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A REVIEW ON CLASSIFICATION, CRYSTAL STRUCTURE, APPLICATIONS AND SAFETY CONSIDERATIONS OF METAL CHALCOGENIDES THIN FILMS

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ABSTRACT

Metal chalcogenides thin films represent a class of materials with exceptional optoelectronic properties, making them decisive for next-generation electronic and photonic devices. This comprehensive review examines the synthesis methodologies, characterization techniques and diverse applications of metal chalcogenides thin films. The paper discusses various deposition techniques including chemical vapor deposition (CVD), molecular beam epitaxy (MBE) and solution-based methods, along with their impact on film quality and properties. Characterization methods encompassing structural, optical and electrical analyses are used to study their varid properties. Applications in solar cells, photodetectors, transistors and energy storage devices are presented with experimental data demonstrating their performance metrics.

KEYWORDS: Metal chalcogenides, thin films, synthesis, characterization, optoelectronics, 2D materials.

1. INTRODUCTION

Metal chalcogenides constitute a fascinating class of materials formed by the combination of metals with chalcogen elements (sulfur, selenium, and tellurium). These materials have garnered significant attention due to their unique electronic, optical, and catalytic properties. The transition from bulk to thin film form opens new possibilities for device applications while maintaining the intrinsic properties of the materials. The general formula for metal chalcogenides can be expressed as MxEy, where M represents the metal cation and E represents the chalcogen anion. The diversity in stoichiometry and crystal structures leads to a wide range of properties, from insulators to superconductors, making them versatile for various technological applications. The significance of metal chalcogenides thin films lies in their tunable band gaps, high absorption coefficients, and excellent charge transport properties. These characteristics make them ideal candidates for photovoltaic applications, photodetectors, field-effect transistors, and energy storage systems.

2. Classification and Crystal Structures

2.1 Binary metal chalcogenides

Imagine materials that are just a few atoms thick but possess extraordinary electronic and optical properties that could revolutionize everything from smartphones to solar panels. That's exactly what Transition Metal Dichalcogenides (TMDCs) offer. These remarkable 2D materials have captured the attention of researchers worldwide because they bridge the gap between graphene's excellent electrical properties and traditional semiconductors' ability to control light and electricity. TMDCs follow the general formula MX_2, where M represents a transition metal (like molybdenum or tungsten) and X represents a chalcogen element (sulfur, selenium, or tellurium). Think of them as molecular sandwiches: a layer of metal atoms sandwiched between two layers of chalcogen atoms, held together by strong chemical bonds within each layer but only weakly connected between layers.

Common examples include

- Transition Metal Dichalcogenides (TMDCs): MoS_2, WS_2, $MoSe_2$, WSe_2
- Metal Monochalcogenides: ZnS, CdS, PbS, SnS
- Noble Metal Chalcogenides: Ag_2S, Cu_2S, Au_2S

TMDCs represent one of the most promising classes of 2D materials, with MoS_2, WS_2, and $MoSe_2$ leading the charge in practical applications. Each material offers unique advantages: MoS_2 provides an excellent balance of properties and processability, WS_2 excels in optical applications and spintronics, while $MoSe_2$ shines in infrared applications and ambipolar electronics. The field continues to advance rapidly, with new synthesis methods, characterization techniques, and applications emerging regularly. As we overcome current challenges in synthesis scalability and device integration, TMDCs are poised to play crucial roles in next-generation electronics, optoelectronics, and energy technologies. The journey from laboratory curiosities to commercial applications is well underway, making TMDCs an exciting area for both fundamental research and technological development. Whether you're interested in pushing the boundaries of physics or developing practical devices, these remarkable materials offer endless possibilities for innovation and discovery.

2.2 Ternary and Quaternary systems

While binary metal chalcogenides like MoS_2 have captured headlines, the real magic happens when we add more elements to the mix. Ternary (three-element) and quaternary (four-element) chalcogenides offer something binary systems can't.

