Thin Film Characterization for Promising PV Layers

Mzoun Almutairi
mzounmutairi@outlook.com

Rawan Aldosari
rawanaldosarii.ii@gmail.com

Shouq Fairaq
shouqfairaq@gmail.com

Mentor: Niladri Banerjee
n.banerjee@imperial.ac.uk

Zeyou Li
zeyou.li22@imperial.ac.uk

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1. Introduction

Solar cell technology is a critical area in the renewable energy sector, playing a vital role in electricity generation to meet the growing global demand caused by rapid population expansion. To reduce material usage and manufacturing costs, thin-film technology has been developed [5]. Among the most prominent thin-film solar cell materials are amorphous silicon, cadmium telluride (CdTe), and copper indium gallium selenide (CIGS), which currently dominate the thin-film market [1].

In perovskite thin-film solar cells (PSCs), hole-transporting materials (HTMs) are crucial for enhancing both device performance and stability. Recently, HTMs incorporating helicene cores have attracted significant attention due to their unique structural and electronic properties. Effective HTMs typically exhibit excellent hole mobility and conductivity, minimal absorption in the visible and near-IR regions of the solar spectrum, as well as strong photochemical, morphological, and thermal stability. Moreover, their hydrophobic characteristics, as demonstrated in water contact angle measurements, are beneficial in preventing moisture penetration into the perovskite layer, thereby improving long-term device stability [2].

Helicenes themselves are a distinct class of organic molecules composed of ortho-fused benzene rings arranged in a spring-like configuration. This structure imparts intrinsic chirality, giving rise to unique optical properties such as exceptionally large optical rotatory dispersion (ORD). Typically, helicenes absorb light in the visible to near-ultraviolet range, with absorption peaks around 350–500 nm, depending on molecular length and type. As the helicene chain length increases, the absorption shifts toward longer wavelengths (lower energy). One major advantage of helicenes lies in their tunable optical absorption, which can be adjusted through variations in length, heteroatom substitution, or functionalization [3].

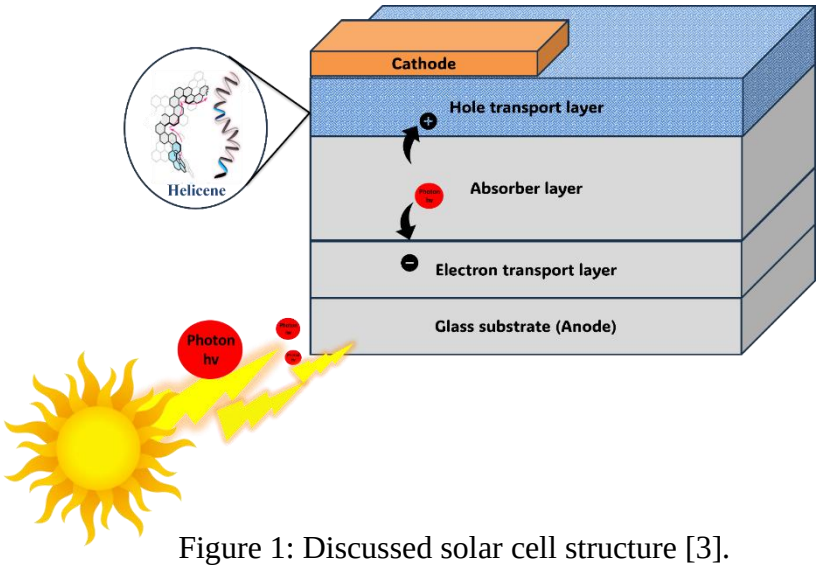


Figure 1: Discussed solar cell structure [3].

In parallel, niobium-based materials have shown promise in energy-related applications, specifically their usage as electrode materials. Niobium nitride (NbN), for instance, possesses a high electrical conductivity of approximately 42.9 S/cm significantly higher than that of semiconducting Nb_2O_5. Its intrinsic nanochannel structure enables efficient charge transport and rapid ion diffusion, leading to high capacitance, excellent rate capability, and low resistance during cycling. These structural and electronic characteristics make NbN a strong candidate for advanced solar cell electrodes and other high-performance energy storage applications [4].

