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Effect of H_2/Ar Ratio on the Photoanodic Currents of Graphene/MoS_2 Films

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Abstract: Enhancing advanced solar energy storage in rechargeable batteries is one of the most critical challenges in clean energy technology aimed at reducing air pollution and dependence on fossil fuels. It has been demonstrated that dye-sensitized electrodes, silicon electrodes, and transition metal-based photoelectrodes can be applied in solar-charged rechargeable batteries to effectively capture visible light. However, potential pollution and cost issues limit their large-scale applications. This study aims to reduce the increased charging potential, caused by the high overvoltage due to the dissolution of compounds such as lithium peroxide and lithium carbonate, through photo-assisted charging. To achieve this goal, efficient graphene/MoS_2 composites are synthesized with chemical vapor deposition (CVD), and their photoelectrochemical properties are characterized to facilitate efficient photocharging. In this context, by positively altering the carrier gas ratio towards H_2 (from 30% to 60%), samples are synthesized at different H_2/Ar ratios to investigate the varying ratio's impact on photoanodic currents.

Keywords: Graphene, Transition metal dichalcogenides, Chemical vapor deposition

Introduction

The MoS_2 material intended to be produced on graphene using CVD is a single-layer transition metal dichalcogenide. It exhibits a range of novel physical properties, including a direct optical bandgap within the visible spectrum and a strong exciton binding energy (Eb), along with distinctive circular dichroism. These characteristics makes MoS2 an appealing semiconductor for use in electronic devices. What's even more fascinating is the recent increase in scientific interest in layer-by-layer stacking of single-layer MX_2 and graphene. This stacking approach has led to the discovery of various captivating physical properties such as superconductivity. Furthermore, it has paved the way for the development of new devices with exceptional performance, such as transistors and light-emitting diodes (Shi et al., 2015).

Chemical vapor deposition (CVD) offers promising opportunities for the synthesis of high-quality graphene films as well as single-layer MoS2 on various substrates, ranging from insulators to metal foils (Shi et al., 2012). In a MoS2/graphene structure with all components produced through the CVD method, graphene offers advantages such as high transparency, high conductivity, and an adjustable work function, while MoS2 provides an advantage with its bandgap (Cai et al., 2018).

The optical absorption of 2D transition metal dichalcogenides is greater than $10^7 m^{-1}$ in the visible range, which means that a 300 nm film will absorb 95% of visible light. However, their conductivity is low, limiting their use in photovoltaic (PV) solar cells. On the other hand, graphene exhibits excellent electrical transport behavior, good transparency, and high carrier mobility, making it a potential candidate for PV solar cells. However, the lack of a bandgap in graphene limits its applicability in PV solar cells. Heterostructures of graphene and 2D

transition metal dichalcogenides can effectively be used in photovoltaics, with graphene serving as a good transparent electrode and transition metal dichalcogenides acting as the photoactive component (Azadmanjiri et al., 2020).

In this study, Ar and H_2 gases were used as carrier gases during CVD synthesis. During the nucleation stage, the density of MoS_2 areas on graphene shows a positive correlation with the Ar flow rate, while extending the growth time can increase the average size of MoS_2 areas. Hydrogen, on the other hand, ensures the survival of graphene at the high temperatures required for MoS_2 crystallization. In this context, the effect of carrier gases on photoanodic currents was investigated by using different H_2/Ar ratios.

Method

Methane was used as the carbon source in graphene production. Graphene is produced on copper substrates and transferred onto Si/SiO_2 wafer. The flowchart for CVD graphene production is provided in Figure 1.