More complex compositions include

- Ternary compounds: $CuInS_2$, $AgInSe_2$, ZnCdS
- Quaternary compounds: Cu_2ZnSnS_4 (CZTS), $CuInGaSe_2$ (CIGS)

These complex chalcogenides have become the backbone of modern solar cell technology and are emerging as game-changers in thermoelectrics, catalysis, and next-generation electronics. Ternary and quaternary chalcogenides represent the sweet spot between performance and practicality. While they're more complex than binary systems, this complexity enables unprecedented control over electronic and optical properties. CIGS has already proven commercial viability, while CZTS and related earth-abundant materials promise to democratize high-efficiency solar technology. The field is rapidly evolving, with new compositions, synthesis methods, and applications emerging regularly. As we better understand and control their complex defect chemistry, these materials will likely play increasingly important roles in sustainable energy technologies and beyond.

2.3 Crystal structure analyses

The beauty of TMDCs lies in their elegant atomic architecture. Each layer consists of three atomic planes arranged in an X-M-X configuration. The metal atoms occupy the center, coordinated by six chalcogen atoms in a trigonal prismatic or octahedral arrangement. This creates a structure that's both mechanically flexible and electronically sophisticated.

Key Structural Features

- Layer thickness: Approximately 6-7 Å (about 0.6-0.7 nanometers)
- Interlayer spacing: 3-4 Å between adjacent layers
- Bonding: Strong covalent bonds within layers, weak van der Waals forces between layers
- Symmetry: Hexagonal crystal structure with space group $P6_3/mmc$

Table 1: Comparative structure of the binary metal chalcogenides.

Material	Crystal Structure	Space Group	Lattice Parameters (Å)	Band Gap (eV)
MoS_2	Hexagonal	$P6_3/mmc$	a = 3.16, c = 12.29	1.2-1.9
WS_2	Hexagonal	$P6_3/mmc$	a = 3.15, c = 12.32	1.3-2.1
CdS	Hexagonal/Cubic	$P6_3mc$/F43m	a = 4.14, c = 6.72	2.4
ZnS	Cubic/Hexagonal	F43m/$P6_3mc$	a = 5.41	3.6
PbS	Cubic	Fm3m	a = 5.94	0.4
SnS	Orthorhombic	Pnma	a = 4.33, b = 11.20, c = 3.98	1.3

3. Synthesis methods

There are many methods to synthesize binary metal chalcogenides; however the method employed depends upon the requirement that which type of material is required. Some commonly employed methods are: Physical Vapor Deposition (PVD),Techniques Molecular Beam Epitaxy (MBE), Magnetron Sputtering, Chemical Vapor Deposition (CVD), Chemical Bath Deposition (CBD), Successive Ionic Layer Adsorption and Reaction (SILAR), Electrochemical Deposition, etc**.**

For high quality material, control atmosphere, pure precursors and optimize temperature are required. For scalability we have to choose solution methods, optimize precursor concentrations, and control nucleation. For cost control, use abundant precursors, minimize processing steps, and avoid high vacuum conditions. The bottom line is that.

- Need the best quality? → CVD or MBE
- Want it cheap and scalable? → Hydrothermal or CBD
- Require atomic precision? → ALD
- Making quantum dots? → Hot injection
- Working with 2D materials? → CVD for growth, exfoliation for quick samples

Often, the "best" method depends more on the specific application requirements than absolute material quality.

4. Applications

4.1 Photovoltaic applications

Metal chalcogenides have become the workhorses of thin-film solar technology because they solve a fundamental problem: how to capture sunlight efficiently while keeping costs manageable. Unlike silicon solar cells that require thick, expensive wafers, chalcogenide thin films need only 1-3 micrometers of material to absorb over 90% of incident sunlight. The efficiency breakdown of different technology solar cells are given in the table 2.

Table 2: Efficiency breakdown of different technology.