To better understand the material characteristics, surface morphology was examined using atomic force microscopy (AFM) in tapping mode, with Gwyddion software applied for data analysis, flattening, and roughness quantification. Line profile analysis was also used to assess feature dimensions across the films. Furthermore, the electronic properties of the niobium component were characterized by Kelvin Probe Microscopy, providing precise measurements of the work function and enabling comparison with established reference values for niobium.

2. Methodology

2.1. Deposition Techniques

Helicene films were prepared from solutions spin-coated onto Si/SiO_2 substrates. Rapid spinning produced uniform films, with solvent evaporation leaving a thin polymer layer Helicene thin films are typically prepared by spin-coating a solution onto Si/SiO_2 substrates. The process begins with the preparation of a helicene solution in an appropriate solvent, while the substrates are carefully cleaned to ensure optimal film adhesion and uniformity. A small amount of the solution is applied to the substrate, which is then rapidly spun at high speeds, causing the solution to spread evenly due to centrifugal force. As the substrate spins, the solvent evaporates, leaving behind a thin, uniform polymer layer. This method produces smooth films with controlled thickness, which can be further optimized by adjusting spin speed, solution concentration, or post-deposition treatments.

NbN films were deposited using pulsed laser deposition (PLD), a precise technique for growing nitride thin films. In this process, a dense NbN target was placed inside a high-vacuum chamber, while the Si/SiO_2 substrate heated to a controlled temperature to promote adhesion and crystallinity. A pulsed laser beam was focused onto the target surface with sufficient fluence to ablate material in the form of a plasma plume. This plume, composed of energetic Nb and N atoms, ions, and clusters, expanded rapidly toward the heated substrate, where the species condensed and nucleated to form a thin film layer.

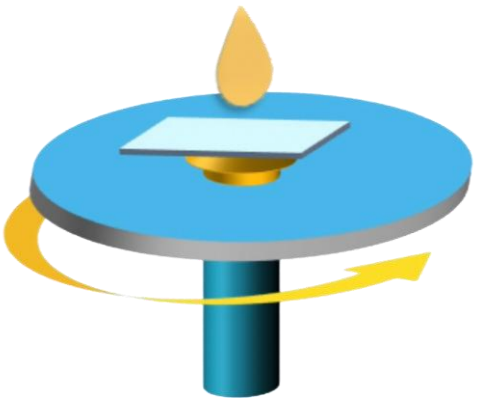


Figure 2: Spin Coating Process.

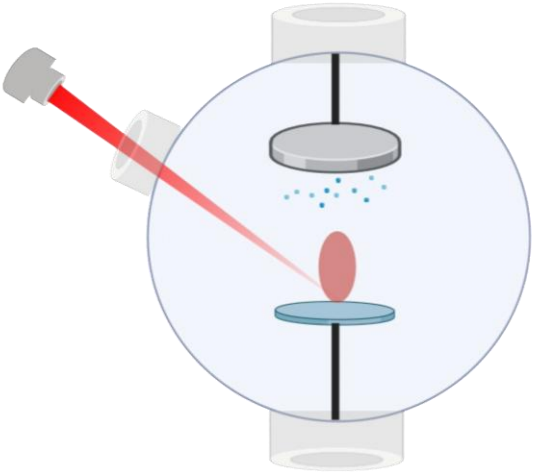


Figure 3:3 Pulsed Laser Deposition (PLD).

Two different film thicknesses were prepared, corresponding to equivalent concentrations of 20 and 35 mg/mL, to systematically study the effect of thickness on morphological and electronic properties.

To examine the impact of thermal processing on film structure and functionality, a subset of samples from each thickness group underwent post-deposition annealing. This process was designed to enhance molecular ordering and crystallinity. The study compared four sample types: annealed and non-annealed films for both concentrations.

