Molybdenum disulphide – Gallium arsenide Heterostructure for Photovoltaic Applications

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Textured MoS_2 films on GaAs have been produced using radio frequency (RF) sputtering and pulsed laser deposition (PLD). The sputtered films showed improved basal plane texture at higher temperatures and relatively low power. The PLD film showed significantly better texture, at the same temperature, and therefore offers the possibility of a low temperature route to textured film growth.

1. **Introduction**

Heterostructures allow for increased absorption of the broad solar spectrum in photovoltaic cells due to the existence of two band gaps. Large lattice mismatch however leads to generation of dislocations at the interface. These dislocations act as minority carrier recombination centres detrimental to cell efficiency. Certain layered transition metal dichalcogenides such as molybdenum disulphide are potential thin film solar cell candidate materials [1]. The layered structure enables a weak Van der Waals interaction at the interface substantially relieving the lattice mismatch problem.

Crystallographic texture with the basal planes parallel to the substrate is essential for high cell performance. Previous investigations have not satisfactorily achieved the required texture [2-4]. Thin metal layers [5] or sodium induced precursor phases [6] have been used, but these impair solar cell efficiency.

In this study, we deposit thin films of MoS_2 on GaAs and Si substrates by RF magnetron sputtering and pulsed laser deposition using a KrF excimer laser. By probing experimentally accessible parameters, we aim to grow the desired texture with large grains and minimal defects.

2. **Experimental**

The undoped GaAs wafers have (111) orientation (± 0.3°) and were Ga terminated on the polished, epi ready face. Ammonium sulphide solution with 8% excess sulphur was spread over the wafer surface for passivation treatment. The wafer was allowed to dry, then placed under vacuum (< 10^{-3} Pa) to remove excess amorphous sulphur by sublimation. Si(111) substrates were sonically cleaned with acetone and ethanol.

Thin films were sputtered on substrates using a 51 mm (2 inch) RF magnetron. The target was 99% purity MoS_2 commercial powder with 2% carbon binder cold pressed at 6000 kg cm^{-2} into a circular geometry. Substrates at a distance of 8 cm were placed on a grounded alloy heater block where substrate temperatures can be varied from ambient (~ 70 °) to a maximum of ~900 °C. The argon working gas pressure was 13.3 Pa (100 milli-torr) and the power applied to the 51 mm target was 40 W.

Pulsed laser deposition was accomplished with a KrF excimer laser at 248 nm UV wavelength with a repetition rate of 10 Hz and fluence 2 Jcm^{-2}. The chamber was evacuated to 1.1 x 10^{-3} Pa (8.3 x 10^{-6} torr) before deposition, and the 25 mm (1 inch) circular target of the same commercial powder and binder was rotated at 5 rev s^{-1} and rastered at 4 scans min^{-1} during operation. The substrate temperature and target-substrate distance were 646 °C and 4.5 cm respectively.

3. **Results**

The usual growth orientation in many previous studies [1-4] has shown that the basal plane orientation is confined to a thin interfacial layer (a few to tens of nm). The x-ray diffraction (XRD) patterns of Fig. 1 show an evolution in bulk texturing with increasing substrate temperature. The relative integrated intensities of the indexed film peaks give a measure of the extent of parallel or perpendicular orientation.

Basal plane orientation (parallel to the substrate) is indicated by a relatively strong (002) peak. Perpendicular orientation of the basal planes is shown as strong (101) and (110) peaks. Fig. 1 clearly shows that the fraction of parallel basal plane orientation in the film increases markedly with increasing substrate temperature on a GaAs substrate. The very low intensity peaks at ambient temperature (~ 70 °C) suggests a low degree of crystallinity at low substrate temperatures consistent with previous workers [1-3].

The XRD curves in Fig. 2 for the films on silicon substrates show a significantly greater change in preferred orientation compared to the results on GaAs. Deposition by PLD in Fig. 3 shows a greater fraction of planar orientation than with sputtering depositions at comparable substrate temperature. Thus PLD may present a low temperature route to the fabrication of basal plane oriented growth of MoS_2, due to the quiescent time between pulses which allow for lattice ordering.

