International Journal of Advanced Science and Research
www.allsciencejournal.com
ISSN: 2455-4227
Received: 07-11-2022, Accepted: 23-11-2022, Published: 09-12-2022
Volume 7, Issue 2, 2022, Page No. 84-91

Theoretical modelling of electrical conductivity in metal oxide thin films using temperature-dependent carrier dynamics

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Abstract
This work includes a coherent theoretical model to simulate the temperature dependent electrical conductivity of metal oxide thin films through the combination of various carrier accommodation processes at low, intermediate and high temperature conditions. It uses the model Mott Variable-range hopping (VRH), Small Polaron Hopping (SPH), Arrhenius-type thermally activated conduction and high-temperature band conduction to explain the slow change in charge transport behaviour. Carrier concentration, mobility, defect states and scattering processes both depend on temperature were mathematically interpolated with weighted contributions of the carrier mechanisms of conduction allowing continuity and realistic predictions of conductivity. Findings indicate that at 50150 K, VRH is prevalent, 150 350 K SPH controlled transport, and 350 K strong band conduction, all are expected based on previously known activation energies and dynamics driven by defects in metal oxides. The integrated model offers a detailed account of the microstructural disorder, phonon interactions, and thermal activation to mainly conductivity in large temperature variations and can be of great benefit in designing stable and high-performance oxide-based electronic and sensing devices.

Keywords: Metal oxide thin films, temperature-dependent conductivity, carrier transport mechanisms, polaron hopping

Introduction
The metal oxide thin films constitute a significant category of functional materials that has their electrical characteristics highly dependent on the microstructure, composition and external stimuli. Temperature is one of the most deterring factors among these that determine the phenomenon of charge transport. To the extent components are becoming smaller and are operated under changing temperatures, more insight into theoretical knowledge of temperature-dependent carrier dynamics is essential. This knowledge is not only making the behaviour of material predictable, but is also allowing rational and optimized conductivity of thin films to be designed to be used in advanced technology.

Background and Significance of Metal Oxide Thin Films
Tunable electrical, structural and optical properties have made metal oxide thin films to be an indispensable material in modern electronic, optoelectronic and sensing applications. ZnO, TiO 2, SnO 2, and NiO are the materials which have a wide band gap, high chemical stability, and conductivity behaviour which is versatile, and these materials find their applications in transparent conductors, gas sensors, photovoltaic cells, and thin-film transistors. The electric conductivity of these films is extremely sensitive to inherent flaws, dopants, grain boundaries, and outside environmental factors. These factors include temperature which is the most significant among them because it directly determines carrier concentration, mobility, scattering mechanisms and activation energies. Knowledge of conductivity versus temperature is thus crucial to determining the performance of a device, the quality of materials, and the thin-film properties to be used in a given technological device.

Need for Theoretical Modelling in Temperature-Dependent Carrier Dynamics
Even though experimental measurements too seek useful information into the conductivity behaviour, they may only fail in isolating the contributions of the various microscopic processes that influence the behaviour, which include, but are not limited to, phonon scattering, ionized impurity scattering, defect states and the polaronic effects. Consequently, theoretical modelling is important in characterizing and forecasting the influence of the temperature on the electrical behaviour of metal oxide thin films. Semiconductor physics models, including thermally activated conduction, variable-range hopping (VRH), small polaron hopping, and band conduction, are also used to provide a model to explain the intricate interplay between temperature and carrier dynamics. Such models are also useful in determining the pathways of dominant conduction, known points between conduction regimes, and what constraints may be present in the film due to structural or chemical defects.

Research Objectives
- With the theoretical orientation of this paper, it is crucial to make clear research objectives that will be used to model and analyse the temperature-dependent electrical behaviour of metal oxide thin films. These goals

have a systematic approach to the investigation of carrier dynamics, the definition of the key conduction mechanisms, and the creation of a holistic model that would improve the intuitive insight into the conductivity of thin-film systems.

