges with the materials needed to build these computers, as current semiconductor materials, such as silicon, have limited properties that are not conducive to building these computers (Kendall & Kumar, 2020).

Opportunities with quantum materials

Quantum materials belong to a category of materials for which the laws of classical physics do not accurately describe their properties. In classical materials, electrons are

considered independent of one another, while for quantum materials, electrons are often strongly correlated (behavior dependent on one another), and therefore have complex electronic states (Cava et al., 2021; Keimer & Moore, 2017). As the composition of these materials is altered, especially through doping, or alloying small amounts of impurities with the material, their properties can be significantly modified (Zunger & Malyi, 2021). Quantum materials have a wide range of applications, from quantum computing to low-power electronics to thermochromic windows, so it is crucial to understand their properties. The model quantum material Vanadium Dioxide (VO_2) is widely studied due to its applicability to a wide range of fields, including brain-inspired computing, so this study focused on VO_2. The main property of interest is the sharp insulator-metal transition (IMT) in this material near room temperature (67 ºC) that can act as a non-linear switching device. Such a device can function as an artificial neuron to emulate switches for information transfer in the brain. The temperature and/or threshold voltage needed for switching and methods to control them are therefore of utmost importance (Chen et al., 2016).

The IMT properties of VO_2 can be further controlled by doping the material. One of the most widely used dopants is tungsten (W 6+), as it has been shown to depress the transition temperature quite effectively (Xue & Yin, 2022). The exact mechanisms of altering the IMT properties are currently unknown, as it is not yet fully clear if the structural distortions or added electrons are the main reason for changes in the IMT behavior. Because tungsten is an n-type dopant, it donates electrons into the lattice causing the conductivity to increase as the band structure is altered. Conductivity increases as electrons at the dopant band are more easily excited to the conduction band, causing the number of free electrons to increase. As conductivity increases, the energy needed to excite electrons into the conduction band decreases, so the

insulator-metal phase transition can happen at lower temperatures. In addition to this, tungsten is a larger ion than vanadium, so it is possible that the addition of tungsten may cause strain on the lattice, resulting in changes in IMT behavior. Therefore, tungsten-doping is a powerful strategy for reducing the phase transition temperature in VO_2 (Xue & Yin, 2022).

The composition of materials can be altered through doping, which is performed by many different processes and introduces small amounts of impurities into materials. Doping can significantly alter the properties of quantum materials, depending on the type of dopant used (Zunger & Malyi, 2021). In semiconductor materials, such as VO_2, dopants are often used for altering the electrical properties of the material. Dopants with a higher valence (n-type) will tend to donate electrons, therefore increasing the conductivity by increasing the number of free electrons. Dopants with lower valence (p-type) will tend to accept electrons (Fiore, 2020). Thus, composition is directly related to electrical conductivity, as based on the dopant that is used, the conductivity of the material will change. This also shows how composition is related to the phase transition, since the conductivity of the material directly correlates to the insulator-metal transition and corresponding properties. Figure 1 illustrates the reduction in insulator-metal transition temperature in VO_2 with electron donor such as W addition. As seen in the schematic, both the insulating state resistance and the transition temperature decrease with increasing tungsten doping. This is because the electrons doped from tungsten weaken the insulating state and enable energy efficient transition from one conducting state to another.

Figure 1: Change in transition temperature as a function of W-doping

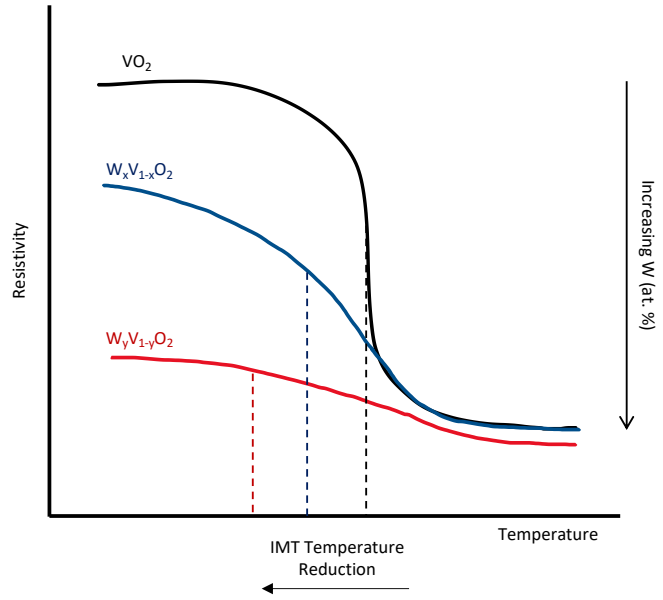

Fig. 1 schematically shows the change in transition temperature as a function of W-doping.

In addition to causing electrical changes, doping can also have structural effects (Zunger & Malyi, 2021). When larger ions are inserted into the lattice, they can cause distortions as the lattice adjusts to compensate for these changes. If the dopant concentration is too high, the lattice can collapse under the strain of the distortions, causing a new crystal structure to form. To prevent this from happening, small amounts of dopant are used.

Challenges in modeling properties of quantum materials

A major challenge that scientists are currently facing with understanding the IMT properties of quantum materials is the limited resources and lack of accurate theoretical models (Stanev et al., 2021). Experiments yield limited datasets and are often expensive and resource intensive to perform. Theoretical models are often inaccurate due to the unique and complex nature of quantum materials, as their properties do not align with physics that these models are based on.

As such, it is necessary to develop new models for quantifying and predicting the properties of quantum materials, especially as they relate to composition.

One significant theoretical model is Adler's model, developed in the late 1960s to explain the mechanism by which impurities cause a reduction in the insulator-metal transition temperature. The Adler Model is represented by the equation:

$$\frac{E_g}{kT_t} = 8.1(1 + 4x_d) + \left(\frac{x_d}{2}\right)\ln\left(\frac{1}{x_d}\right)$$

where E_g is the band gap, k is the Boltzmann constant, T_t is the transition temperature, and x_d is the dopant concentration. Adler's model states that as impurities are introduced into the material, the band gap reduces. The model elegantly combines semiconductor theory with novel properties of phase transition materials. This reduction in the band gap, combined with the introduction of the impurity band, allows for greater electrical conduction at lower temperatures, since less energy is required to excite electrons into the conduction band (Adler & Brooks, 1967). The model is shown below.

