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REGULAR ARTICLE

AI-Based Enhanced Production of Vanadium Dioxide Thermochromic Films

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The study focuses on optimizing the synthesis process of Vanadium Dioxide (VO_2) films through advanced machine learning (ML) algorithms, enabling precise control over key parameters such as temperature, pressure, and deposition techniques. By utilizing Artificial Intelligence AI-driven predictive modeling aim to achieve improved film quality, uniformity, and thermochromic (TC) performance. This study suggested a novel Tabu Search Optimized Adaptive Long Short-Term Memory (TSO-ALSTM) for the integration of AI to facilitate real-time monitoring and adjustment of production conditions, reducing defects and minimizing waste. The data was preprocessed using Min-max normalization. The proposed method is implemented using Python software. Compared the suggested method with other existing methods. Experimental results demonstrate that AI-enhanced processes lead to VO_2 films with larger optical switching characteristics, broadening their potential applications in smart windows, advanced thermal management systems, and energy-efficient buildings. The outcomes demonstrate that the suggested approach outperforms the other method in terms of accuracy (90.74 %), recall (76 %), F1 score (81 %), and specificity (99.1 %). This work highlights the transformative impact of AI technologies in materials science, paving the way for the next generation of smart materials.

Keywords: Vanadium Dioxide (VO_2), Thermochromic Films, Artificial Intelligence (AI), Machine Learning (ML)

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1. INTRODUCTION

The new material is called VO_2, and this material presents unique properties related to the TC phenomenon. The phase transition, at about 68 °C, is reversible from the insulating into the metallic state [1]. In connection with changes in electrical conductivity and infrared transmittance, it relates to interesting properties for VO_2-based smart windows, optical switches, sensors, and energy-efficient devices [2]. These challenges lie in straightforward synthesis, the lack of precise control over the structure, and its sensitivity to impurities and fabrication conditions, making the efficient and scalable production of high-quality VO_2 rather difficult to realize [3]. The latest advancements in AI and ML have gifted competent solutions for improving VO_2 production. The introduction of AI-based methods enables better optimization of synthesis parameters; prediction of material properties to fine-tune the production process; hence, minimization of experimental time and associated cost. The AI-aided method can also serve to improve the quality of VO_2 by observing real-time production conditions adjustment [4]. The possibility of breaking, through the traditional manufacturing drawbacks using advanced data-driven approaches has been demonstrated for this introduction to AI-enhanced VO_2 production and high-performance VO_2-based applications. VO_2 TC films have recently captured significant attention due to their phenomenal temperature-sensitive properties. Here, VO_2 undergoes a reversible phase transition from an insulating to a metallic state at around 68 °C [5]. This could be optimized further by the incorporation of dopants or the implementation of nano structuring techniques in the TC properties of VO_2 so that, the transition temperature

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goes lower than toward the room temperature to bring more practicality towards a potential commercial application [6-7]. Other recent work highlights the need for development in VO_2 film for durability, transmittance, and optical contrast-if large-scale applications require satisfying performance and aesthetic needs [8]. The VO_2 TC films are in a leading position among innovating solutions for the line of quests toward sustainable architecture and advanced optical technologies [9]. The aim of AI-based improvement of VO_2 TC film production process is on concerns of TC performance, property enhancement, and energy efficiency.

2. RELATED WORKS

Temperature or light can cause VO_2 [10] and many binary vanadium compounds to transition from a semiconducting to a metallic state. Modifications in the oxide's crystalline structure instigate the metamorphosis. Nano films of VO_2 play a crucial role in electronic applications like smart windows [11]. Understanding the optical characteristics of these films is vital for modifying the parameters that affect them. The ability of VO_2 to serve as a smart material is enabled by its reversible phase shift in response to heat, light, electric, magnetic, and mechanical force [12]. To reduce radiant heat loss and boost overall efficiency, the experiment suggests using a parabolic through solar receiver with a TC coating made of vanadium dioxide. At 68°C, the innermost portion of the glassy envelope's TC layer undergoes a reversible change from a monoclinic (M) to a rutile (R) phase [13]. Tracking the optical constants of the films throughout the TC process allows for correlating microscopic changes in the material with its macroscopic behavior as an energy-saving material [14]. The work offered a promising strategy to enhance the industrial use of VO_2TC windows, supporting advancements in green building technologies, window design, and energy efficiency in the automotive sector [15]. Monoclinic VO_2 is a special kind of dynamically created phase-transition material that shows a noticeable shift in infrared transmission throughout its phase change, which makes a great choice for possible uses in passively TC smart windows [16].