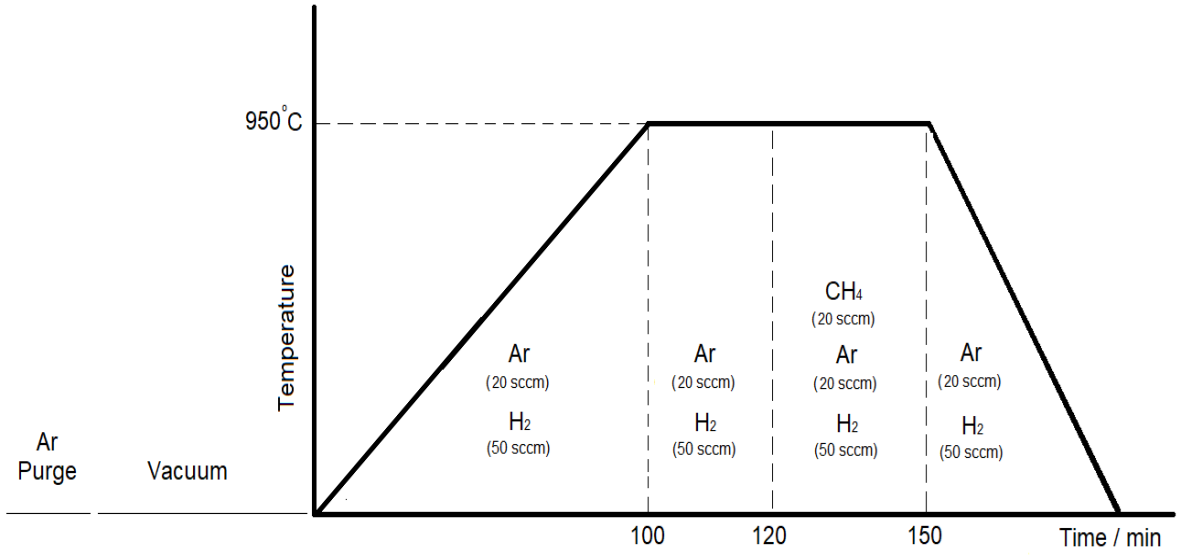

Figure 1. Production flow chart of graphene

Following synthesis of graphene, MoS_2 was performed on a Graphene/Si substrate located inside CVD furnace at 770°C, with various flow rates and the delivery of H_2 (30-40-50-60%), Ar (70-60-50-40%) as carrier gases. The quantities of the solid precursors MoO_3 and S used were 2 mg and 150 mg, respectively. Figure 2 schematically illustrates the positions of the precursors and the substrate inside the CVD furnace.

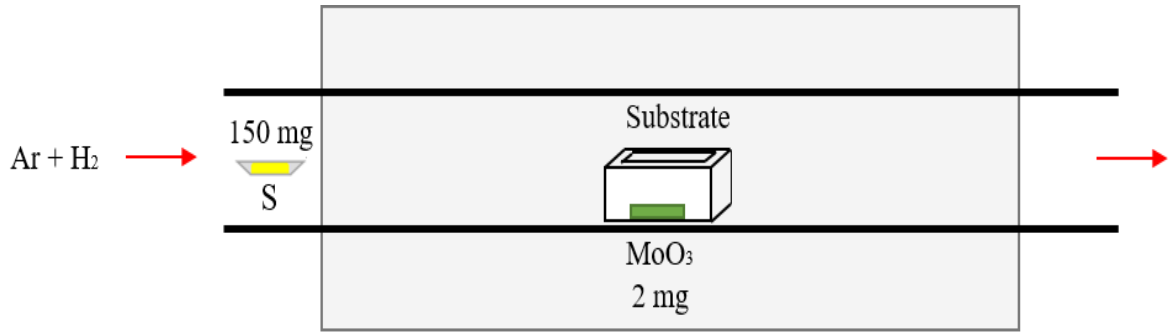

Figure 2. Schematic illustration of the CVD furnace setup for MoS_2 synthesis.

The samples prepared for photo-current experiments were coated on indium tin oxide (ITO) glass and dried in a vacuum-controlled atmosphere at 100°C for 12 hours. Linear Sweep Voltammetry experiments conducted with a GAMRY Reference 3000 potentiostat in a 0.1 M KCl / 0.1 M H2PO4 solution (pH 7), light from a solar simulator (Type A 150 W, 1-3 SUN, Xenon lamp, 1.5 AM Filter) was directed onto the ITO surface (wavelength range of 400 nm - 700 nm). Raman spectroscopy was performed using a RENISHAW inVia Microscope Raman Spectroscopy system, and measurements were carried out at a wavelength of 532 nm.

Results and Discussion

In the Raman spectrum of graphene, you can observe two distinct Raman features known as the G and 2D bands, which are typical characteristics in almost all sp2 materials. The G band, situated at 1583 cm^{-1}, is a first-order scattering phenomenon resulting from the stretching of bonds between all sp2 atom pairs. In contrast, the 2D band, located at 2670 cm^{-1}, is a second-order scattering effect, and the D band is a specific peak at 1350cm^{-1}. Regarding the 2D mode, it connects two zone-boundary phonons, while the D mode links a single phonon and a defect. Consequently, in high-quality, pristine graphene, D band is absent (Childres et al., 2013). In the Raman spectrum of MoS_2, you can observe two characteristic Raman peaks, one at about 405.7 cm^{-1} (A_{1g}) corresponding to the out-of-plane vibration of sulfur atoms and another at around 385.5 cm^{-1} (E^1_{2g}) corresponding to the in-plane vibration of both molybdenum and sulfur atoms (Shi et al., 2015).