Figure 2: Comparison of classical semiconductor band model and Adler models

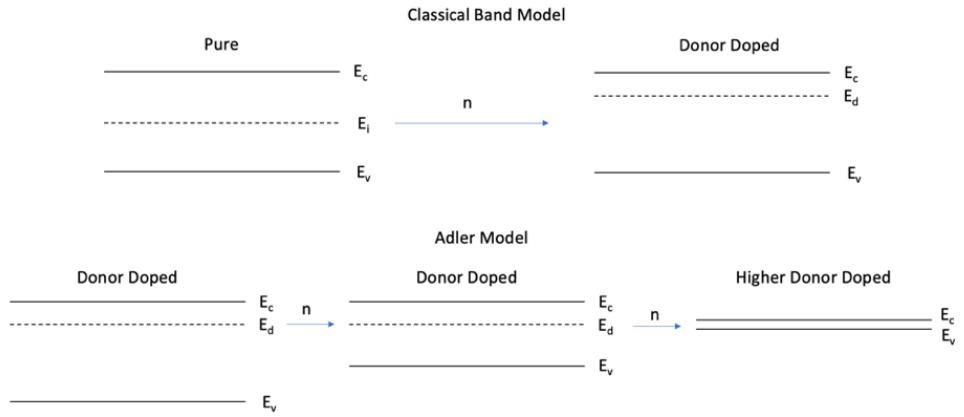

Fig. 2 shows the Adler model wherein adding an electron donor reduces the band gap of the parent crystal.

Another grand challenge lies in determining the composition of the alloyed material after the dopant is added. Rutherford Backscattering Spectroscopy (RBS) is a characterization technique used to determine the composition of thin film materials. A particle accelerator is used to excite helium ions to high energies, which are then fired towards the target sample. A detector is used to measure the energy of the backscattered ions. The backscattered ions have varying energies depending on where in the sample they have backscattered from and the mass of the element that they collided with. For example, an ion that collided with a heavier element will have a lower backscattered energy, since it will have lost more energy in the collision. Based on the energies that the detector measures, a spectrum is produced with different peaks at varying energy levels that correspond to the amount of the element present in the compound. Through analysis of the spectrum, it is possible to determine the composition of the compound being characterized. The high sensitivity of technique is especially useful for characterizing materials that may have low concentrations of certain components. Therefore, RBS is a powerful tool for characterizing doped thin films (Evans et al., 1992).

In this study, a comprehensive review of literature from the past 20 years was conducted to develop models that relate the composition of pure and cation doped VO_2 and various IMT properties. Phase transition temperature was focused on given its central role in optimization of this material for various applications, and due to the larger volume of data found. Other characteristics studied include the effect of ionic radius on transition temperature, the effect of tungsten (W) concentration on threshold voltage, and the effect of W-concentration on the activation energy for electron conduction. It was hypothesized that as the tungsten concentration increased, the IMT temperature would decrease, and that a similar trend would occur for threshold voltage (Zunger & Malyi, 2021; Xue & Yin, 2022). It was hypothesized that the

activation energy will decrease as tungsten is added (Mulchandani et al., 2021). It was also hypothesized that larger ionic radii would cause the transition temperature to decrease (Shao et al., 2018). Using the software package SimNRA, the RBS spectra of varying compositions $W_xV_{1-x}O_2$ were studied. It is hypothesized that using this technique we will be able to distinguish these compositions based on examination of the spectrum even when the doping concentrations are close in value.

Broader significance of the research project

Besides interest in brain-inspired electronics, VO_2 has a wide range of applications due to its tunable electrical and optical properties. VO_2 is used as a coating in thermochromic windows, as its transition from insulator to metal also results in a change in the thermal emissivity of the material (Cui et al., 2018). Through this transition, the coating on the window changes from clear to opaque, causing light to be reflected beyond a critical temperature. These windows have a huge potential to reduce energy consumption by heating and cooling systems in buildings and homes, as the reflection or absorption of thermal energy will result in a reduced need for these systems (Cui et al., 2018). VO_2 also has applications in defense and space technology, as it can act as a coating on spacecrafts and rovers, thereby reflecting the heat of the sun and protecting the technology from overheating (Yamagata et al., 2023). In all these studies, it is of great importance to be able to tune the transition temperature to suit the application domains. Hence, the results from this project should be of interest in these emerging applications. The models produced provide insight into the transition phenomena of VO_2, which is incredibly important for optimizing this material.

Materials & Methods

In this study, papers from the past 20 years were reviewed and data from these papers was used to analyze and develop the model. A few review papers were chosen first for developing a broad understanding of the current state of the field. Some of the papers with relevant experimental results were extracted from the reference sections of these papers. Other literature was found through key-word searches. A full list of papers is included in the references section. From the papers, data was selected, initially relating to the relationship between tungsten concentration (atomic percent) and insulator-metal transition temperature (Kelvin). The data collected was then recorded in tables in a spreadsheet, alongside information regarding the procedures for material synthesis, any relevant definitions or notes, and the reference. Once data compilation was completed, the data was plotted, and lines of best fit were generated. Following this, the source material was re-read to gain an understanding of the properties observed. A similar procedure was followed to study the effect of dopant ionic radius (pm) on the IMT temperature (K) at a fixed concentration (at. %) and on the rate of change in the IMT (K/at. %), and the effect of tungsten concentration on activation energy (meV) and threshold voltage (V).

Through the literature search, the Adler model was found. After reading more about the Adler model, it was compared with the linear model developed to evaluate the predicted values of change in the insulator-metal transition temperature. This comparison was done through using varying values of dopant concentration to determine the magnitude of difference in the transition temperature. The exact value of the transition temperature was not directly compared because of the difference in scaling factor between the two models.

Following the literature search, the software package SimNRA was used to simulate the Rutherford Backscattering Spectroscopy (RBS) spectra of varying compositions of $W_xV_{1-x}O_2$.

Four concentrations were simulated: Pure VO_2, 0.5 at. % tungsten ($W_{0.005}V_{0.995}O_2$), 1 at. % tungsten ($W_{0.01}V_{0.99}O_2$) and 1.6 at. % tungsten ($W_{0.016}V_{0.984}O_2$). The spectra were overlaid to examine differences. The doping concentrations were chosen such that the transition temperature is shifted down towards room temperature that is of interest to the above-mentioned applications.

Results

A series of linear models are depicted below which show the relationship between composition and phase transition characteristics.