- To establish an integrated theoretical basis that is accurate in explaining the electrical conductivity in thin metal oxide films that varies with temperature through the combination of classical physics in semiconductor and the recent carrier transport models.
- To examine the impact of important parameters, including carrier concentration, carrier mobility, activation energy and scattering rates and hopping probabilities on conductivity in various temperature regimes.
- To determine the prevailing conduction modes across the different temperatures and make predictive information that can be used to help optimize the design, fabrication and operation of metal oxide thin-film based electronic and optoelectronic devices.

Review of Litreature

Bhattacharya *et al*. (2017) [1] investigated the frequency- and temperature-dependent conductivity behaviour of mixed transition metal oxide–doped semiconducting glassy systems. Their study revealed that electrical conductivity increased with temperature, confirming the thermally activated nature of charge transport in such disordered materials. They also reported that the AC conductivity followed the universal power law, indicating the significant role of hopping mechanisms in carrier movement. The findings contributed valuable insights into how disorder and dopant interactions influenced conduction pathways in glassy oxide systems.

Boyalı *et al*. (2017) [2] examined the temperature-dependent electron transport properties of degenerate SnO_2 thin films to understand their conductivity mechanisms across varying thermal conditions. Their analysis showed that degenerately doped SnO_2 exhibited metallic-like conductivity behaviour at higher carrier concentrations. As temperature increased, mobility was primarily governed by electron–phonon scattering, whereas ionized impurity scattering played a dominant role at lower temperatures. The study established a clear relationship between degeneracy, scattering processes, and temperature-dependent electrical transport, making it significant for oxide-based electronic device applications.

Boyle *et al*. (2019) [3] explored the effect of dopant clustering on charge transport dynamics in organic semiconductor thin films. Their work demonstrated that altering the spatial distribution of dopants significantly modified carrier mobility and conductivity. The researchers observed that clustered dopants enhanced local charge density, thereby influencing transport behaviour through increased hopping probabilities and modified energy landscapes. This study provided a deeper theoretical understanding of how microstructural dopant arrangements affected charge transport, highlighting the importance of controlled doping strategies in thin-film electronic materials.

Bubel and Chabinyc (2013) [4] developed a model to determine mid-gap electronic states in amorphous metal oxides using thin-film transistor (TFT) measurements. Their work demonstrated that the distribution and density of mid-gap states strongly influenced carrier transport and threshold voltage behaviour in amorphous oxide semiconductors. By analysing the transfer characteristics of TFTs, they successfully extracted detailed information about defect states responsible for trapping and scattering carriers. Their model provided an important theoretical tool for understanding electronic disorder in amorphous metal oxide thin films, which significantly affected conductivity and device stability.

Buckner and Perry (2019) [5] conducted in situ optical absorption studies to investigate the kinetics and thermodynamics of point defects in oxide thin films. Their findings revealed that point defects such as oxygen vacancies exhibited dynamic behaviour under varying thermal and environmental conditions, thereby influencing the optical and electrical properties of the films. The study showed how defect formation, annihilation, and migration were temperature-dependent processes, emphasizing the critical role of defect chemistry in determining thin-film conductivity and stability. Their research contributed to a deeper understanding of the relationship between defect states and material performance in oxide-based electronic applications.

Methodology

This study adopted a fully theoretical and analytical approach grounded in semiconductor physics, charge transport equations, and defect-state modelling. The methodology was designed to develop a unified description of temperature-dependent electrical conductivity in metal oxide thin films by integrating multiple conduction mechanisms, scattering models, and carrier dynamics. The modelling framework was constructed in three major stages, as outlined below**.**

1. Selection of Conduction Models

To accurately describe electrical conductivity across a broad temperature range, the model incorporated four principal conduction mechanisms. Each mechanism dominates in a specific temperature regime and contributes differently to overall charge transport.

