2D LAYERS OF MOS₂ GROWN BY THE METHOD OF PULSED LASER DEPOSITION ON GLASS AND POLYIMIDE SUBSTRATES

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Abstract. We presents the results of the synthesis and studies of the properties of MoS_2 monolayer and multilayer films deposited by pulsed laser deposition on glass and flexible polyimide substrates. Atomic force microscopy (AFM), X-ray diffractometry, Raman scattering spectroscopy, optical absorption, photoluminescence and Hall measurements used to characterize the structural, morphological, optical and electrical properties of the films confirm the correlation between the strain effects and properties of the films appearing due to the large mismatch between thermal expansion coefficients (TEC) of the substrate and ultrathin MoS_2 layers.

1. Introduction

Currently, two-dimensional (2D) materials are attracting great interest for applications in post-silicon electron devices, particularly in next-generation flexible electron devices [1]. The physical properties of MoS_2 can be significantly affected by its interaction with substrate [2]. One of the prominent substrate effects is the strain created in the MoS_2 layer due to the large lattice mismatch between the TEC of the substrate and MoS_2 [3]. A large TEC mismatch between the substrate and MoS_2 will introduce internal biaxial tensile or compressive strain to the MoS_2 layer and therefore TEC mismatch may become a prominent temperature factor that modulates all the films properties. In this study large-area MoS_2 films of a few atomic layer thicknesses were successfully prepared by the pulsed laser deposition (PLD) technique on a polyimide and glass substrates under the same deposition conditions. The observed experimental features indicate the evolution of all properties of such a two-dimensional material with an increase in the number of atomic layers and the role of strain effects due to a large mismatch between the substrate and MoS_2 .

2. Experimental procedure and sample preparation

To deposit thin films up to seven of atomic mono-layers, a Q-switched neodymium laser with the following parameters was used: wavelength 1.064 µm, pulse duration 30 nsec, pulse energy 0.35J, pulse repetition rate 0.1 Hz, beam diameter 20 mm. Polyimide film of 40 µm thickness were chosen as a flexible substrate on the bases of its ability to maintain excellent physical, electrical and mechanical properties over a wide temperature range (up to 400° C). Polyimide films and glass substrates are characterized by TEC about $20 \cdot 10^{-6} K^{-1}$ and $9.10^{-6} K^{-1}$, correspondingly, which are much larger than nor few-layer thick ($0.5 \cdot 10^{-6} I/C$) MoS_2 [4]. The substrate was heated up to 350° C.



Fig.1 XRD pattern of 2L MoS₂ films of thickness 4.7 nm (7L) grown on polyimide (a) and glass (b) substrates

The results of measurements of the X-ray diffraction spectra of the films deposited on polyimide and glass substrates are illustrated in Fig. 1 (a) and (b), respectively. The film thickness in both cases was 4.7 nm (i.e. about 7 atomic layers). A clearly pronounced diffraction peaks are seen at $2\vartheta = 14,2^{0}$, which is characteristic of the crystallographic plane (002) of both a bulk MoS_2 material and thin films consisting of several of its atomic layers.

Raman spectroscopy was used in order to define the number of layers and strain effects in the film. We found the thickness dependent Raman spectra for MoS_2 films deposited on both glass and polyimide substrates.

It is seen from Fig.2 (a) that there are small shifts in the peak position among samples, deposited on glass and polyimide substrates due to different residual strain arising from different TEC mismatch. As it is expected the frequency of in-plane E_{2g}^1 Raman mode is less sensitive to strain, which red-shifts with respect to the bulk sample by 1-1.5cm⁻¹ as the strain increases in the films grown on glass and polyimide. Meantime the frequency of out-of-plane A_{1g} Raman mode is changed more significantly (about 2.4 cm⁻¹) under strains introduced by polyimide substrate [5,6].



Fig. 2 Raman scattering (a) and photoluminescence spectra of 2L *MoS*₂ films deposited on glass and polyimide substrates

The strain-caused band-gap shift was validated in PL spectra as it is shown in Fig.2 (b), where PL spectra are plotted for $2LMoS_2$, deposited on glass and polyimide substrates under the same technological conditions. From the PL spectra two peaks at 659 nm (1.887eV) and 616 nm (2.013eV) were clearly observed, corresponding to a direct transition between the top valence band K point and the bottom conduction K points in the Brillouin zone [4]. In comparison with the MoS_2 films grown on polyimide, a blue shift (about 12 meV) of the direct band transition was observed in MoS2 films grown on glass. Also the PL intensity sharply increases with decreasing film thickness and the transition to a direct-gap semiconductor in the limit of a monolayer film. The PL intensity of the films grown on polyimide is substantially larger than that of deposited on glass, probably due to better crystalline quality of the film.

We have measured also the optical absorbance of the MoS_2 films deposited on polyimide and glass substrates. These absorbance spectra also show the formation of excitons of types A and B [4]. The difference between the exciton binding energies for the samples of MOS2 grown on different substrates can be caused by strain shift of the band gap, arising due to TEC mismatch between the film and substrate.

Conclusions:

In conclusion, we demonstrated the possibility of growing by PLD technique high quality few-layer MoS_2 on glass and flexible polyimide substrates. The studies of XRD, Raman scattering, PL and optical absorption spectra revel the correlation between the strain effects and properties of the films.

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