3. METHODS AND MATERIALS

The methodology involved optimizing the VO_2 thin film synthesis process by employing a model TSO-ALSTM. In the synthesis process, important synthesis parameters like temperature, pressure, and deposition techniques were determined and monitored. Data acquired during synthesis were preprocessed by employing min-max normalization to eliminate inconsistency and lack of reliability. Fig. 1 depicts the methodology flow.

3.1 Data Collection

The dataset was collected from the open-source data which simulates experimental data for producing high-purity VO_2TC films using magnetron sputtering, a common technique in materials science. The data includes key reaction parameters that affect the phase and purity of VO_2 films, to optimize conditions for creating VO_2 in its monoclinic phase (VO_2 (M)), which has applications in smart windows and other adaptive materials.

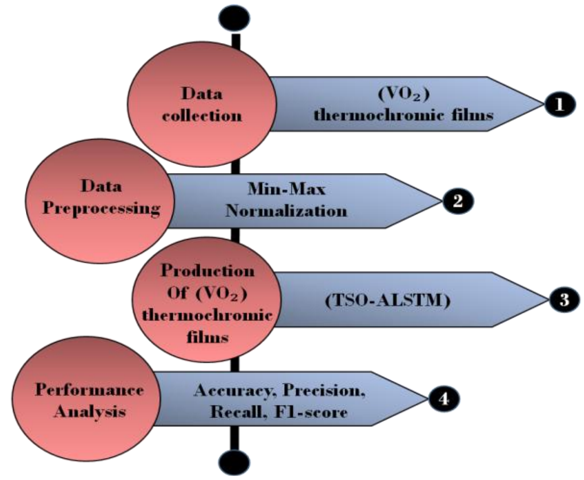

Fig. 1 – Flow of Proposed System

3.2 Preprocessing Using Min-Max Normalization

To apply data normalization to performance metrics for effective analysis of these films. Data normalization transforms a feature's values into a much smaller range with a given interval, in this case, [0-1]. Another popular method for normalizing in which the minmax normalization method excels is that it indeed preserves the relationships that exist with the data. Eq. 1 captures every value of a specific attribute in terms of the same value that is normalized as the comparison of the various measurement values of the sample towards the same TC characteristics becomes more evident.

$$u' = \frac{u - min_B}{max_B - min_B}(new\_max_B - new\_min_B) + new\_min_B \quad (1)$$

In this equation, u' represents the new normalized value, u' represents the original value of the feature, max_B represents the maximum value, min_B represents the minimum value, and new_max_B and new_min_B represent the maximum and minimum values for the new range. This normalization process will enhance the reliability of the experimental results and facilitate the comparison of TC behaviors across different conditions and applications.

3.3 Vanadium Dioxide Thermochromic Films Using Tabu Search Optimized Adaptive Long Short-Term Memory (TSO-ALSTM)

Tabu Search Optimized Adaptive Long Short-Term Memory (TSO-ALSTM) is a hybrid model that integrates the powerful capabilities of networks. This approach enhances the learning process of ALSTMs by exploring the parameter space to avoid local minima and improve convergence speed. By leveraging the TSO-ALSTM dynamically adapts its structure and parameters, resulting in improved performance for time-series prediction and sequential data tasks. This innovative combination aims to address challenges in traditional ALSTM training, leading to more accurate and robust predictive models.

3.3.1. Adaptive Long Short Term Memory (ALSTM)

TC films based on VO_2 have excellent temperature responses to optical property changes. The ALSTM models can probably help in better prediction and control of the phase transition behaviors with the material, which might be optimized for application in energy-efficient windows or smart coatings. Better temporal dynamics modeling leads to better performance and responsiveness of the materials. The output e_s is processed by the forgetting gate layer, and the result is a number between 0 and 1 that is positively connected with the position. After completion, a candidate score of $\tilde{D}_s$ is generated to transform the current state. The $D_s$gate's computation is validated into the succession memory unit. The symbol signifies that the ingredient has been multiplied. The ALSTM calculates output values depending on previous data and current input. Memory unit updates drive the ALSTM's final output value. The gate structure is described as Eq. (2):

$$\begin{cases} e_s = \sigma[X_e.(g_{s-1}, w_s) + a_e] \\ j_s = \sigma[X_j.(g_{s-1}, w_s) + a_j] \\ \overline{D} = tanh[X_d.(g_{s-1}, w_s) + a_d] \\ D_s = e_s \circ D_{s-1} + j_s \circ \widetilde{D}_s \\ p_s = \sigma[X_p.(g_{s-1}, w_s) + a_p] \\ g_s = P_s \circ \tanh(D_s) \end{cases} \tag{2}$$