Figure 3: IMT Temperature as function of W-doping Concentration

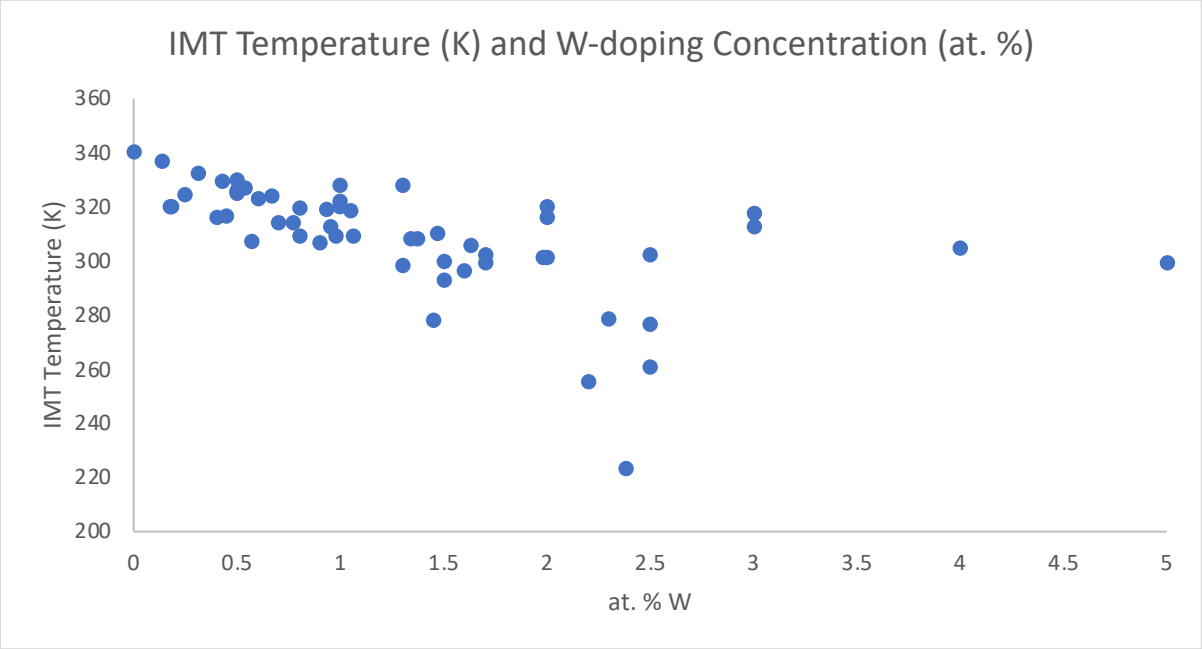

Fig. 3 shows the relationship between the insulator-metal transition temperature and tungsten doping concentration. There is a clear decrease in temperature due to doping. At higher doping concentration, the slope is flatter than at lower doping concentration. This clearly indicates that as doping concentration increases, the transition behavior is modified and is discussed further in the project. Data was obtained from references 15-27.

Figure 4: IMT Temperature as a function of W-doping Concentration (<1.8 at. % doping)

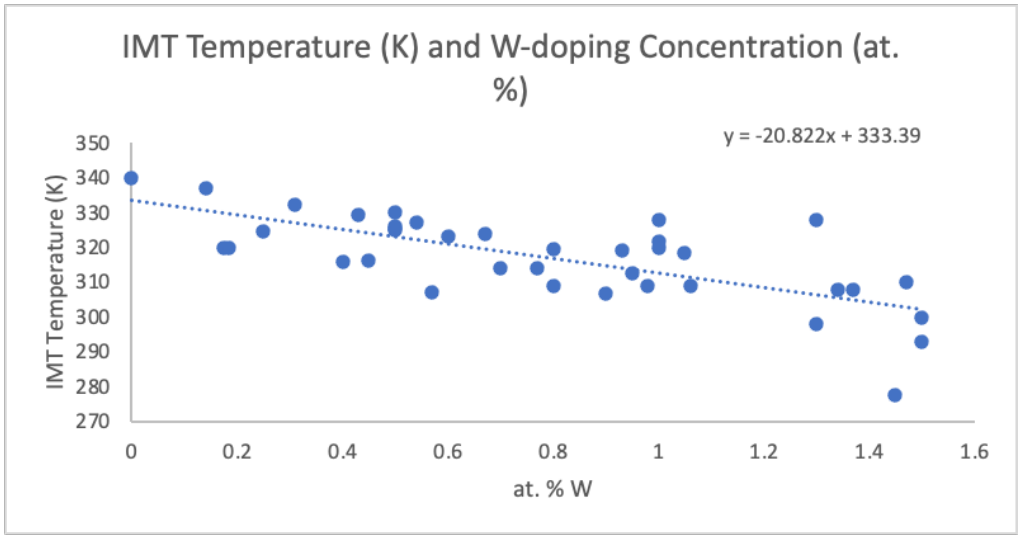

Fig. 4 shows the relationship between the insulator-metal transition temperature and tungsten concentration. As tungsten concentration increases, the temperature decreases. This slope agrees well with both experimentally obtained and theoretically calculated relationships. Data was obtained from references 15-27.

Figure 5: Rate of Decrease in IMT Temperature versus Dopant Ionic Radius

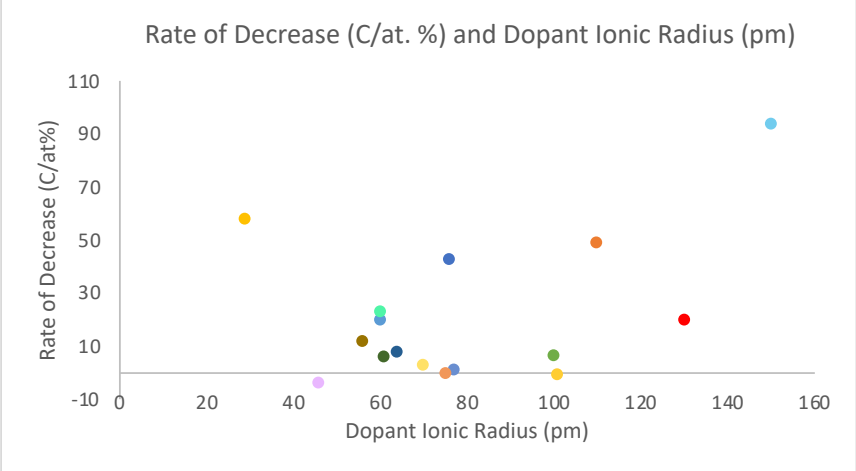

Fig. 5 shows that there is no clear correlation between the rate of decrease in the IMT temperature and dopant ionic radius. Data was obtained from references 11, 16, 28, and 32. Each color represents a different dopant (Li^{+}(76), Na^{+}(110), K^{+}(150), Be^{2+}(29), W^{6+}(60), Eu^{3+}(100), Mg^{2+}(70), F^{-}(130), Mo^{6+}(56), Nb^{5+}(64), Fe^{3+}(61), Sb^{3+}(74), Zr^{4+}(75), Ge^{4+}(46), and Tb^{3+}(101)).

