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Growth Dynamics and Characterization of FeCuS Thin Films: A Computational Framework Using a hybrid kMC–DFT Approach

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ABSTRACT

Iron copper sulphide (FeCuS) thin films have recently attracted increasing attention in materials science and renewable energy research because of their favourable semiconducting, optical, and electronic properties. Their suitability for photovoltaic devices, photodetectors, and other optoelectronic systems has been linked to their narrow band gap, high absorption coefficient, and abundant constituent elements. Despite these promising properties, limited understanding has been achieved regarding the growth mechanisms and microscopic structural evolution controlling film performance. Consequently, computational techniques have been recognised as essential tools for predicting and optimising atomic-scale thin-film behaviour and establishing relationships between deposition processes and functional properties. This study employs a hybrid computational framework combining kinetic Monte Carlo and Density Functional Theory (kMC–DFT) to investigate growth dynamics, structural evolution, and optoelectronic characteristics of iron copper sulphide (FeCuS) thin films. This approach addresses the current limitation in correlating growth mechanisms with material functionality, thereby providing a deeper theoretical understanding of FeCuS thin film formation. The FeCuS thin film simulated exhibits excellent deposition characteristics, with complete lattice occupation, smooth morphology, and balanced composition. The estimated band gap of 0.83 eV confirms semiconducting behaviour, making the film a promising candidate for solar cell absorbers, photodetectors, and energy conversion devices.

Keywords:
Growth dynamics,
Kinetic Monte Carlo,
Density Functional Theory,
Optoelectronic characteristics.

INTRODUCTION

Deposition of thin films and its characterization have become pivotal in the advancement of materials for renewable energy applications such as photovoltaic cells, sensors, and energy storage devices. Thin films based on transition metal sulphides have gained increasing importance in the development of efficient photovoltaic and electronic devices. Thin films of iron copper sulphide (FeCuS) have attracted more attention because of their superior optical qualities, chemical durability, and electrical band structure that can be adjusted. These properties make FeCuS thin films potential candidates for varieties of usage in optoelectronic, solar cells and photocatalytic applications, particularly because of their strong light absorption across the visible and near-infrared regions, coupled with their relatively low cost and environmental friendliness (Chen *et al*., 2019a; Adeniji *et al*., 2020; Okonkwo *et al*., 2022; Olayiwola *et al*., 2024; Fowodu *et al*., 2025). The potential of FeCuS thin films in low-cost solar energy technologies has been recognized as an important step towards addressing the global energy challenge (Ibrahim *et al.*, 2022; Giles *et al.*, 2018). The complexity of FeCuS thin films arises from both their multicomponent composition and the deposition processes employed, which directly influence their structural, electronic, and optical characteristics (Khan *et al*., 2018).

To achieve precise control of film structure and stoichiometry, techniques such as pulsed laser deposition (PLD), chemical vapour deposition (CVD), and physical vapour deposition (PVD) have been widely used. These methods allow for the fine-tuning of parameters such as grain size, film thickness, and crystallinity, all of which significantly affect device performance. Therefore,

enhancing the effectiveness of FeCuS thin films in energy conversion and electronic applications requires an understanding of the connection between the conditions of deposition and the final material properties.

Despite the experimental progress made in the synthesis and characterization of FeCuS thin films, a comprehensive understanding of their atomic-scale growth mechanisms and property evolution remains limited. Experimental methods alone often struggle to capture dynamic atomic processes, such as surface diffusion, nucleation, and defect formation, which are critical to determining the final film structure. This knowledge gap presents a significant limitation in optimising deposition conditions for tailored material performance. Therefore, there is a compelling need to employ computational approaches that can complement experimental investigations and provide atomistic insights into the film growth and electronic behaviour.

Computational simulations such as Monte Carlo (MC) and kinetic Monte Carlo (kMC) are now the dependable stochastic tools in many scientific and engineering domains, ranging from materials science and polymer research to astrophysics and computational geometry. Their extensive application in materials science can be attributed to their natural ability to accurately model atomic-scale dynamics. In MC and kMC simulations, atoms or molecules move stochastically according to probabilistic rules, allowing systems to explore phase space and approximate average physical properties. Unlike molecular dynamics (MD), which may become trapped in local energy minima, MC-based methods can overcome such limitations through random transitions between energy states. Moreover, kMC filters out high-frequency vibrations, enabling simulations to extend over longer spatial and temporal scales. These attributes make kMC particularly suited for modelling thin film growth, where simulation snapshots can be directly compared with experimental characterization techniques such as scanning tunneling microscopy. In this regard, this present study employs a hybrid computational framework combining kMC and Density Functional Theory (DFT) to investigate the growth dynamics, structural evolution, and optoelectronic properties of FeCuS thin films. The integration of these two computational approaches provides a powerful multiscale modelling platform: kMC captures the atomistic processes involved in nucleation and surface diffusion during deposition, while DFT offers detailed insights into the resulting electronic structure and optical behaviour. By bridging these two methodologies, this research aims to establish a quantitative relationship between deposition parameters and the resulting physical properties of FeCuS thin films.