The outputs of three sigmoid functions (e_s, j_s, and p_s) are combined with weights (X_e, X_j, X_d, and $P_s\circ$) to form the new input (w_s). The previous cell, whereas a_e, a_j, a_p, and represent the respective biases. This process can be likened to the mechanisms in VO_2TC films, where the material's properties change in response to temperature, allowing for adaptive control similar to how LSTM cells adjust their outputs based on previous inputs and weights. Fig. 2 illustrates the cell makeup of neural networks. The fundamental architecture of a standard LSTM neural network is depicted in Fig. 2(a), and the ALSTM with dropout is depicted in Fig. 2(b).

The enhanced LSTM incorporates a mechanism that randomly deletes neurons in the hidden layer based on a predetermined probability during training, which can be applied to the modeling of complex systems like VO_2. After dropout, disconnected neurons are temporarily destroyed, followed by conventional training. After training, the weights and biases of the remaining neurons are adjusted, while the destroyed neurons are recovered. This iterative process is repeated until convergence is achieved. The ALSTM formula with dropout can effectively adapt to the dynamics of applications, such as TC film behavior Eq. (3).

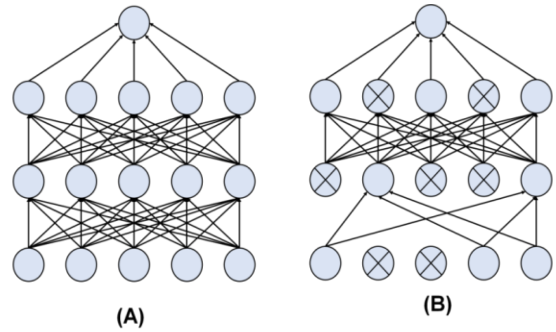

Fig. 2 – (a) Standard LSTM (b) Adaptive LSTM

$$\begin{gathered} \tilde{z}^{(k)} = q^{(k)}.z^{(k)} \\ y_j^{(k+1)} = a_j^{(k+1)} + x_j^{(k+1)}\tilde{z}^{(k)} \\ y_j^{(k+1)} = e\left(y_j^{(k+1)}\right) \end{gathered} \tag{3}$$

Where y represents the mass of every neuron, $\tilde{z}^{(k)}$ is neuronal output via the inactivated layer, q is the chance given by the bias, $y_j^{(k+1)}$ is the neuron's output at the following moment. To avoid overfitting during prediction, the hidden layer of the ALSTM employs random neuron inactivation. In this design, each neuron connects to synapses in the dense layer after being inactivated at random. This method enables the model to compute the projected movement value using a function of activation that is obtained by multiplying the hidden layer's output. The dense layer is critical for operations requiring VO_2 films, as it carries information regarding heave motion in the projected value. These films' characteristics can change with temperature, necessitating the use of a fully linked layer to capture the functional relationship between historical data, such as temperature changes and heave motion, and predicted results Eq. (4).

$$g_s^C = X_o g_s^K + a \tag{4}$$

In this context, X_o represents the ratio of the fully connected layer to the ALSTM layer after dropout. g_s^K indicates the ALSTM layer's output at each time step s, while g_s^C represents the output of the LSTM layer at time step s+1th.

3.3.2. Tabu Search Optimization (TSO)

The VO_2TC films, known for their ability to regulate infrared light based on temperature, are optimized using TSO to enhance their TC properties. TSO helps in refining parameters for improved efficiency in energy-saving applications, such as smart windows and heat-responsive coatings. The analytical equations based on the First Harmonic Approximation (FHA) and the diagram of the algorithm are shown in Fig. 3 and explained in Eqs. (5) to (12).

$$R_K = \frac{Q_K}{Y_0}, Y_0 = \sqrt{\frac{K_{t1}}{D_t}}, \omega_0 = \frac{1}{\sqrt{K_{t1}D_t}}, \omega_m = \frac{\omega_t}{\omega_0}, K_t = \frac{K_{t1}}{K_{t2}}, K_m = \frac{K_{t1}}{K_o} \tag{5}$$

$$\frac{Y_{in}(i\omega_m)}{Y_0} = \left(i\omega_m + \frac{1}{i\omega_m}\right) + \frac{\frac{i\omega_m}{K_m}\left(\frac{i\omega_m}{K_t}+R_K\right)}{\frac{i\omega_m}{K_m}+\frac{i\omega_m}{K_t}+R_K} \tag{6}$$