Figure 6: IMT Temperature versus Dopant Ionic Radius (at 3 at. % dopant concentration)

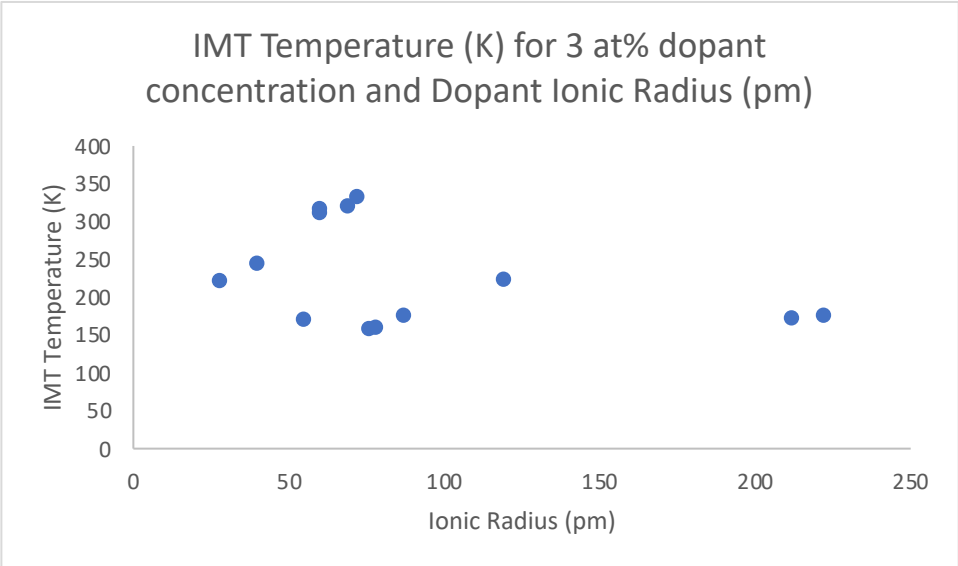

Fig. 6 shows that there is no clear relationship between insulator-metal transition temperature (at a fixed 3 at. % doping level) and dopant ionic radius. Data was obtained from references 11, 16, 24, and 32.

Figure 7: Activation Energy versus W-doping Concentration

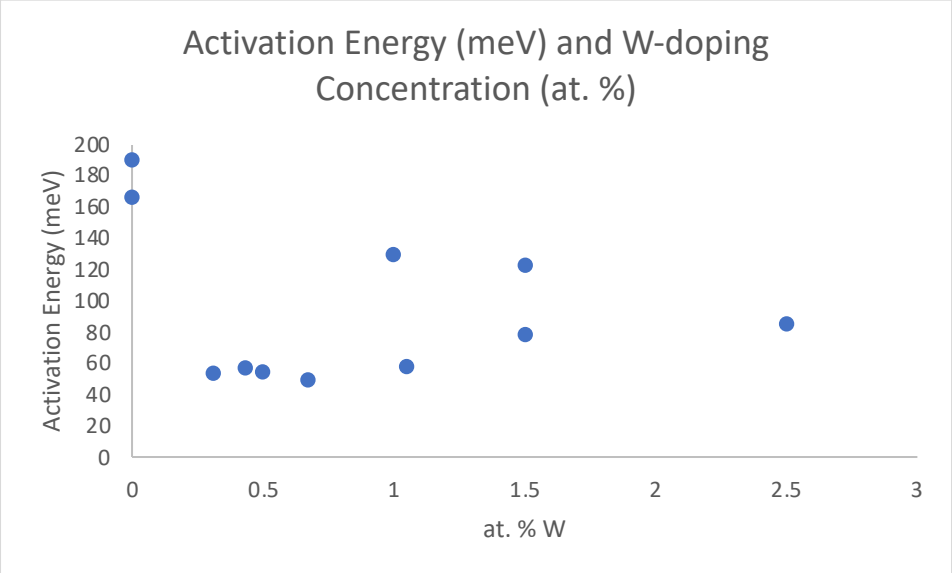

Fig. 7 shows the relationship between activation energy and tungsten doping concentration. Activation energy drops immediately following doping, although there is not a significant difference between low doping and high doping concentrations. Data was obtained from references 12, 19, and 26.

Figure 8: Threshold Voltage and W-doping Concentration

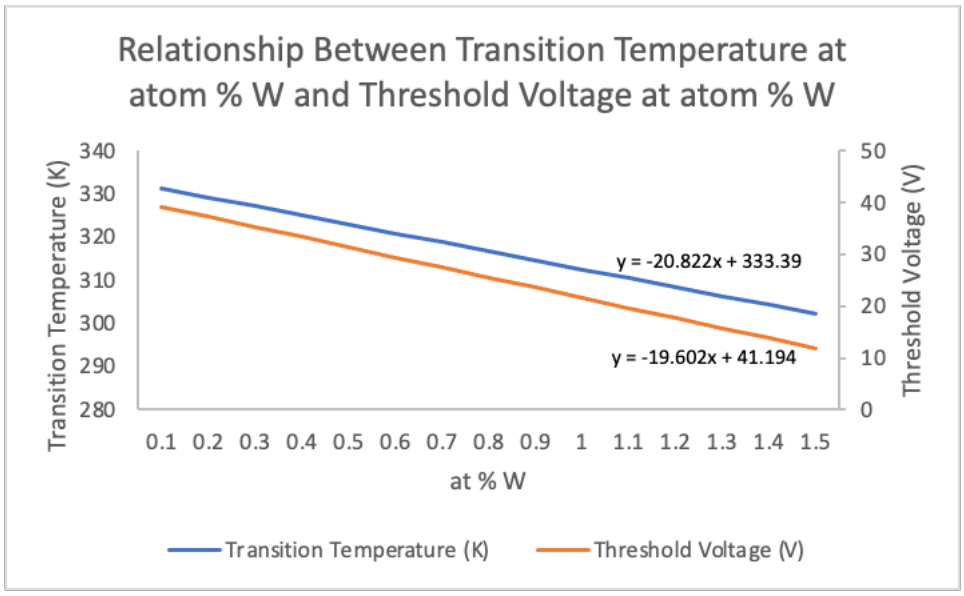

Fig. 8 shows the relationship between transition temperature and tungsten concentration as well as threshold voltage and tungsten concentration. Threshold voltage decreases at a very similar rate to transition temperature, indicating that the mechanisms behind this decrease are likely similar. Data obtained from references 15-27 and 29.