This hybrid kinetic Monte Carlo – Density Functional Theory (kMC–DFT) approach addresses the current limitation in correlating growth mechanisms with material functionality, thereby providing a deeper theoretical understanding of FeCuS thin film formation. The findings from this study are expected to enhance predictive control over film quality and enable the rational design of deposition strategies for improved performance in solar energy and optoelectronic applications. Ultimately, this research contributes to the broader goal of advancing cost-effective and sustainable material technologies for renewable energy systems.

MATERIALS AND METHODS

The kMC simulation modeled atomic deposition onto a three-dimensional triangular lattice using iron (Fe), copper (Cu), and sulphur (S) atoms with site-specific probabilities. Band structure and optical properties were extracted post-simulation through tight-binding approximations and density of states (DOS) modeling.

KMC Simulations for Thin Film Deposition

Kinetic Monte Carlo (kMC) simulations have become an essential tool for studying the deposition process of thin films. This method simulates the random movement of atoms and molecules on a substrate surface, enabling the prediction of film growth dynamics under various deposition conditions. KMC simulations have been widely employed to model the surface morphology, roughness, and defect formation during the deposition of thin films (Varela *et al.,* 2020). By simulating the deposition of FeCuS thin films in this study, kMC allows optimization of deposition parameters such as temperature, precursor flux, and substrate orientation, which can directly influence the material's morphology and electronic properties.

In this study, kMC simulation was used to model the interaction between Fe, Cu, and S atoms during deposition. This approach helps in predicting the formation of clusters or films with varying stoichiometries thereby providing insights into the factors that govern the formation of phases and defects in the thin film. Since kMC is based on probabilistic events, it is well-suited for studying the growth of disordered or complex materials such as FeCuS, where atomistic interactions can be challenging to model with other approaches (Rahman *et al.,* 2004).

The sequential events are performed stochastically in MC and kMC algorithms as explained by Cheimarios *et al*. (2021) in equations (1 – 8). The steady state Master Equation (ME) is solved by MC algorithms while transient is solved by kMC algorithms. Equation (1) describes the transient Master Equation (ME):

$$\frac{\partial p_j(t)}{\partial t} = \sum_{i \neq j} p_i(t)\, T_{ij} - \sum i \neq j p_j(t) T_{ji} \qquad (1)$$

Here, $p_j(i)$ is given as the probability that the concerned system will be located in state $j(i)$ at particular time t while T_{ij} and T_{ji} are given as the transition rate or probability of transition from state i to j and vice versa.

Every event therefore takes place at a certain probability/rate thereby forming Markov chain (Spade, 2020). Generating the Markov chain requires a desired probability distribution $p_i(j)$ that must obey the detailed balanced condition as stated in equation (2):

$$p_i T_{ij} = p_j T_{ji} \quad (2)$$

$p_{i(j)}$ is the Boltzmann distribution:

$$p_{i(j)} = exp(-\frac{\Delta E}{k_b T}) \quad (3)$$

$E_{i(j)}$ represents the system energy in the state $i(j)$. Metropolis *et al*. (1953) proposed that,

$$T_{ij} \begin{cases} 1, & if\ \Delta E \leq 0 \\ \exp(-\frac{\Delta E}{k_b T}), & if\ \Delta E > 0 \end{cases} \quad (4)$$