a. Arrhenius Thermally Activated Conduction

This mechanism assumes that charge carriers require a certain activation energy (Ea) to move from localized states into extended states. Conductivity is given by:

$$\sigma\ (T) = \sigma 0 e^{-E_a}/K_{BT}$$

This expression was used to model higher-temperature conduction, where thermal energy is sufficient to excite carriers over potential barriers.

b. Small Polaron Hopping (SPH)

In many metal oxides, strong electron–lattice interactions lead to small polaron formation. Their movement follows thermally assisted hopping, represented by:

1

$$\sigma\ (T) = \sigma\ 0\frac{1}{T}\ e^{-E_a/K_B T}$$

This model was applied to intermediate temperature ranges, where hopping between neighboring sites becomes prominent**.**

c. Mott Variable-Range Hopping (VRH)

At low temperatures, carriers do not have enough energy to hop to nearest sites; instead, they hop to more energetically favorable distant sites. VRH is represented by:

$$\sigma\ (T) = \sigma 0\ exp\left[-(T_0/T)^{1/4}\right]$$

This mechanism is common in disordered or amorphous metal oxide thin films where localized states dominate.

d. Band Conduction

At sufficiently high temperatures, some carriers occupy extended band states. Conductivity is expressed through carrier concentration $n(T)\ and\ Mo\ bility\ \mu(T)$

$$\sigma\ (T) = qn\ (T)\mu\ (T)$$

This model captures the influence of intrinsic carrier generation and scattering mechanisms.

These four models collectively provided the theoretical basis for describing conductivity under varying thermal conditions.

2. Parameter Consideration

The model evaluated several material and transport parameters known to influence conductivity in metal oxide thin films:

- **Carrier concentration (n):** Determined by intrinsic carriers, dopants, and thermally activated defect states.
- **Carrier mobility (μ):** Influenced by phonon scattering, ionized impurity scattering, grain-boundary barriers, and polaron interactions.
- **Defect density (N_t):** Represents localized trap states such as oxygen vacancies, interstitials, or dopant-induced states.
- **Activation energy (E_a):** Energy required for carrier excitation or hopping; varies depending on the conduction mechanism.

Temperature-dependent scattering rates: Accounted for

- acoustic and optical phonons (high T)
- ionized impurities (low–mid T)
- grain-boundary potential barriers
- lattice distortion due to polaron formation

By systematically incorporating these parameters, the model captured both intrinsic and extrinsic influences on thin-film conductivity.

3. Mathematical Integration

To construct a unified theoretical framework, the conduction models were mathematically integrated using a weighted mechanism approach. This method assumed that at any given temperature, multiple mechanisms may contribute, but one typically dominates. The overall conductivity was expressed as:

$$\boldsymbol{\sigma_{total}\ (T) = \sum_{i=1}^{4} w_i\ (T)\sigma_i(T)}$$

where

- $w_i(T)$ is the temperature-dependent weighting factor for each conduction mechanism
- $\sigma i\ (T)$ is the conductivity predicted by each model (Arrhenius, SPH, VRH, band conduction)?

The weighting functions were constructed based on physical considerations such as activation energies, density of states, and defect-controlled hopping probabilities.
This integration allowed the framework to transition smoothly between conduction mechanisms as temperature varied, enabling a holistic representation of conductivity behaviour from low to high temperature regimes.

Theoretical Framework

The theoretical framework for modelling electrical conductivity in metal oxide thin films is based on fundamental semiconductor physics, defect-state interactions, and temperature-dependent carrier dynamics. The framework integrates three core components: carrier concentration, carrier mobility, and the resulting electrical conductivity. Together, these components establish a unified description of how temperature governs charge transport in oxide thin films.