The frequency gap (Dk) between the E^1_{2g} and A_{1g} modes in MoS_2 is related to the number of layers. As the thickness of MoS_2 decreases, the difference between the E^1_{2g} and A_{1g} modes also decreases. It was noted that for a single layer MoS_2, the Dk for E^1_{2g} and A_{1g} modes is less than 21 cm^{-1}, around 21-22 cm^{-1} for a double layer, and greater than 25 cm^{-1} for bulk MoS_2. The intensity ratios for E^1_{2g} and A_{1g} are roughly 0.31 for a single-layer MoS_2 and about 0.45 for bulk MoS_2 (Shi et al., 2012).

The Raman spectrum in Figure 3 corresponds to the sample labeled as 30-70, which contains the highest Ar content at 70%. The peaks at 520 and 964 cm-1 are attributed to the Si substrate. The intensity ratio for the E^1_{2g} and A_{1g} modes is 0.45, and the frequency difference (Δk) between these modes is 25 cm^{-1}. These features indicate that the sample exhibits bulk characteristics.

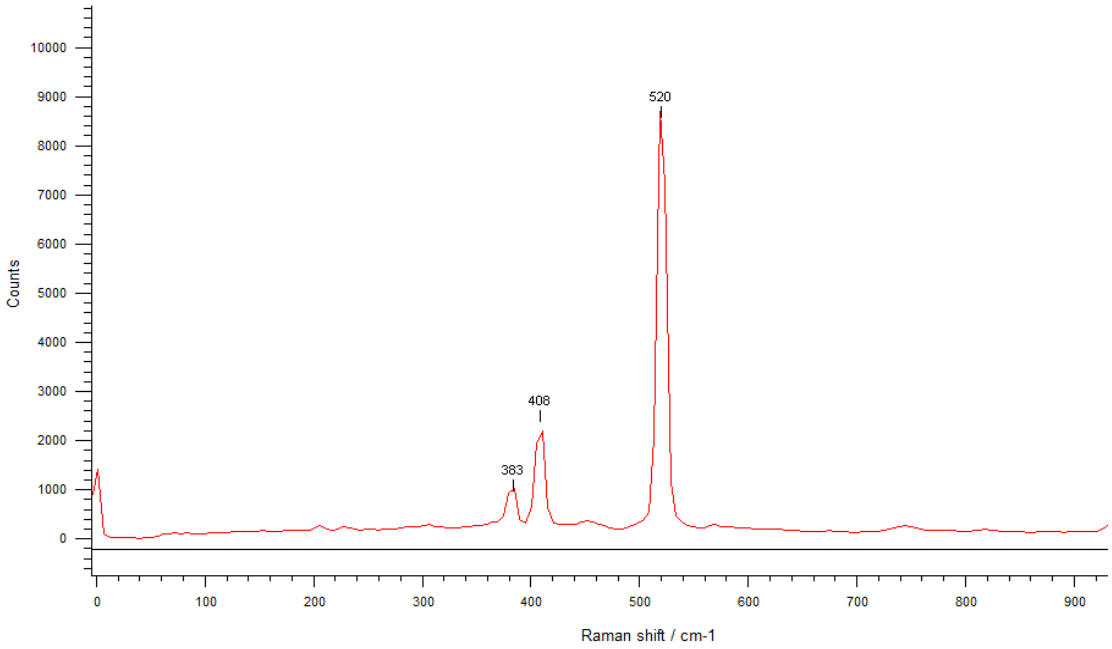

Figure 3. Raman spectrum of %30 H_2 – %70 Ar (30-70) sample

With the increasing H_2 density (60%), the frequency difference between the Raman modes has decreased. In the 60-40 sample, the frequency difference has reached the empirically defined limit of 21 for a single-layer structure. The Raman spectrum for this sample is presented in Figure 4.

The photoanodic currents of the samples were measured using the linear sweep voltammetry method, and the results of these experiments are presented in Figure 5. As can be seen from the figure, in experiments conducted with intermittent potential changes (20 seconds of polarization under light followed by 20 seconds of polarization in dark). The photoanodic currents generated by the samples were clearly detectable. It was observed that the current values of the samples increased as the hydrogen ratios were raised, and it was determined that the samples with the highest hydrogen content (50-50 and 60-40) were capable of producing significantly higher photoanodic currents compared to the other two samples.