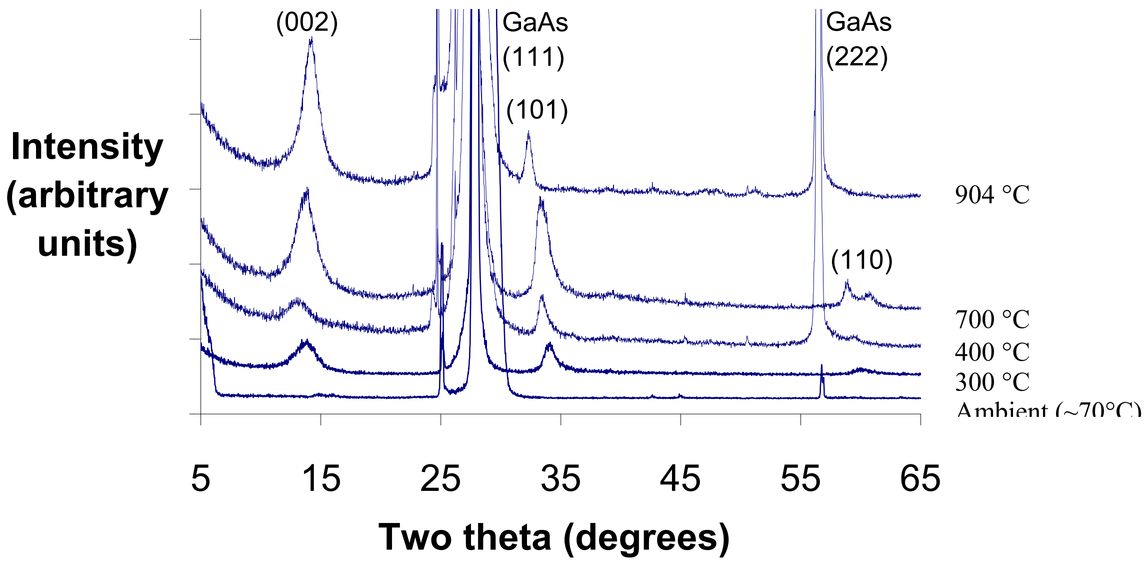

Fig. 1. XRD of sputtered MoS_2 films on GaAs substrates at various substrate temperatures. Other parameters are 40 W power and argon pressure 100 milli-torr.

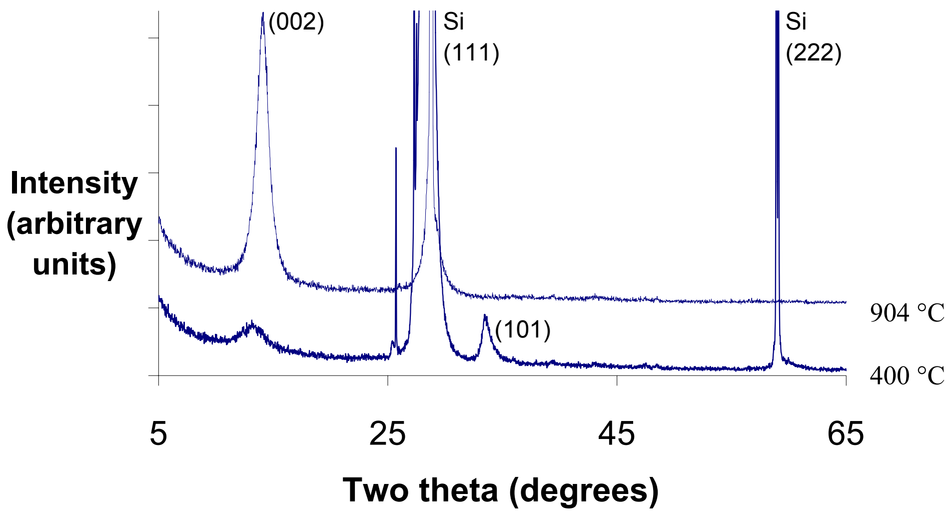

Fig. 2. XRD of sputtered MoS_2 films on Si substrates at two substrate temperatures. Other parameters are 40 W power and argon pressure 100 milli-torr.

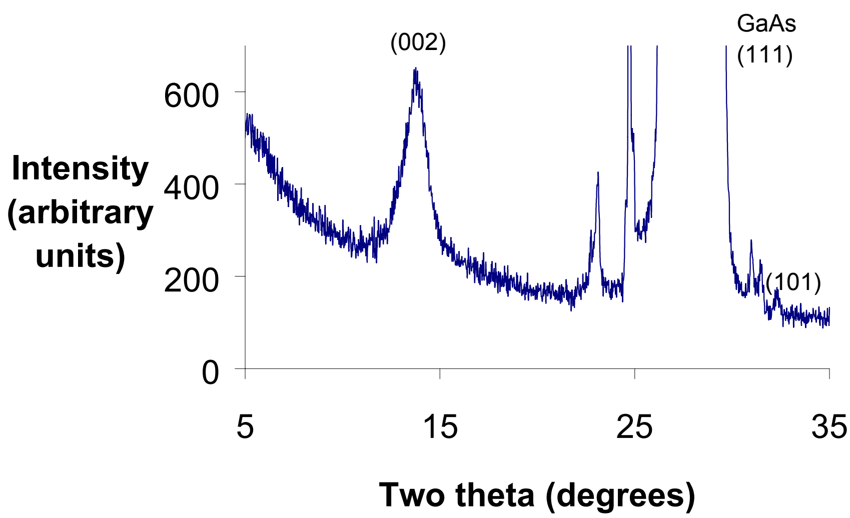

Fig. 3. XRD of PLD MoS_2 film on GaAs substrate with fluence 2 Jcm^{-2} and substrate temperature 646 °C.

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