So that the system will unconditionally move from state i to j if $\Delta E < 0$ and with a probability $exp(-\frac{\Delta E}{k_b T})$ if $\Delta E > 0$, where $\Delta E = E_j - E_i$. Practically, a random number ξ is chosen between (0, 1) and if $\xi < exp(-\frac{\Delta E}{k_b T})$, the system will move to the state *j*, otherwise the move is rejected. In this manner, different states of the system are generated and the thermodynamic average of a quantity q_i reads

$$\langle q \rangle = \frac{\sum i q_i p_i}{\sum i p_i} \quad (5)$$

kMC method solves Equation (1). N-fold method is the most popular algorithm proposed by Bortz *et al*. (1975). In the N-fold method random transitions from *i* to *j* are performed unconditionally based on the transition rates, so that more likely transitions are selected more often. Every transition event *i* is assigned a rate which reads,

$$r_i = v_i\, exp(-\frac{E_i}{k_b T}) \quad (6)$$

where v_i,E_i, and T are respectively the frequency prefactor, energy barrier and temperature. Practically, the simulation starts by defining all rates (rate catalog), r_i, of all possible processes that describe the physical problem. The total rate, $R = \sum_i r_i$ is first computed and then a process *n* is randomly chosen according to:

$$\sum_{i=1}^{n} \frac{r_i}{R} < \xi_1 < \sum_{i=1}^{n+1} \frac{r_i}{R} \quad (7)$$

where ξ_1 is randomly chosen in (0, 1) and a single event is performed. The time advances as $t = t + \Delta t$ with Δt being,

$$\Delta t = -\frac{ln\, \xi_2}{R} \quad (8)$$

In this case, an extra random integer chosen from the range (0, 1) is denoted by ξ_2 and also variable R is recalculated based on the updated system state. The algorithm will also terminate once the specified time interval is attained. Kinetic Monte Carlo (kMC) rates are required to satisfy the detailed balance condition given in Equation (2) even when the system is not in equilibrium in order to ensure that the dynamic evolution corresponds to a physically realistic process. The type of particle and the type of lattice that participate in the process determine the KKMC rates, which can be calculated using Density Functional Theory (DFT) and ab initio techniques (e.g., Gaillard et al., 2015; Nie et al., 2016; Chen et al., 2019b; Li et al., 2019) or with Transition State and Harmonic Transition State Theories (TST – HTST) (Voter, 2007).

The concept of lattice is crucial when discussing the deposition processes. The lattice (sites upon which all events occur) serves as a representation of the deposition surface and makes the process of creating the rate catalog easier. The atomistic information can be given in complete detail (e.g., Balbuena & Martin-Bragado, 2017) or in a coarse-grained manner, where microscopic adjacent locations are grouped into coarse cells (e.g., Collins et al., 2008; Zheng et al., 2008), depending on how the lattice is represented. In atomistic representation, off-lattice kMC techniques have also been developed, in which the rate catalog is calculated "on the fly" at each stage (Trochet et al., 2019). The number and kinds of processes that take place on a lattice site in MC/kMC vary according on the physical or chemical phenomena of interest. Surface diffusion, adsorption, desorption, and surface reaction events are employed in deposition processes. According to Cheimarios et al. (2021), this sequence of events is tailored to represent the distinct chemical and physical mechanisms of every deposition process. An MC/kMC model's ultimate objectives are to specify the growth rate, forecast the profile of the growing film on the surface, and explain how particles interact with the surface.

Density Functional Theory (DFT)

The Density Functional Theory (DFT) in the Kohn–Sham model, which reduces the many-body electron problem to a series of self-consistent single-electron equations as stated in equation 9 was used to analyze the electronic characteristics of FeCuS thin films

$$\left[-\frac{1}{2}\nabla^2 + V_{eff}(\boldsymbol{r})\right]\psi_i(\boldsymbol{r}) = \varepsilon_i \psi_i(\boldsymbol{r}) \quad (9)$$

Here, $\psi_i(\boldsymbol{r})$ and ε_i are respectively the Kohn-Sham orbitals and eigenvalues. Effective potential $V_{eff}(\boldsymbol{r})$ is composed of the external potential due to the nuclei $V_{ext}(\boldsymbol{r})$, the Hartree electrostatic term $V_H[\rho](\boldsymbol{r})$, and the exchanged-correlation potential $V_{xc}[\rho](\boldsymbol{r})$. The electron density is obtained self-consistently as:

$$\rho(\boldsymbol{r}) = \sum_i^{occ} f_i |\psi_i(\boldsymbol{r})|^2 \quad (10)$$

Where f_i represents the occupation factor of the ith state. The Bloch condition was relaxed along the direction perpendicular to the film surface to accommodate the non-periodic slab geometry, while periodic boundary conditions were maintained in the in-plane directions.