2.2. Characterization Tools

Surface morphology characterization was performed using atomic force microscopy (AFM) in tapping mode, which provides high-resolution topographic imaging. Scans were performed at two different sizes: 20 µm X 20 µm, 5 µm X 5 µm. The AFM data were analyzed with standard flattening procedures applied to remove background tilt. Quantitative analysis included measurement of surface roughness parameters, and line profile analysis was employed to characterize feature dimensions and spatial distribution across the film surfaces.

Complementary to morphological analysis, the electronic properties of NbN component were characterized using a Kelvin Probe Microscopy to determine the work function by measuring the contact potential difference between a conductive tip and the sample surface. The variation in reported values may be attributed to differences in experimental conditions, such as ambient atmosphere, surface preparation, and measurement protocols. This technique provided precise measurements of the material's surface potential, allowing for direct comparison with reference values for NbN.

3. Results Discussion

3.1. AFM results

The surface morphology of the helicene thin films was investigated using AFM over a scan area of 5 µm × 5 µm. To further examine the topography, line scans were employed to trace the height profiles of the films. The RMS roughness of the film surfaces was calculated for all samples and was found to be strongly influenced by the annealing process.

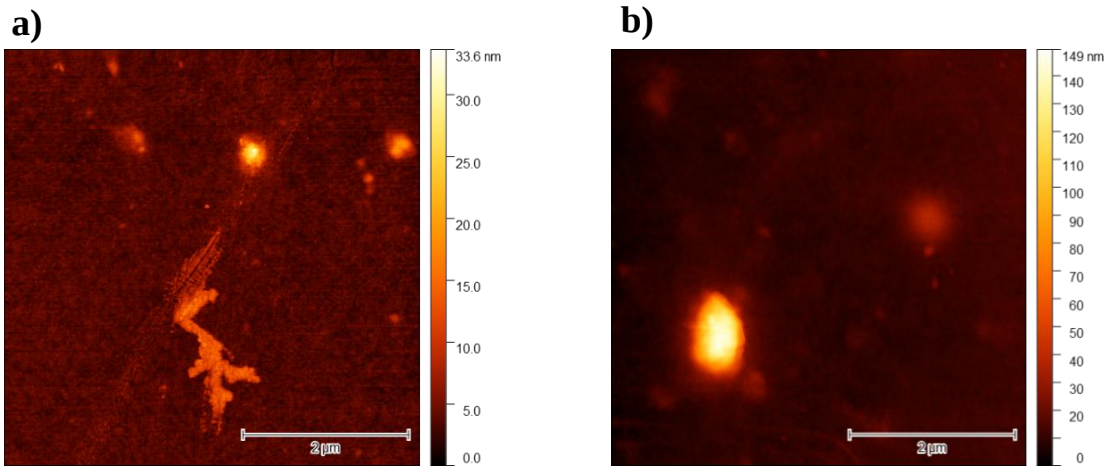


Figure 4: Non-annealed samples 5 µm × 5 µm AFM image at concentrations (a) 20 mg/mL (b) 35 mg/mL

Figure 4 (a) and (b) show the surface morphology of non-annealed films at concentrations of 20 mg/mL and 35 mg/mL, respectively. The AFM images of the non-annealed films show a relatively uniform and featureless surface, with only a slight increase in height observed at the 35 mg/mL concentration. This is further confirmed by the line scan profiles presented in Figure 5. The RMS roughness values were 0.571 nm (20 mg/mL) and 1.928 nm (35 mg/mL) at a scan size of 5 µm × 5 µm.

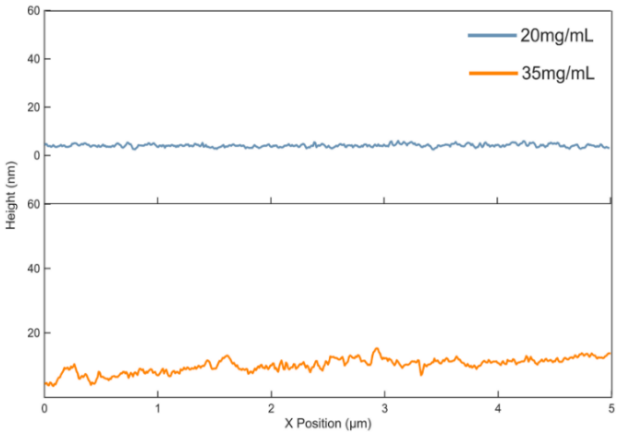


Figure 5: Line scans for non-annealed samples

In contrast, the AFM images for the annealed films in both concentrations are provided in Figure 6 (a) 20 mg/mL and (b) 35 mg/mL. Annealed samples exhibited more distinct peaks and troughs, with a notable increase in height observed at the 35 mg/mL concentration, as shown by the line scan in Figure 7.