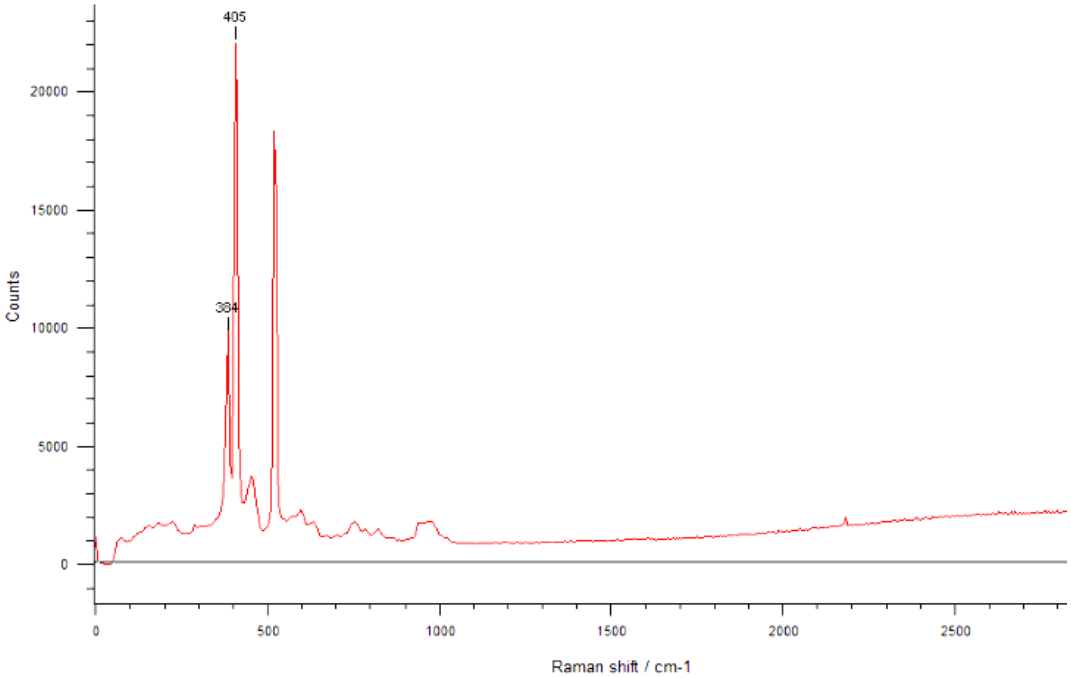

Figure 4. Raman spectrum of %60 H_2 – %40 Ar (60-40) sample

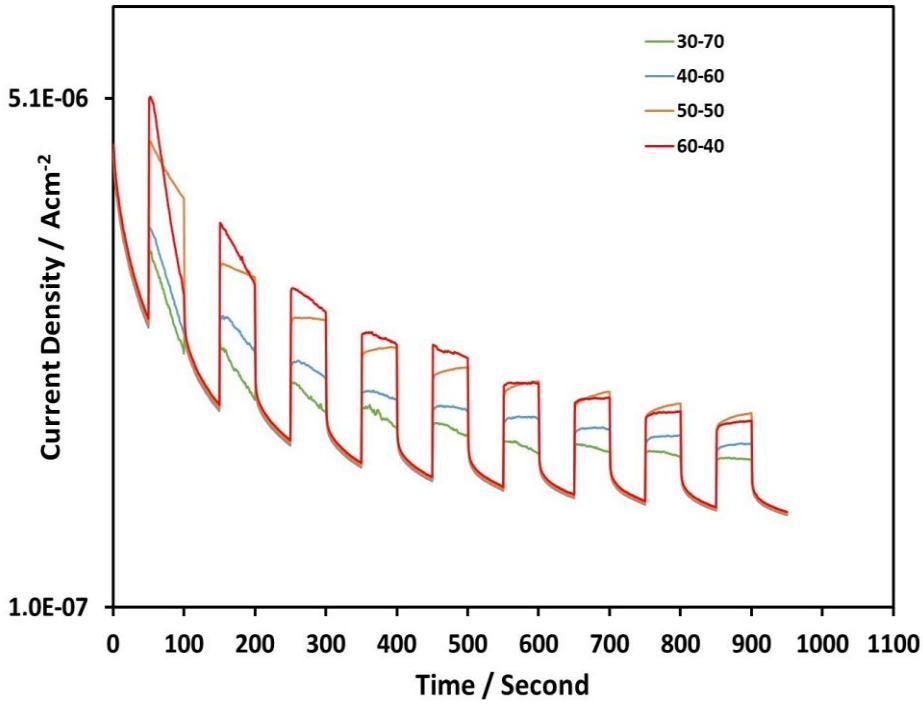

Figure 5. The photoanodic currents of the samples

Conclusion

In this study, graphene/MoS_2 films were produced using the CVD method, and the photoanodic characteristics of the films produced with varying H_2/Ar ratios were determined. According to the results:

1) When the hydrogen content fell below a certain level (50%), the structure was found to be multilayered.

2) Significantly higher photoanodic currents were observed in single-layer or bi-layer coatings. This indicates that single-layer structures offer a distinct advantage in terms of photoanodic performance.

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Acknowledgments or Notes

* This article was presented as an oral presentation at the International Conference on Technology, Engineering and Science (www.icontes.net) held in Antalya/Turkey on November 16-19, 2023.

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