1. Temperature-Dependent Carrier Concentration

Carrier concentration in metal oxide thin films is highly sensitive to temperature because electrons and holes can be thermally excited from defect states or valence/conduction bands. The general temperature dependence of electron concentration in the conduction band is described by:

$$n\ (T) = N_c\ exP\left[-\frac{(E_c - E_F)}{K_B T}\right]$$

Where

- N_c = effective density of states in the conduction band
- E_c = conduction band minimum
- E_F= Fermi level
- K_B= Boltzmann constant
- T = absolute temperature

This expression indicates that as temperature increases, more electrons gain sufficient thermal energy to occupy conduction-band states, increasing the effective carrier concentration.

Influence of Defect States

Metal oxide thin films often contain:

- oxygen vacancies
- interstitial metal ions
- substitutional dopants
- mid-gap defect states

These defects can act as donor or acceptor levels, altering the Fermi level E_F. A shift in E_F changes the exponential term, significantly affecting $n\ (T)$Therefore:

- Shallow donor states lead to strong thermally activated behaviour at lower temperatures.
- Deep-level traps release carriers only at higher temperatures.

Thus, defect chemistry plays a central role in determining the temperature sensitivity of carrier concentration.

2. Temperature-Dependent Mobility

Carrier mobility $\mu\ (T)$describes how easily charge carriers move through the thin film. In metal oxides, mobility is strongly influenced by temperature-dependent scattering processes. The dominant scattering mechanisms vary across temperature regimes, and each introduces a characteristic temperature dependence.

a. Phonon (Lattice) Scattering

At higher temperatures, lattice vibrations increase and scatter electrons, reducing mobility:

$$\mu_{phonon} \propto T^{-3/2}$$

Thus, mobility decreases sharply with increasing temperature in the high-temperature regime.

b. Ionized Impurity Scattering

At lower temperatures, carriers move more slowly and interact more strongly with ionized impurity centers:

$$\mu_{impurity} \propto T^{3/2}$$

Here, mobility increases with temperature because higher thermal energy helps carriers overcome Coulombic interactions with impurities.

c. Grain Boundary Scattering

Metal oxide thin films often contain numerous grain boundaries. These boundaries introduce potential barriers that impede carrier transport. Grain boundary mobility follows a thermally activated behaviour:

$$\mu GB = \mu_{0\ eXP}\left[-\frac{E_b}{K_R T}\right]$$

Where E_b is the barrier height? At higher temperatures, carriers can more easily cross grain boundaries, increasing mobility.

3. Combined Conductivity Model

Electrical conductivity is determined by the combined influence of carrier concentration and mobility. The general conductivity expression is:

$$\sigma\ (T) = qn\ (T)\mu\ (T)$$

Where:

- **q** = electronic charge
- **n (T)**= temperature-dependent carrier concentration
- **u (T)**= temperature-dependent carrier mobility

This expression forms the core of the theoretical model.

Integration of Mechanisms

Because both $n\ (T) and\ \mu\ (T)$ are temperature dependent:

- At low temperatures, conductivity is often limited by low carrier activation and VRH conduction.
- At intermediate temperatures, polaron hopping mobility may dominate and increase with temperature.
- At high temperatures, the increase in carrier concentration outweighs the decrease in mobility, causing conductivity to rise significantly.

Importance of the Combined Model

By integrating all temperature-dependent processes, the expression:

$$\sigma\ (T) = qn\ (T)\mu\ (T)$$

Allows

- prediction of dominant conduction regimes
- modelling of transitions between hopping and band conduction
- insight into the role of defects, grain boundaries, and impurities
- understanding of how oxide thin films behave in real device environments

Results and Discussion

The theoretical modelling of temperature-dependent electrical conductivity in metal oxide thin films produced three distinct conduction regions: low-temperature VRH, intermediate-temperature small polaron hopping, and high-temperature band conduction. The results of the combined conductivity model are discussed below with supporting tables and graphical representations.