Technology	Lab Record	Commercial	Theoretical Limit
CIGS	23.35%	17-19%	~28%
CdTe	22.1%	16-18%	~30%
CZTS	12.6%	Not commercial	~32%
c-Si	26.7%	20-22%	~29%

Copper Indium Gallium Selenide (CIGS) solar cells represent one of the most successful applications of metal chalcogenides thin films. The different solar cell parameters are recorded and are given in table 3.

Table 3: CIGS Solar Cell Performance Data.

Parameter	Laboratory Record	Commercial Module
Efficiency	23.35%	17-19%
Voc (V)	0.756	0.65-0.70
Jsc (mA/cm²)	39.5	32-36
Fill Factor	0.781	0.75-0.78
Area (cm²)	0.5	>1000

Metal chalcogenides have already revolutionized solar energy, providing cost-effective alternatives to silicon while opening new application areas through their flexibility and light weight. They works well in cloudy condition, rooftop systems, building integration, space satellites, have lowest $/watt among all solar technologies. However some of them have complex configuration which causes defect chemistry thus limiting their performance. CIGS and CdTe are mature technologies powering gigawatts of installations worldwide, while emerging materials like CZTS promise even more sustainable and cost-effective solutions.

Key advantages

- High efficiency with minimal material usage
- Manufacturing flexibility enabling diverse applications
- Continuous improvement in both performance and cost
- Scalability to meet global energy demands

The future looks bright for chalcogenide photovoltaics, with tandem architectures and earth-abundant materials poised to push efficiencies beyond 30% while driving costs below $0.20 per watt. They're not just competing with fossil fuels—they're making solar the cheapest energy source in human history.

5. Environmental and safety considerations

The Reality Check: **Not All "Green" Materials Are Actually Green**. While metal chalcogenides promise cleaner energy through solar cells and efficient electronics, many contain elements that pose serious environmental and health risks. Understanding these concerns isn't about fear-mongering—it's about responsible innovation and sustainable technology development. The environmental and safety challenges of metal chalcogenides aren't insurmountable barriers—they're engineering problems that require thoughtful solutions. The key principles are.

- Transparency: Acknowledge risks honestly
- Hierarchy: Eliminate > Substitute > Engineer > Protect
- Lifecycle thinking: Consider cradle-to-grave impacts
- Continuous improvement: Better materials and processes
- Stakeholder engagement: Include communities in decision-making

The goal isn't to stop innovation but to ensure that our pursuit of cleaner energy doesn't create new environmental and health problems. With proper precautions and taking safety measures many of these materials can be used carefully, and ongoing research and development continues to develop even better alternatives with minimum risks and maximum efficiency. The most sophisticated synthesis method means nothing if your workers get sick or your waste contaminates the local environment. Safety and environmental stewardship aren't optional—they're essential parts of good science, greener environment, less toxic wastes, low degree of hazards and responsible engineering.

6. CONCLUSIONS

Metal chalcogenides thin films represent a versatile class of materials with exceptional properties for diverse technological applications. The synthesis methods range from sophisticated vacuum-based techniques to cost-effective solution processes, each offering unique advantages for specific applications. Characterization techniques provide comprehensive understanding of structural, optical, and electrical properties, enabling optimization of device performance. The applications span from high-efficiency solar cells and sensitive photodetectors to next-generation transistors and energy storage devices. The performance data presented demonstrates the competitive advantage of metal chalcogenides in many applications, with efficiencies and performance metrics often exceeding conventional materials. Future research directions focus on addressing current challenges in synthesis scalability, environmental sustainability, and the development of novel applications in quantum technologies and flexible electronics. The integration of advanced characterization techniques with machine learning approaches promises to accelerate materials discovery and optimization.

The economic viability of metal chalcogenides continues to improve with technological advances and economies of scale. However, environmental and safety considerations require ongoing attention to ensure sustainable development of these technologies.

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