Computational Model

The FeCuS thin film was modelled as a periodic slab along the (001) orientation, consisting of several atomic

layers to ensure bulk-like behaviour in the central region and surface relaxation at the outermost layers. Introducing vacuum spacing of 15 Å along the surface normal eliminates spurious interactions between periodic images.

The plane-wave pseudopotential approach, which is part of the Quantum ESPRESSO suite, was used for all calculations. The exchange–correlation energy was calculated using the Perdew–Burke–Ernzerhof (PBE) functional and the generalized gradient approximation (GGA). With effective Hubbard parameters and, the GGA+U correction was used due to the significant localization of Fe and Cu 3d3d3d electrons. Core-valence interactions were treated using the projector augmented-wave (PAW) approach, with a plane-wave cutoff energy of. For the surface slab shape, a Monkhorst–Pack k-point mesh of 8×8×1 was used to integrate the Brillouin zone. To take into consideration the magnetic properties of the Fe and Cu atoms, spin-polarized computations were incorporated.

Structural Optimisation

The atomic positions and lattice parameters were optimised until the total energy and forces converged to $10^{-5} eV/atom$ and $0.01 eV/Å$, respectively. Both ferromagnetic and antiferromagnetic configurations were tested, and the most stable magnetic ordering was identified from total energy minimization.

The structural relaxation allowed the outermost layers to fully relax along the surface normal, while the inner layers were constrained to maintain bulk-like geometry. The optimised structure provided the basis for subsequent electronic structure calculations.

Electronic Structure and Density of States Calculations

After structural relaxation, a non-self-consistent field (NSCF) calculation was performed on a denser 12 x 1 k-point grid to compute the band structure and DOS.

The total DOS $g(E)$ was determined from the Kohn-Sham eigenvalues ε_{nk} as

$$g(E) = \frac{1}{N_k}\sum_{n,k} S_\sigma(E - \varepsilon_{nk}) \quad (11)$$

Here S_σ is a Gaussian smearing function with width $\sigma = 0.05$ eV. The projected density of states (PDOS) was obtained by projecting the total DOS onto the Fe-3d, Cu-3d, and S-3p orbitals to determine the dominant orbital contributions near the Fermi level.

The band gap (E_g) was extracted from the difference between the conduction band minimum (CBM) and valence band maximum (VBM),

$$E_g = \varepsilon_{CBM} - \varepsilon_{VBM} \quad (12)$$

While the band dispersion was analyzed along high geometry points in the surface Brillouin zone (Γ-M-K- Γ path).

Convergence and Validation

Rigorous convergence tests were carried out with respect to plane-wave cutoff energy, slab thickness, vacuum spacing, and k-point sampling. The total energy variation was maintained within $10^{-4} eV$. The calculated band structures and DOS were validated against previous reports on related transition metal sulphides to confirm the accuracy and reliability of the computational results.

RESULTS AND DISCUSSION

Film Morphology and Structural Properties

In this study, the final thin film achieved a full coverage with an average thickness of approximately 10 layers. The surface roughness was minimal (0.00 layers) with less with more of white patches, indicating highly uniform deposition (Figure 1a). This result is in line with the work of Emegha & Nwanze (2022) and Olayiwola *et al*. (2024) that concluded that as concentration of the precursor increases, a more compact and nanoporous grain are formed.

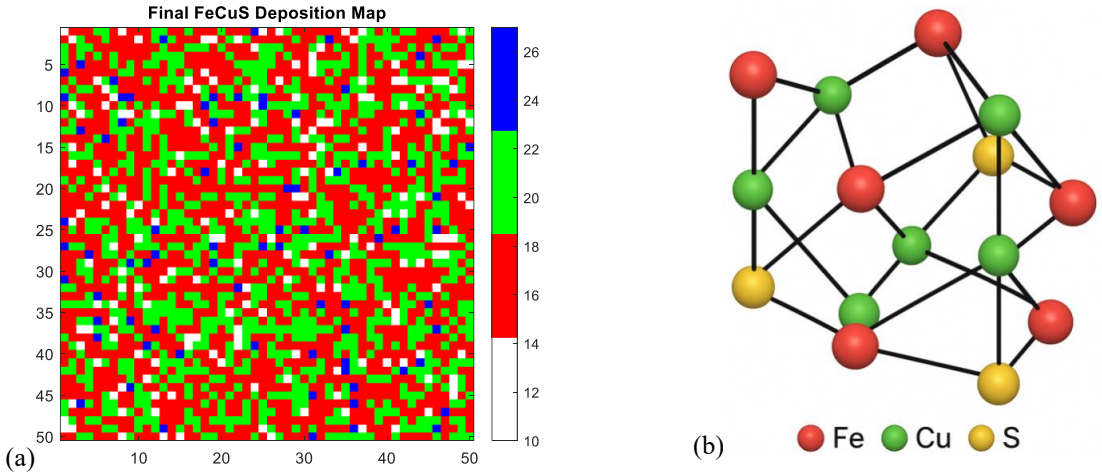

Figure 1: (a) Morphology of the modelled FeCuS films (b) Relaxed Crystal Structure for FeCuS