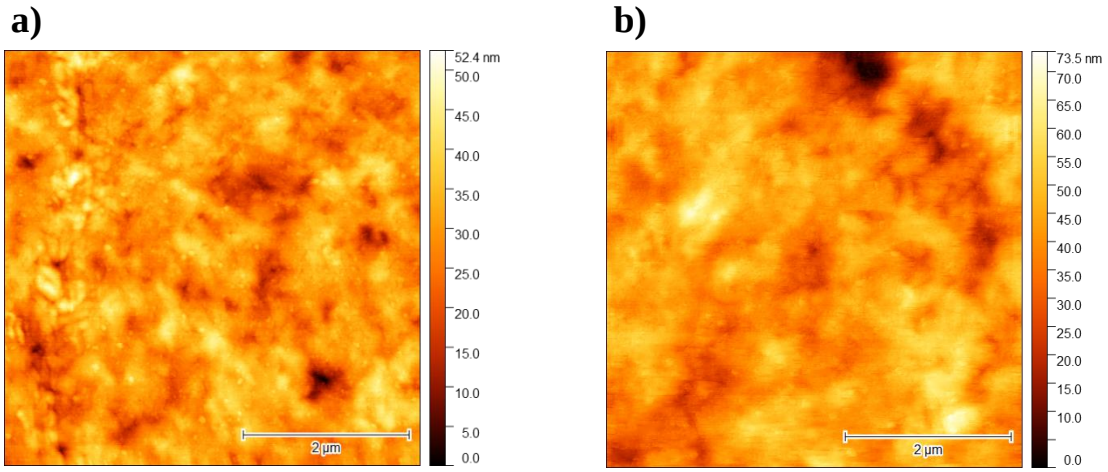


Figure 6: Annealed samples 5 µm × 5 µm AFM image at concentrations (a) 20 mg/mL (b) 35 mg/mL.

The annealed films exhibit a significant increase in roughness, with RMS values of 5.796 nm and 8.607 nm at sample concentration of 20 mg/mL and 35 mg/mL respectively. This suggests enhanced structural rearrangement and surface diffusion, leading to increased roughness and the formation of fibrillar features. These observations indicate that annealing plays a crucial role in modifying the surface morphology

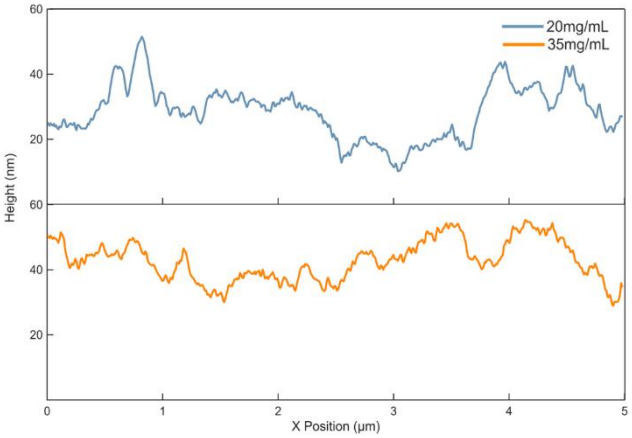


Figure 7: Line scans for annealed samples

A histogram of fibril size distribution plotted for each sample is illustrated in Figure 8. At 20 mg/mL concentration sample in Figure 8 (a), the dominant fibril sizes were 34 nm and 38 nm, whereas at 35 mg/mL concentration sample in Figure 8 (b), the fibril size distribution shifted to 25, 27, 30, and 37 nm.