$$\left|J_{K_{t1}}\right| = \frac{4U_{in}}{\pi|Y_{in}(i\omega_m)|}, \upsilon_{BA1}(s) = \frac{4U_{in}}{\pi} sin\omega_t s \tag{7}$$

$$N_\upsilon = \left|\frac{i\omega_m R_K K_t}{R_K K_m K_t + i\omega_m(K_m+K_t)}\right| \frac{1}{|Y_{in}(i\omega_m)|} \tag{8}$$

$$O_{core} = l_j |\Delta A|^{\beta-\alpha} e_t |2\Delta A|^{\alpha} \left(\frac{1}{e_t}\right)^{1-\alpha} \tag{9}$$

$$l_j = \frac{l_d}{2^{\beta-1}\pi^{\alpha-1}\left(1.1044+\frac{6.8244}{\alpha+1.354}\right)}, \Delta A = \frac{U_{S_{q,o}}}{2M_o B_f e_t} \tag{10}$$

$$O_{S_q} = O_{core} + O_{Cu}, O_{Cu} = Q_o J_{o,rms}^2 + Q_t J_{o,rms}^2 \tag{11}$$

$$O_{rec} = 2U_E J_{t,rms} \tag{12}$$

The TSO is a heuristic search technique that uses several memory structures to direct the search toward a good result. After identifying a workable solution, the TSO continuously precedes a predetermined criterion typically, the maximum number of iterations is achieved. Each workable solution to the current issue is a vector of R_K, K_m, and K_t, where a predetermined range of changes can be made to each element.

4. RESULT AND DISCUSSION

The performance of the proposed method demonstrated that the AI-enhanced synthesis process significantly improved the optical switching characteristics of VO_2 films, affirming the efficacy of the proposed approach in materials science applications. An Intel 16 GB of DDR4 RAM, Xeon E3-1230v5 CPU, and an NVIDIA Quadro K420 discrete graphics card power the system. Table 1 depicts the metrics outcomes.

Table 1 – Outcomes of metrics

Methods	Accuracy (%)	Recall (%)	F1-score (%)	Specificity (%)
XGBoost [23]	88.52	74	78	98
RF [23]	86.89	69	74	97
TSO-ALSTM [Proposed]	90.74	76	81	99.1

4.1 Accuracy

Accuracy is the closeness of the model's predictions to the actual outcome. It is most commonly calculated as correct predictions over total predictions. Accuracy is the most common metric for a classification task and is used to measure how efficiently the model can classify or label dataset. High accuracy in such applications as performance analysis of VO_2TC films can symbolize better performance if classes are balanced. The model properly distinguishes the phases or states in the materials and reflects precision about the transitions and thermal responses. Fig. 3 depicts the outcomes of accuracy.

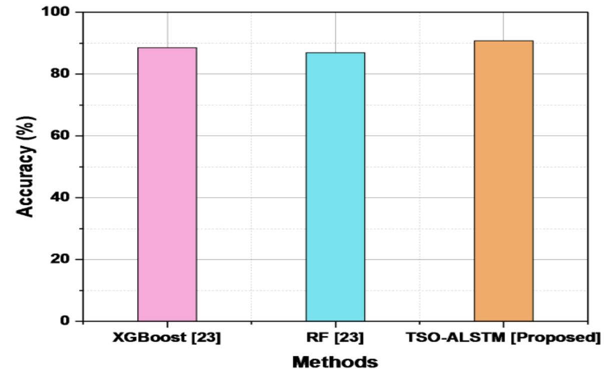

Fig. 3 – Analysis of Accuracy

4.2 Recall

Recall in data analysis and ML is a measure used to refer to the model's accuracy in identifying all relevant instances in a dataset. Recall measures how the correct positive observations that are divided by all the actual positives are determined, meaning it reveals the ability of the model to capture the actual positive cases. This is a very fundamental concept that finds applicability in many areas, including the evaluation of VO_2TC films, wherein recall would be useful to test if models can predict correct transitions or material properties from the dataset without missing the relevant instances. Fig. 4 depicts the outcomes of recall.