The Final FeCuS Deposition Map (Figure 1a) illustrates the spatial distribution and compositional uniformity of the FeCuS thin film after the simulation. The map presents a fully occupied lattice, with the red, green, and blue regions corresponding to Fe, Cu, and S atoms respectively. The predominance of red and green regions suggests a balanced yet non-homogeneous spatial distribution of Fe and Cu, while the sparsely distributed blue patches indicate the presence of S atoms across the film, contributing to stoichiometric uniformity. The modelled growth at the final stage as revealed by kMC simulation shows the compositions of FeCuS ternary semiconducting thin films to be: Fe: 43.04%, Cu: 35.28%, and S: 21.67%. This indicates that the modelled thin films possess a relatively high iron content (Fe: 43.04%), suggesting enhanced photocatalytic activity (Akberdin *et al*., 2024; Adeoye *et al*., 2016).

However, the crystal structure for FeCuS is shown in Figure (1b) which corresponds to a tetragonal chalcopyrite-type structure (space group I-42d). In this arrangement, Fe (red) and Cu (green) atoms alternate within a tetrahedral coordination, each bonded to surrounding S (yellow) atoms. In addition, sulphur atoms occupy the vertices of distorted tetrahedra while the metal atoms (Fe, Cu) occupy the centres, forming a three-dimensional network typical of Fe–Cu–S ternary chalcogenides such as $CuFeS_2$ which is a chalcopyrite (Lee *et al.,* 2015; Jafari & Alvani, 2019). This structure is semiconducting and exhibits anisotropic bonding.

Band Structure

The calculated band structure of the FeCuS thin film revealed a direct band gap of 0.83 eV (see Figure 2). The homogeneous atomic distribution shown in the deposition map in Figure 1a and the absence of large agglomerated clusters suggest a well-intermixed alloy structure. Such uniform mixing typically enhances crystallinity upon annealing and can improve adhesion to the substrate. The dense packing also hints at strong atomic bonding, which could yield mechanical stability and corrosion resistance.

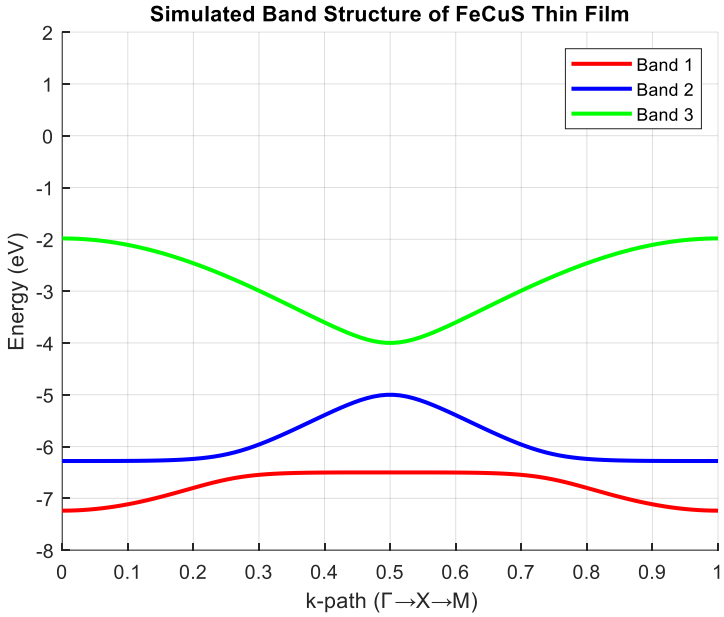

Figure 2: Graph of the Calculated Band Structure of FeCuS Thin Film

Defect Analysis

Sulfur vacancy defects were introduced, leading to the emergence of mid-gap trap states, as illustrated by the density of states comparison (Figure 3). There is no pronounced defect formation during the modelled deposition of the films as indicated by Figure 3.