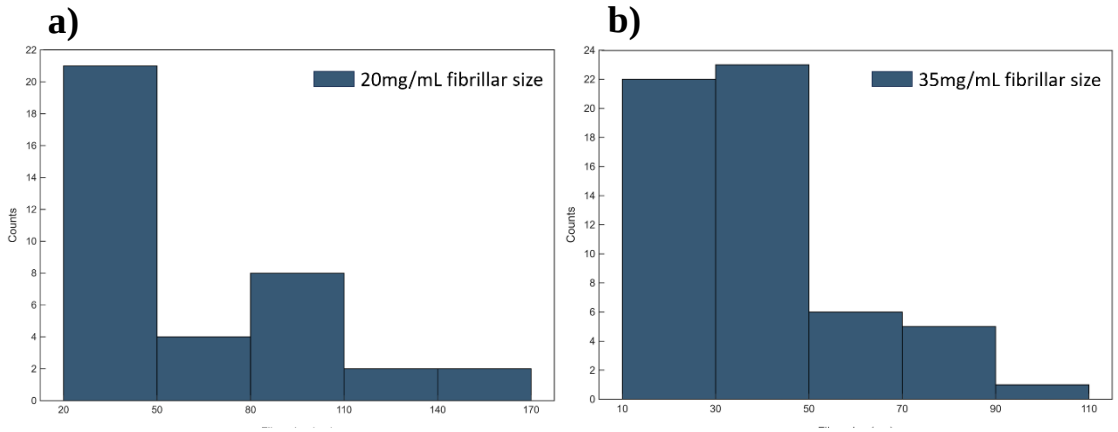


Figure 8: Histograms showing the distributions of fibril size for (a) 20 mg/mL, (b) 35 mg/mL annealed sample

3.2. Kelvin probe microscopy result

Figure 9 shows the Kelvin probe result for NbN, with a relative shift from -170 to -154 mV. Converting this shift with respect to the probe reference gives a work function of 4.612 eV, which falls within the reported range of 4.6–4.9 eV [5] [6]. The gradual upward trend indicates possible surface stabilization or oxidation. Precise work function measurement is essential for optimizing NbN thin films in electronic and device applications.

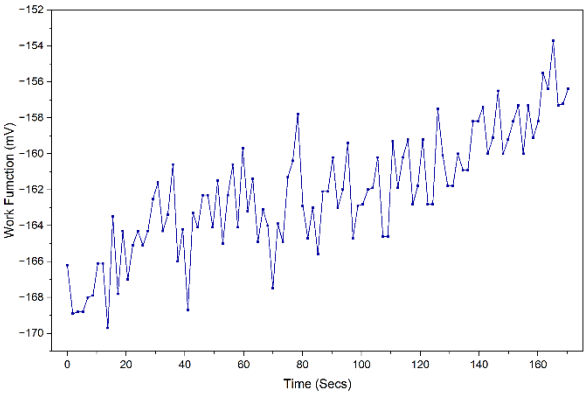


Figure 9: NbN work function variation with time

4. Challenges

Engineering of thin films to enhance PV devices represents a particularly difficult challenge: while in essence the devices are simple, characterization reveals the materials to be complex. It is understood that the device performance cannot wholly be described by taking the properties of the component materials in their bulk or simple forms and applying junction theory to them. Instead, either an empirical or a multidisciplinary approach is required. Given that increasing the efficiency of solar cells has been in demand, there is a strong case that work should continue in making links between the materials' properties (in thin-film form) and the properties of the devices made from them. This requires the cooperative effort of many techniques and of many laboratories.

5. Conclusion and Future Work

This study successfully demonstrated the surface characteristics of helicene thin films and confirmed that the work function of niobium nitride thin films falls within the expected theoretical range, indicating high-quality fabrication. We strongly recommend further characterization using advanced optical techniques such as photoluminescence and Electronic Circular Dichroism (ECD) to explore the chiral optical properties of helicene. Additionally, helicene shows promising potential as an organic material for application in OLED technologies.

6. References

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