Figure 9: Comparison of Linear Model with Adler Impurity Conduction Model

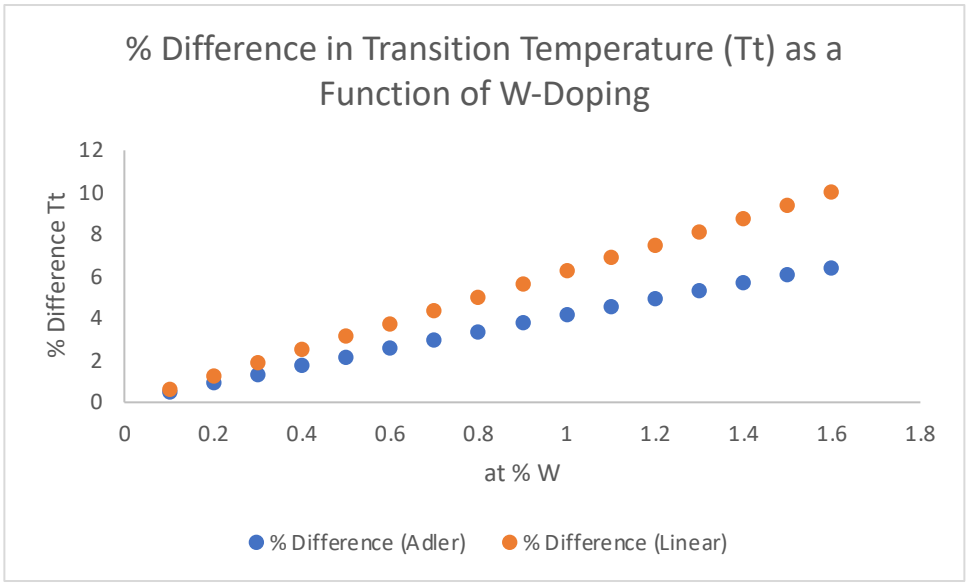

Fig. 9 shows the difference between the linear model and Adler's model. The two models agree closely at low doping concentrations and begin to diverge at higher concentrations.

Table 1: Rate of Decrease of Insulator-Metal Transition Temperature

Source	Rate of Decrease (K/at%)
Linear Model (This Work)	20.82
Zhang et al., 2013 (Density Functional Theory – hybrid functionals)	18.6
Zhang et al., 2013 (Density Functional Theory – GGA + U)	27

Table 1 shows the values for the rate of decrease in the insulator-metal transition temperature for W-doping. The linear model developed in this project agrees with the experimentally observed and theoretically calculated rate of change.

Figure 10: RBS Spectra of VO_2, $W_{0.005}V_{0.995}O_2$, $W_{0.01}V_{0.99}O_2$, $W_{0.016}V_{0.984}O_2$

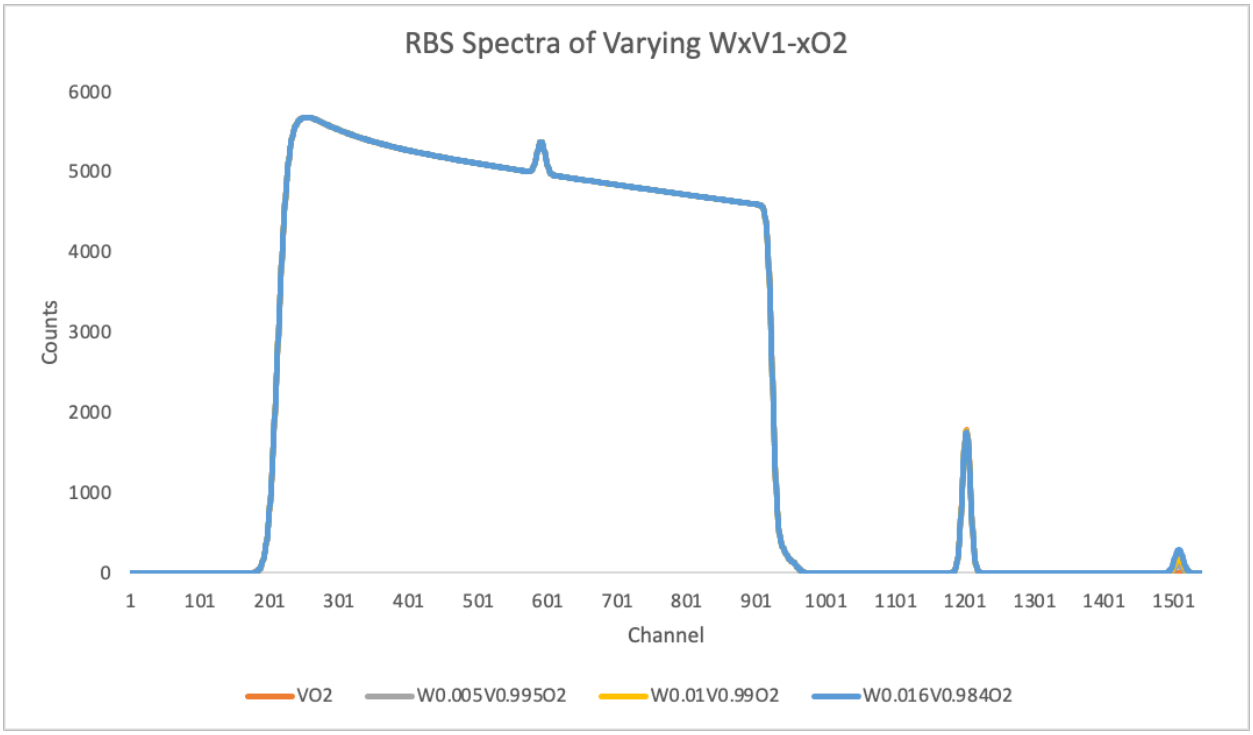

Fig. 10 shows the RBS spectra of varying compositions of $W_xV_{1-x}O_2$ ($100 * 10^{15}$ atoms/cm^2) on a silicon substrate ($10000 * 10^{15}$ atoms/cm^2) as simulated using the software package SimNRA. Except for the W peak, rest of the spectrum is quite similar as expected. As shown in the zoomed in region in next figure, it is possible to distinguish the compositions from one another.

Figure 11: RBS Spectra of Tungsten Peak of VO_2, $W_{0.005}V_{0.995}O_2$, $W_{0.01}V_{0.99}O_2$, $W_{0.016}V_{0.984}O_2$