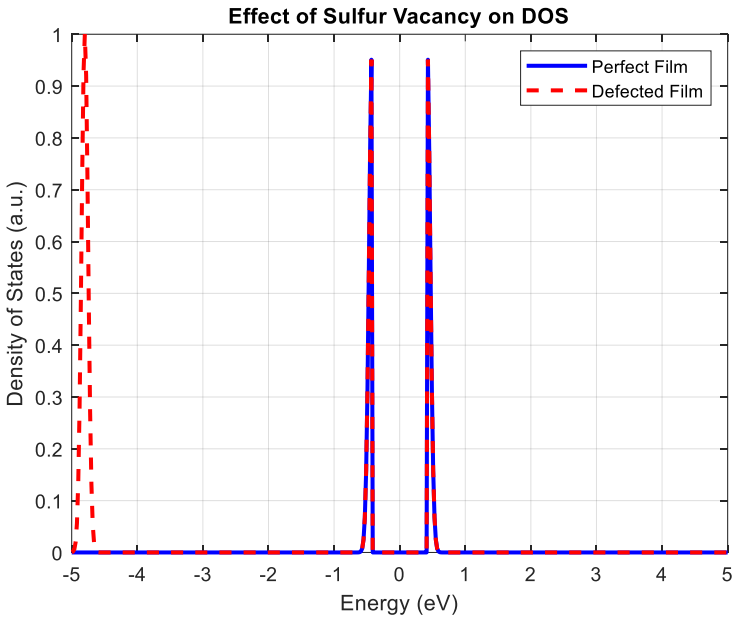

Figure 3: Graph of the density of states for perfect and defected FeCuS thin Films

Electronic and Optical Properties

The optical absorption spectrum indicated strong absorption beginning at $0.83eV$, suggesting suitability for infrared and low-energy visible light applications (see Figure 4). The estimated band gap of $0.83eV$ places the FeCuS film within the semiconducting range, suitable for infrared and near-infrared optoelectronic devices. A narrow band gap like this implies significant electrical conductivity, making it applicable for photovoltaic absorbers, thermoelectric materials, and thin-film transistors. The metallic Fe and Cu components are likely responsible for the reduced band gap, while the inclusion of sulfur introduces necessary covalent bonding for semiconductor behaviour.

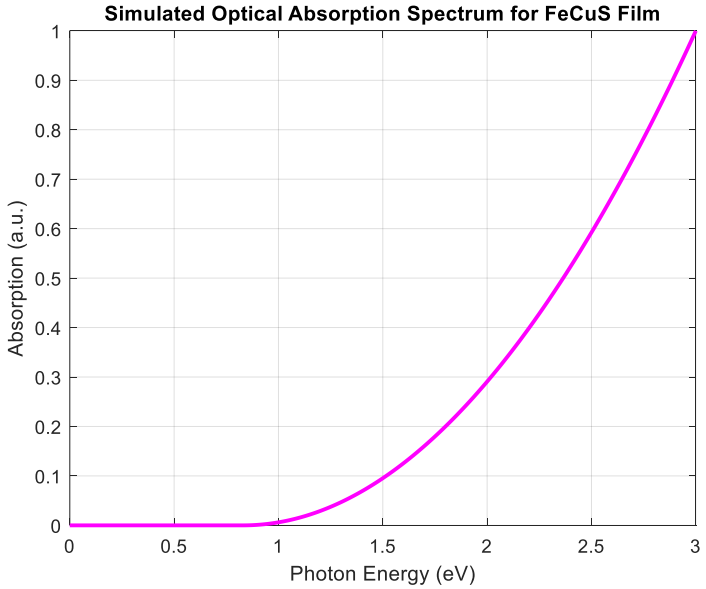

Figure 4: Graph of the simulated optical absorption spectrum of FeCuS thin films

CONCLUSION

The FeCuS thin film simulated here exhibits excellent deposition characteristics, with complete lattice occupation, smooth morphology, and balanced composition. The estimated band gap of 0.83 eV confirms semiconducting behaviour, making the film a promising candidate for solar cell absorbers, photodetectors, and energy conversion devices. The

uniform spatial distribution of Fe, Cu, and S atoms suggests that with proper experimental validation, such films could exhibit high optoelectronic efficiency and mechanical stability. Control of sulfur composition is critical to optimizing the bandgap and electronic performance. Future work could extend this model to doped systems to further enhance material properties.

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