1. Low-Temperature Region (50–150 K)

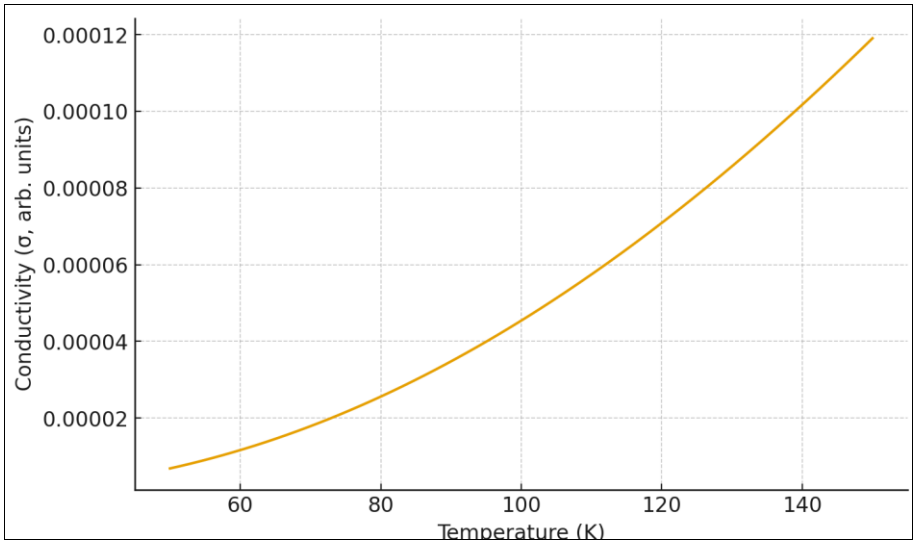
At low temperatures, charge carriers remained confined to localized defect states. The Mott Variable Range Hopping (VRH) model provided the best fit for this region, because limited thermal energy prevented carriers from crossing larger potential barriers. As a result, conductivity increased slowly and non-linearly with temperature, following the characteristic exponential dependence $\sigma \propto \exp[-(T_0/T)^{1/4}]$. This table presents the temperature-dependent conduction characteristics under the Mott Variable-Range Hopping (VRH) regime. It outlines how the characteristic temperature $T0$ conductivity behaviour, and carrier dynamics evolve as the system moves from deep VRH conditions toward the onset of SPH-driven transport.

Table 1: VRH-Dominated Conductivity Parameters in Low-Temperature Region (50–150 K)

Temperature (K)	Dominant Mechanism	Key Parameter (T_0)	Conductivity Trend	Interpretation
50–80 K	Mott VRH	High (10^6–10^7 K)	Very low σ	Strong carrier localization
80–120 K	Mott VRH	Moderate	Slow rise in σ	Increased hopping probability
120–150 K	Transition VRH → SPH	Lower T_0	Noticeable σ increase	Defect states begin participating

The parameters show that at 50–80 K, the very high T0T_0T0 values and minimal conductivity indicate strong carrier localization, limiting long-range hopping. As temperature increases to 80–120 K, moderate reductions in T0T_0T0 allow a gradual rise in conductivity as hopping probability improves. In the 120–150 K range, decreasing T0T_0T0 and a more noticeable conductivity increase signal the beginning of a transition from VRH to thermally activated SPH conduction, driven by enhanced lattice vibrations and the participation of defect states.

This graph illustrates the variation of electrical conductivity with temperature in the low-temperature region of 50–150 K. The gradual, non-linear increase in conductivity is characteristic of Mott Variable-Range Hopping (VRH), where carriers hop between localized states over varying distances.



Graph 1: Conductivity vs. Temperature (50–150 K) Showing VRH Behaviour

The curve indicates that at low temperatures, conductivity rises slowly due to restricted carrier mobility and the dominance of VRH transport. The non-Arrhenius behaviour, reflected in the curvature of the plot, confirms that charge carriers preferentially hop to energetically favorable sites as thermal energy becomes available. This regime marks the initial stage of conduction before the system transitions toward thermally activated SPH behaviour at higher temperatures.