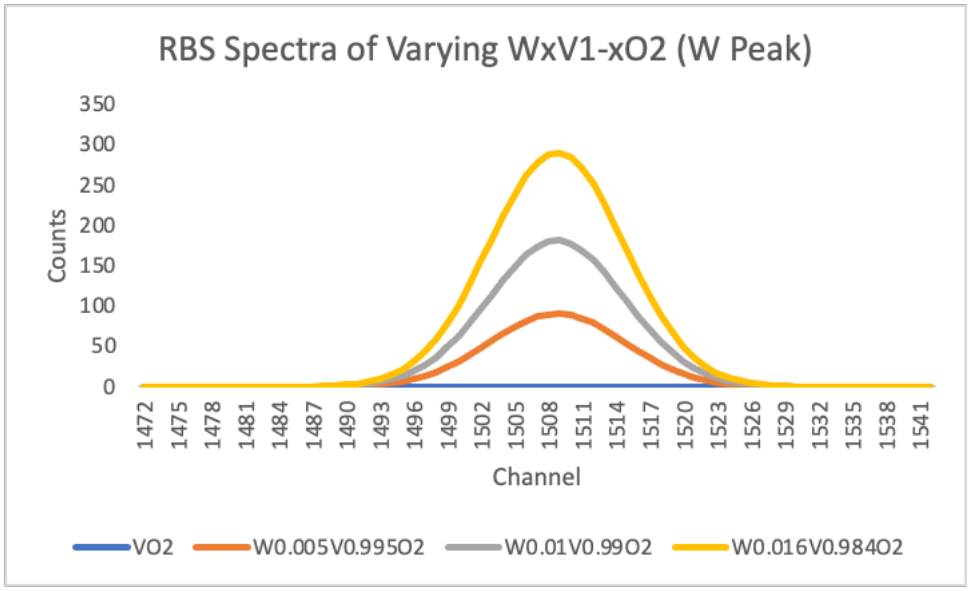

*Fig. 11 shows the RBS spectra of the tungsten peak of varying compositions of $W_xV_{1-x}O_2$ (100 * 10^{15} atoms/cm^2) on a silicon substrate (10000 * 10^{15} atoms/cm^2) as simulated using the software package SimNRA. This further shows the visibility of the difference in tungsten peak height, demonstrating that it is possible to distinguish very similar concentrations using this technique.*

Discussion

The insulator-metal transition of VO_2 was studied to determine the relationship between various IMT properties and the composition of doped-VO_2. Linear models were developed to represent these relationships. The insulator-metal transition temperature was focused as the main property of interest due to its wide range of applications, from brain-inspired electronics to space technologies and thermochromic windows.

It was hypothesized that the insulator-metal transition temperature would decrease as tungsten concentration increased. This hypothesis was supported by the data, as the IMT temperature decreased with increasing W-doping (Figure 3). This relationship follows a linear trend at low doping concentrations (< 1.8 at. % W), as the transition temperature decreases at a rate of roughly 21 K/at. % W (Figure 4). The rate of decrease extracted from our study aligns with both experimentally observed rates of change and theoretically calculated rates of change (Table 1). Zhang et al. (2013) reports a rate of change in transition temperature between 18.6 and 27 K/at. % depending on the theory technique. It is observed that there is a difference in the rate of decrease between low and high doping concentrations. This suggests that new physics may be governing the mechanisms of the IMT at higher doping concentration.

The linear relationship between W-doping concentration and IMT temperature was compared with Adler's model. It was found that these two models agree at low doping concentrations but begin to diverge at higher concentrations (Figure 9). The Adler model is further supported by the drop in activation energy. The activation energy can be obtained from fitting the conductivity vs. temperature according to the equation:

$$\sigma = e^{\frac{-E_a}{kT}}$$

where σ is the conductivity, E_a is the activation energy (eV), k is the Boltzmann constant, and T is temperature (Kelvin).

Activation energy drops immediately after doping, although no distinct relationship exists between activation energy and increasing W-concentration (Figure 7). This result supports the hypothesis that activation energy will decrease with the addition of tungsten. This finding supports Adler's theory, as it demonstrates that the band gap must reduce after doping, since the energy needed to excite electrons into the conduction band reduces.

The relationship between structural effects and the transition temperature was also investigated through examining the relationship between ionic radius and transition temperature. No distinct relationship was observed between the effect of ionic radius on the rate of change in the transition temperature (Figure 5). The effect of the size of the dopant's ionic radius on the transition temperature at a fixed dopant concentration of 3 at. % was also examined. There does not seem to be a clear correlation between these two properties either. Therefore, it is possible to determine that the structural properties of the dopant do not have a significant impact on the insulator-metal transition compared to the electrical properties of the dopant.

The threshold voltage for switching was also explored. Threshold voltage was shown to decrease at a rate of 19.6 V/at. % W which is similar to the transition temperature (Figure 8). This is significant because it reveals that the mechanisms behind the decrease in transition temperature (thermal) and threshold voltage (electrical) are quite similar. Hence, it is possible to conclude that the change in the temperature to initiate IMT can be electrically driven, as the threshold voltage is affected due to electrical properties of dopants. This reaffirms the idea that the electrical properties of the dopant have a more significant effect on the insulator-metal transition temperature than the structural properties.

The discrepancies between the Adler model and the linear model found in this study can be attributed to the non-linear term in the Adler model. At lower doping concentrations, the non-linear term does not have a major impact on the predicted value, and therefore, it behaves like the linear function. At higher doping concentration, the non-linear terms begin to dominate the equation, causing a difference in the predicted values.

Through the reduction of both the transition temperature and the threshold voltage of VO_2, low power electronics can be realized. By lowering the insulator-metal transition temperature, the switch between states can occur at lower temperatures and therefore will require reduced electrical energy. For example, to achieve transition at room temperature, ~1.6 at. % tungsten doping concentration is required. This will allow transistor-like devices built from W-VO_2 to function at lower temperatures, which will in turn allow the computer to function at lower temperatures. This means that less energy will be required to run brain-inspired computers, thereby reducing the power consumption of these devices. Additionally, since the threshold voltage decreases with tungsten doping, the voltage needed for devices to function will decrease. The relationship found between threshold voltage and increasing tungsten concentration predicts that through tungsten doping, the threshold voltage of VO_2 decreases by 76% indicating that the power consumption of VO_2 devices per switch is expected to be 76% lower with W-doping.

Since the discovery of VO_2, there has been argument surrounding the exact mechanisms by which doping affects the insulator-metal transition. Some scientists argue that structural strain have a greater effect on the transition, while others maintain that the electrical effects are the dominant effect. Though both structural and electrical properties have some level of influence on the IMT transition characteristics, the results of this study strongly suggest that the electrical effects of doping have a greater effect on the transition temperature. When tungsten is added to

VO_2, the lattice parameters shift, with parameters *a* and *b* increasing, *c* decreasing, and the β-angle decreasing (Mulchandani et al., 2021; Zhang et al., 2013). This means that the lattice of VO_2 increases with the addition of tungsten, likely to account for the larger ionic radius, which favors a higher symmetry. This also causes VO_2 to adopt a more metallic or rutile structure, which results in higher conductivity and the switch to the metallic state (Mulchandani et al., 2021). When the lattice expands, the transition temperature also decreases (Zhang et al., 2013). The Adler model depends on the structural distortion of the VO_2 lattice, so this change in the lattice supports the model as the flow of electrons is increased through the symmetrical, metallic structure (Adler & Brooks, 1967).