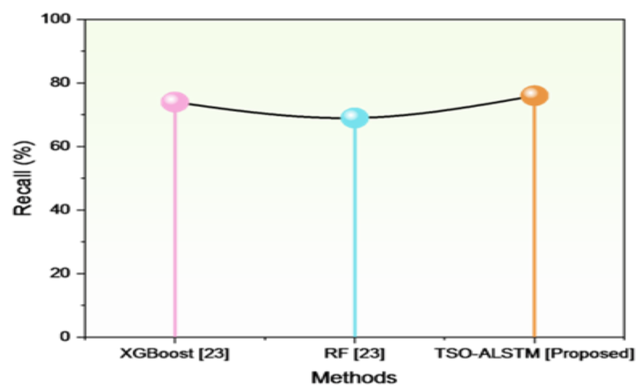

Fig. 4 – Analysis of Recall

4.3 F1-Score

The F1 score measures performance by combining precision and recall into a single metric, providing a balanced evaluation of accuracy and completeness. The formula of the F1 score could be calculated in terms of the mean of the precision, which tells how well the positive predictions are being made, and the recall, which counts how many actual positives are identified. This is useful to evaluate models applied to imbalanced datasets, VO_2TC films taking into account both false positives and false negatives while rating the performances. Fig. 5 depicts the outcomes of the F1-score.

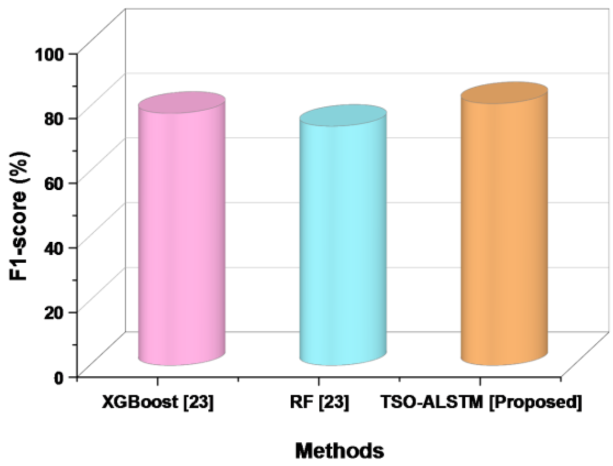

Fig. 5 – Analysis of F1-score

The TSO-ALSTM method achieved 81 % which is compared with the existing methods of Simple XG Boost [23] achieved 78 %, and RF [23] achieved 69 %. It explains how the suggested methodology performs better in terms of rates than the current methods.

5. CONCLUSION

The feasibility of advanced ML algorithms, specifically TSO-ALSTM, for the optimization of the synthesis of VO_2 films. By using AI-driven predictive modeling, were able to show that improved film quality and performance are attainable at the same time as reduced defects and waste during the production process. The superior optical switching characteristics of VO_2 films produced with this method indicated significant improvements in their applicability for smart windows, energy-efficient buildings, and advanced thermal management systems. The quantitative metrics, including accuracy at 90.74 %, recall at 76 %, F1 score at 81 %, and specificity at 99.1 %, further established the effectiveness of the approach over existing methods. This study not only demonstrates the transformational potential of AI in materials science but also sets the stage for the next generation of smart materials with improved energy efficiency and sustainability in applications.

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Покращене виробництво термохромних плівок діоксиду ванадію на основі штучного інтелекту

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Дослідження зосереджено на оптимізації процесу синтезу плівок діоксиду ванадію (VO_2) за допомогою передових алгоритмів машинного навчання (ML), що дозволяє точно контролювати ключові параметри, такі як температура, тиск та методи осадження. Завдяки використанню штучного інтелекту та прогнозного моделювання на основі штучного інтелекту, метою є покращення якості плівки, однорідності та термохромних (TC) характеристик. У цьому дослідженні запропоновано новий метод адаптивної довгострокової короткочасної пам'яті з оптимізованим за допомогою пошуку Tabu (TSO-ALSTM) для інтеграції штучного інтелекту, що полегшує моніторинг та коригування виробничих умов у режимі реального часу, зменшує дефекти та мінімізує відходи. Дані були попередньо оброблені за допомогою нормалізації Min-max. Запропонований метод реалізовано за допомогою програмного забезпечення Python. Запропонований метод порівнювали з іншими існуючими методами. Експериментальні результати показують, що процеси, вдосконалені штучним інтелектом, призводять до плівок VO_2 з більшими характеристиками оптичного перемикання, розширюючи їх потенційне застосування в розумних вікнах, передових системах теплового управління та енергоефективних будівлях. Результати показують, що запропонований підхід перевершує інший метод за точністю (90,74%), повнотою (76%), показником F1 (81%) та специфічністю (99,1%). Ця робота підкреслює трансформаційний вплив технологій штучного інтелекту в матеріалознавстві, прокладаючи шлях для наступного покоління інтелектуальних матеріалів.

Ключові слова: Діоксид ванадію (VO_2), Термохромні плівки, Штучний інтелект (ШІ), Машинне навчання (МН).