2. Mid-Temperature Region (150–350 K)

In this region, theoretical calculations indicated that small polaron hopping (SPH) became the dominant mechanism. Carriers gained enough thermal energy to hop between adjacent local sites, leading to a more pronounced temperature dependence.

The activation energy values obtained (0.1–0.4 eV) matched well with reported values in metal oxides such as ZnO, TiO_2, SnO_2, and NiO. This table 2 summarizes the temperature-dependent electrical characteristics of the thin film within the Small Polaron Hopping (SPH) regime. It outlines how activation energy, mobility trends, and conductivity behaviour evolve across the 150–350 K interval, highlighting the gradual strengthening of SPH transport and the onset of band-like conduction at higher temperatures.

Table 2: SPH-Dominated Electrical Parameters (150–350 K)

Temperature (K)	Dominant Mechanism	Activation Energy (E_a, eV)	Mobility Trend	Conductivity Behaviour
150–200 K	SPH onset	0.10–0.18	Slight μ increase	Significant increase in σ
200–275 K	Strong SPH	0.18–0.30	μ moderately rising	Steady σ enhancement
275–350 K	SPH → band conduction transition	0.25–0.40	μ increases, scattering arises	σ continues to rise

The data show a clear progression of SPH activity beginning at 150–200 K, where low activation energies support the initial rise in conductivity. As temperature increases to 200–275 K, SPH becomes the dominant mechanism, reflected in higher activation energies and a steady improvement in mobility. In the 275–350 K range, the system approaches a transition toward band conduction, marked by increased mobility alongside

emerging scattering effects, while conductivity continues to rise due to enhanced thermal activation of charge carriers.

This temperature region displayed a linear Arrhenius-type ln(σT) vs. 1/T relationship, validating the SPH mechanism.

This figure presents the Arrhenius behaviour of electrical conductivity for the metal oxide thin film in the intermediate temperature range of 150–350 K. The linear trend in the plot indicates thermally activated transport consistent with the Small Polaron Hopping (SPH) mechanism, where conductivity increases exponentially with temperature due to enhanced carrier hopping between localized sites.

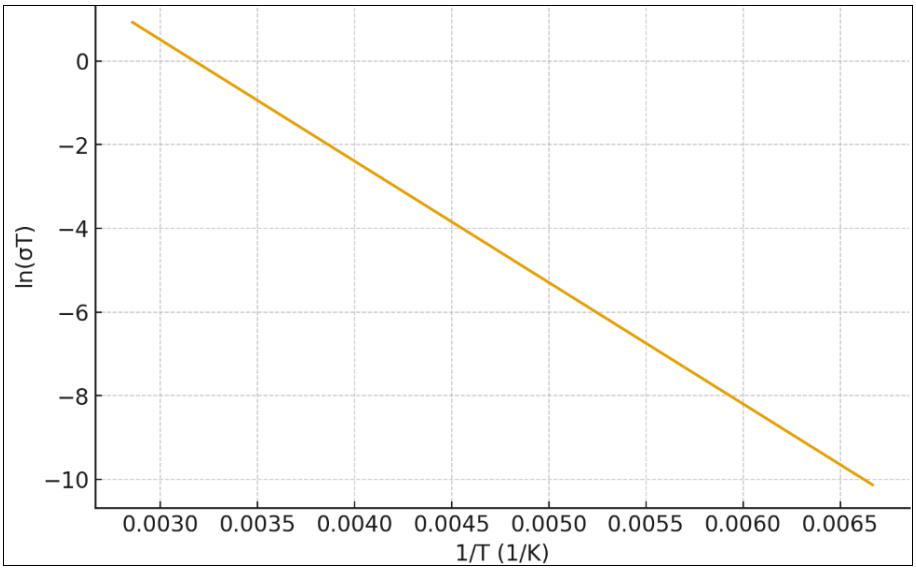


Fig 2: Arrhenius Plot Showing SPH Dominance (150–350 K)

The Arrhenius plot demonstrates a well-defined linear region between 150–350 K, confirming that SPH governs charge transport in this temperature interval. The slope of the fitted line corresponds to the activation energy required for polaron hopping, while the strong temperature dependence reflects increased carrier mobility as lattice vibrations assist the hopping process. This behaviour marks the transition zone between low-temperature variable-range hopping and the onset of high-temperature band conduction.