Finally, the characterization technique Rutherford Backscattering Spectroscopy was investigated through the simulation software SimNRA. SimNRA was shown to be able to distinguish between compositions of $W_xV_{1-x}O_2$ in the low doping region (Figure 10-11). As seen in Figure 11, the differences between W concentration are clearly visible in the peak height. This demonstrates that RBS is a well-suited technique for characterizing the composition of W-doped VO_2 thin films. Further, it is also possible to obtain the chemical composition of the parent V:O crystal stoichiometry to validate the quality of the material through analysis of the peak height ratio.

In the future, this study will be extended to focus on the synthesis methods used for doping VO_2. Since synthesizing materials with an exact concentration is incredibly difficult, it is necessary to develop precise techniques that help reduce the error in creating these materials. It will be useful to understand how different synthesis procedures yield different experimental results, and to see if the synthesis procedure influences the IMT behavior.

The results of this study are of broad relevance to both the scientific community and the public. The linear models developed can be used for predicting the behavior of W-VO_2, and therefore can greatly reduce the need for wider experimentation. Researchers can now begin to fine tune W-VO_2 for exact conditions and applications, since the overall trend has been established. These models will not only reduce the need for experimentation but will also provide insight into designing materials for brain-inspired computing devices. Since the composition of W-VO_2 required for a certain IMT temperature or threshold voltage is now known, it will be possible to synthesize materials with these compositions and then start assembling the circuits and transistors that will be used in future computers. These devices will allow for lower power consumption, which will greatly benefit all.

Conclusion

Principal Results of this Study

1. Derived a universal equation relating tungsten doping concentration to insulator-metal transition temperature by considering over two decades of experimental data. The slope determined from this work is consistent with theoretical predictions.
2. From analysis of the influence of dopant ionic radii on the IMT temperature, it can be concluded that electron doping is the dominant factor for tuning the transition temperature, rather than structural effects.
3. The semiconductor impurity model agrees with the linear model for low doping concentration (< 1.8 at. %).
4. The slope obtained from the linear model is in excellent agreement with the scaling of the threshold voltage reduction, suggesting a common mechanism between the two processes. This enables predictive modeling of artificial neuron devices built with W-VO_2.
5. RBS can be utilized to determine the composition of the VO_2 films in the transition temperature ranges of interest.

Vanadium Dioxide (VO_2) is an important material for a variety of applications, with the most prominent being low power electronics. The results of this study provide two important mathematical relationships which can be used for predicting the insulator-metal transition properties of W-doped VO_2 at different concentrations of tungsten. It is observed that there is a linear, decreasing relationship between tungsten concentration and IMT temperature for low doping concentrations (< 1.8 at. %), and it is hypothesized that there are undiscovered physics phenomena that govern the transition mechanisms beyond this limit, as well as a non-linear

relationship that explains the transition temperature at higher concentrations. The linear model found agrees nicely with theoretical reports as well as Adler's theory. The relationship between tungsten concentration and threshold voltage follows a similar trend, suggesting that similar mechanisms affect the IMT temperature. Additionally, there is no clear correlation between dopant ionic radius and transition temperature. These findings suggest that the electronic effects of doping are dominant over structural effects. This study reaffirms the usage of RBS as a robust characterization technique for analysis of the W dopant and can differentiate between low doping concentrations. The results of this study are crucial towards developing predictive models for quantum materials, unraveling the mechanisms of W-doped VO_2, and optimizing this material for its applications in low-power electronics, as W-VO_2 has the potential to reduce power consumption by up to 76%.

References

1. Ludvigsen, K. G. A. (2023, March 5). ChatGPT's Electricity Consumption. Medium. https://towardsdatascience.com/chatgpts-electricity-consumption-7873483feac4
2. de Vries, A. (2023). The growing energy footprint of artificial intelligence. Joule, 7(10), 2191-2194.
3. Kendall, J. D., & Kumar, S. (2020). The building blocks of a brain-inspired computer. Applied Physics Reviews, 7(1).
4. Cava, R., De Leon, N., & Xie, W. (2021). Introduction: quantum materials. Chemical Reviews, 121(5), 2777-2779.
5. Keimer, B., & Moore, J. E. (2017). The physics of quantum materials. Nature Physics, 13(11), 1045-1055.
6. Zunger, A., & Malyi, O. I. (2021). Understanding doping of quantum materials. Chemical reviews, 121(5), 3031-3060.
7. Chen, P. Y., Seo, J. S., Cao, Y., & Yu, S. (2016, November). Compact oscillation neuron exploiting metal-insulator-transition for neuromorphic computing. In 2016 IEEE/ACM International Conference on Computer-Aided Design (ICCAD) (pp. 1-6). IEEE.
8. Fiore, J. M. (2020, June 23). 1.4: Doped Materials. Engineering LibreTexts. https://eng.libretexts.org/Bookshelves/Electrical_Engineering/Electronics/Book%3A_Semiconductor_Devices_-_Theory_and_Application_(Fiore)/01%3A_Semiconductor_Fundamentals/1.4%3A_Doped_Materials

9. Stanev, V., Choudhary, K., Kusne, A. G., Paglione, J., & Takeuchi, I. (2021). Artificial intelligence for search and discovery of quantum materials. Communications Materials, 2(1), 105.
10. Adler, D., & Brooks, H. (1967). Theory of semiconductor-to-metal transitions. Physical Review, 155(3), 826.
11. Xue, Y., & Yin, S. (2022). Element doping: a marvelous strategy for pioneering the smart applications of VO 2. Nanoscale, 14(31), 11054-11097.
12. Mulchandani, K., Soni, A., Pathy, K., & Mavani, K. R. (2021). Structural transformation and tuning of electronic transitions by W-doping in VO2 thin films. Superlattices and Microstructures, 154, 106883.
13. Shao, Z., Cao, X., Luo, H., & Jin, P. (2018). Recent progress in the phase-transition mechanism and modulation of vanadium dioxide materials. NPG Asia Materials, 10(7), 581-605.
14. Cui, Y., Ke, Y., Liu, C., Chen, Z., Wang, N., Zhang, L., ... & Long, Y. (2018). Thermochromic VO2 for energy-efficient smart windows. Joule, 2(9), 1707-1746.
15. Yamagata, M. R., Wakita, Y., Tsuruda, Y., & Miyata, K. (2023). Feasibility study of low-temperature operable electric power supply for CubeSats using passive thermal control with VO2-based solid–solid phase change material. Thermal Science and Engineering Progress, 37, 101601.
16. Bleu, Y., Bourquard, F., Barnier, V., Loir, A. S., Garrelie, F., & Donnet, C. (2023). Towards Room Temperature Phase Transition of W-Doped VO2 Thin Films Deposited by Pulsed Laser Deposition: Thermochromic, Surface, and Structural Analysis. Materials, 16(1), 461.

17. Piccirillo, C., Binions, R., & Parkin, I. P. (2008). Synthesis and characterisation of W-doped VO2 by aerosol assisted chemical vapour deposition. Thin Solid Films, 516(8), 1992-1997.
18. Sun, K., Wheeler, C., Hillier, J. A., Ye, S., Zeimpekis, I., Urbani, A., ... & de Groot, C. H. (2022). Room Temperature Phase Transition of W-Doped VO2 by Atomic Layer Deposition on 200 mm Si Wafers and Flexible Substrates. Advanced Optical Materials, 10(23), 2201326.
19. Reyes, J. M., Sayer, M., & Chen, R. (1976). Transport properties of tungsten-doped VO2. Canadian Journal of Physics, 54(4), 408-412.
20. Whittaker, L., Wu, T. L., Patridge, C. J., Sambandamurthy, G., & Banerjee, S. (2011). Distinctive finite size effects on the phase diagram and metal–insulator transitions of tungsten-doped vanadium (iv) oxide. Journal of Materials Chemistry, 21(15), 5580-5592.
21. Ling, C., Zhao, Z., Hu, X., Li, J., Zhao, X., Wang, Z., ... & Jin, H. (2019). W doping and voltage driven metal–insulator transition in VO2 nano-films for smart switching devices. ACS Applied Nano Materials, 2(10), 6738-6746.Reyes et al., 1975, Canadian Journal of Physics
22. Shen, N., Chen, S., Shi, R., Niu, S., Amini, A., & Cheng, C. (2021). Phase transition hysteresis of tungsten doped VO2 synergistically boosts the function of smart windows in ambient conditions. ACS Applied Electronic Materials, 3(8), 3648-3656.
23. Tan, X., Yao, T., Long, R., Sun, Z., Feng, Y., Cheng, H., ... & Wei, S. (2012). Unraveling metal-insulator transition mechanism of VO2 triggered by tungsten doping. Scientific reports, 2(1), 466.

24. Wang, X., Chen, L., Lu, H., Fang, W., Li, H., Yin, W., ... & He, Y. (2021). Enhancing visible-light transmittance while reducing phase transition temperature of VO2 by Hf–W co-doping. Applied Physics Letters, 118(19).
25. Ersundu, A. E., Ersundu, M. Ç., Doğan, E., & Güven, M. B. (2020). A comparative investigation on thermal, structural and optical properties of W and Nb-doped VO2-based thermochromic thin films. Thin Solid Films, 700, 137919.
26. Chaillou, J., Chen, Y. F., Émond, N., Hajlaoui, T., Torriss, B., Malviya, K. D., ... & Chaker, M. (2022). Combined Role of Substrate and Doping on the Semiconductor-to-Metal Transition of VO2 Thin Films. ACS Applied Electronic Materials, 4(4), 1841-1851.
27. Wang, N., Duchamp, M., Dunin-Borkowski, R. E., Liu, S., Zeng, X., Cao, X., & Long, Y. (2016). Terbium-doped VO2 thin films: reduced phase transition temperature and largely enhanced luminous transmittance. Langmuir, 32(3), 759-764.
28. Krammer, A., Magrez, A., Vitale, W. A., Mocny, P., Jeanneret, P., Guibert, E., ... & Schüler, A. (2017). Elevated transition temperature in Ge doped VO2 thin films. Journal of Applied Physics, 122(4).
29. Pattanayak, M., Hoque, M. N. F., Ho, Y. C., Li, W., Fan, Z., & Bernussi, A. A. (2023). Ultrahigh tunability of resistive switching in strongly correlated functional oxide. Applied Materials Today, 30, 101642.
30. Zhang, J., He, H., Xie, Y., & Pan, B. (2013). Theoretical study on the tungsten-induced reduction of transition temperature and the degradation of optical properties for VO2. The Journal of chemical physics, 138(11).

31. Sun, C., Yan, L., Yue, B., Liu, H., & Gao, Y. (2014). The modulation of metal–insulator transition temperature of vanadium dioxide: a density functional theory study. Journal of Materials Chemistry C, 2(43), 9283-9293.
32. R.D. Shannon (1976). Acta Crystallographica. A32, 751.
33. Dietrich, M. K., Kuhl, F., Polity, A., & Klar, P. J. (2017). Optimizing thermochromic VO2 by co-doping with W and Sr for smart window applications. Applied Physics Letters, 110(14).
34. Jin, P., Nakao, S., & Tanemura, S. J. T. S. F. (1998). Tungsten doping into vanadium dioxide thermochromic films by high-energy ion implantation and thermal annealing. Thin Solid Films, 324(1-2), 151-158.
35. Koch, D., & Chaker, M. (2022). The Origin of the Thermochromic Property Changes in Doped Vanadium Dioxide. ACS Applied Materials & Interfaces, 14(20), 23928-23943.
36. Leffer, L. (2023, October 13). The AI Boom Could Use a Shocking Amount of Electricity. Scientific American. https://www.scientificamerican.com/article/the-ai-boom-could-use-a-shocking-amount-of-electricity/
37. Netsianda, M., Ngoepe, P. E., Catlow, C. R. A., & Woodley, S. M. (2008). The displacive phase transition of vanadium dioxide and the effect of doping with tungsten. Chemistry of Materials, 20(5), 1764-1772.
38. Niklasson, G. A., Li, S. Y., & Granqvist, C. G. (2014, November). Thermochromic vanadium oxide thin films: Electronic and optical properties. In Journal of Physics: Conference Series (Vol. 559, No. 1, p. 012001). IOP Publishing.

39. Romanyuk, A., Steiner, R., Marot, L., & Oelhafen, P. (2007). Temperature-induced metal–semiconductor transition in W-doped VO2 films studied by photoelectron spectroscopy. Solar Energy Materials and Solar Cells, 91(19), 1831-1835.
40. US, K. S. C. (2023, May 25). A Computer Scientist Breaks Down Generative AI's Hefty Carbon Footprint. Scientific American. https://www.scientificamerican.com/article/a-computer-scientist-breaks-down-generative-ais-hefty-carbon-footprint/
41. Whittaker, L., Patridge, C. J., & Banerjee, S. (2011). Microscopic and nanoscale perspective of the metal− insulator phase transitions of VO2: some new twists to an old tale. The Journal of Physical Chemistry Letters, 2(7), 745-758.
42. Wu, Y., Fan, L., Liu, Q., Chen, S., Huang, W., Chen, F., ... & Wu, Z. (2015). Decoupling the lattice distortion and charge doping effects on the phase transition behavior of VO2 by titanium (Ti4+) doping. Scientific reports, 5(1), 9328.
43. Evans, C., Wilson, L., & Wilson, G. (1992). Medium-energy ion scattering spectrometry with channeling and blocking, MEISS 502 9.0 INTRODUCTION. https://glass.rutgers.edu/sites/default/files/uploads/virtual/dir.cullity/B-ch.9-ISS-RBS.pdf