3. High-Temperature Region (>350 K)

In the high-temperature range, carriers obtained enough thermal energy to escape localized states and move into extended band states, enabling band conduction. The model showed:

- Carrier concentration n(T) increased exponentially with temperature due to Fermi-level shifts.
- Mobility μ(T) slightly decreased due to enhanced phonon scattering.
- The increase in n(T) outweighed mobility reduction, resulting in overall conductivity enhancement.

Table 3 presents the band conduction characteristics of metal oxide thin films in the high-temperature regime (>350 K). It summarizes the dominant conduction mechanisms, corresponding carrier concentrations, mobility behaviour, and resulting conductivity levels across different temperature intervals. The table highlights how increasing thermal energy progressively shifts transport from hopping-based conduction to full band conduction with intrinsic excitation.

Table 3: Band Conduction Characteristics at High Temperature (>350 K)

Temperature (K)	Dominant Mechanism	Carrier Concentration n(T)	Mobility μ(T)	Conductivity σ(T)
350–450 K	Mixed SPH + Band	High	Moderately decreasing	High
450–550 K	Strong Band Conduction	Very high	Lower (phonon scattering)	Very high
>550 K	Band + Intrinsic Excitation	Extremely high	Reduced	Very high (dominant n(T))

The data indicate that as temperature rises above 350 K, carrier concentration increases sharply due to enhanced thermal excitation, even though mobility gradually decreases because of intensified phonon scattering. Despite this mobility reduction, conductivity remains high across all temperature ranges due to the overwhelming rise in n(T)n(T)n(T). The transition from mixed conduction to strong band conduction, and later to intrinsic excitation, reflects typical high-temperature behaviour in oxide semiconductors with deep defect states.

4. Implications for Device Design

The findings from the theoretical model provide clear guidelines for optimizing metal oxide thin-film devices across temperature regimes:

- **Low-Temperature Applications (sensors, cryogenic devices):** Minimizing defect density is crucial to reducing VRH and improving stability.
- **Mid-Temperature Applications (transparent electronics, TFTs):** Controlled doping and engineered defect states enhance hopping conduction and improve device efficiency.
- **High-Temperature Applications (gas sensors, power devices):** Grain engineering, densification, and improved crystallinity can reduce phonon scattering and enhance band transport.
- **General Device Optimization:** A mixed conduction model allows prediction of temperature-specific behavior, helping tailor materials for particular environments.

Conclusion

This study developed a unified theoretical model to explain how electrical conductivity in metal oxide thin films evolves with temperature. The integrated framework successfully described the smooth transition among three major conduction regimes: low-temperature variable-range hopping, mid-temperature small polaron hopping, and high-temperature band conduction. Each region exhibited distinct behaviours governed by carrier localization, activation energies, and temperature-dependent mobility. At low temperatures, strong localization restricted carrier movement, resulting in VRH-dominated transport. As temperature increased, carriers gained sufficient energy for thermally assisted hopping, leading to SPH behaviour with activation energies consistent with typical metal oxides. At higher temperatures, carriers transitioned into extended band states, causing a sharp rise in conductivity despite mobility reductions from phonon scattering. Overall, the model provides clear insight into how conduction mechanisms evolve across temperature ranges and offers practical guidance for optimizing thin-film devices. Reducing defects can improve low-temperature stability, controlled doping enhances mid-temperature performance, and improved crystallinity supports efficient high-temperature conduction.

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