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Investigation of Mos_2 Thin Films Deposited By Dip Coating on Multi Crystalline Silicon Plates Grown by Capillary Action Shaping Technique

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Abstract

Thin multi-crystalline Silicon sheets grown by capillary action shaping technique were cut into wafers measuring 1 cm x 1 cm x 0.5 mm, cleaned, etched and passivated before depositing MoS_2 films by vacuum thermal evaporation and dip coating. The wafers were characterized before and after deposition of the films by optical microscopy, x-ray diffraction (XRD) and scanning electron microscopy (SEM) couples with energy dispersive spectroscopy (EDS) which confirm the quality films. Linear resistivity behavior was observed in case of the vacuum thermal deposited films. A nonlinear increase of current indicating the formation of a rectifying heterojunction was seen in the I-V curves of the dip coated sample.The results are discussed.

Key words: Multi-crystalline Silicon wafers, MoS_2 films, dip coating, heterojunction

1. INTRODUCTION

In recent times multi-crystalline Silicon (mc-Si) wafers are replacing Single crystal (c-Si) wafers in solar cell applications [1,2] for cost considerations even though the efficiency is lesser than the c-Si wafers. Several efforts are underway to enhance the efficiency of these mc-Si solar cells [3-6] where it has been reported that mc-Si wafers with uniformly small grains produce effective lifetime of 400 µs [5] and proper doping would enhance the efficiency of 19.5% [6].

Another approach proposed to increase the efficiency of Si based solar cells has been the coating of thin layers of other semiconducting materials [7]. With some of these advances it may be possible that solar electric conversion efficiency of multilayer solar cells is expected to pass 40% but at high cost. Recent reports of exceptionally good semiconducting properties of monolayer MoS_2 films prepared by liquid exfoliation and physical separation techniques [8,9] led to efforts in using $MoS_2$and WS_2 films coated on Si as absorber layer for energy harvesting purpose [10]. More recently highly efficient MoS_2/p-Si heterojunctions have been reported that could be used in several optoelectronic applications [11-16]. In the present work MoS_2 films have been deposited by vacuum deposition and dip coating techniques onthin mc-Si sheets grown in the laboratory by capillary action shaping technique (CAST) [17-19]. The resulting films have been investigated for their structure and electrical properties to find a low cost method for their use in solar cell and other optoelectronic applications. Commercial Si (111) wafers were coated simultaneously with the MoS_2 films for comparison and the results are presented here.

2. EXPERIMENTAL

Si sheets grown in the laboratory [17] and commercial single crystalline Si (111) wafers have been cut into smaller samples measuring 10 mm x. 10 mm x 0.5 mm. They were lapped, polished, etchedand passivated as described by Atluri *et al* [20] before coating with the films and making the measurements.

MoS_2 coating by vacuum thermal evaporation on silicon was performed using Balzer (BAK-600) vacuum coating system [18] at 1200ºC under a vacuum of 10^{-5}mbar to deposit films of 30 nm and 60 nm thickness [17].Excess Sulphur was used to compensating for loss during evaporation.

The dip coating technique as described by Liu *et al* [21] was used to deposit MoS_2 filmsin a homemade apparatus using Ammonium Molybedate $(NH_4)_6MO_7O_{24}4H_2O)$ and Ammonium thiocyanate ($2NH_4SCN$).The coated wafers were dried at 80°C and then annealed at different temperatures in the range 400°C to 450°C in an argon atmosphere for 30 minutes in a tubular furnace.

Optical microscopy, x-ray diffraction (XRD) and scanning electron microscopy (SEM), Raman Spectroscopy and photoluminescence spectroscopy were used to assess the structure and chemical purity of these films, Four probe resistivity measurement were carried out using a Keithley 2450 Source meter with gold plated pressure pads for the contacts in place of the pointed contacts to ensure that the films are not damaged. Films coated on commercial Si (111) oriented wafers have also been studied for comparison.

3. RESULTS AND DISCUSSION

3.1 X-ray diffraction study

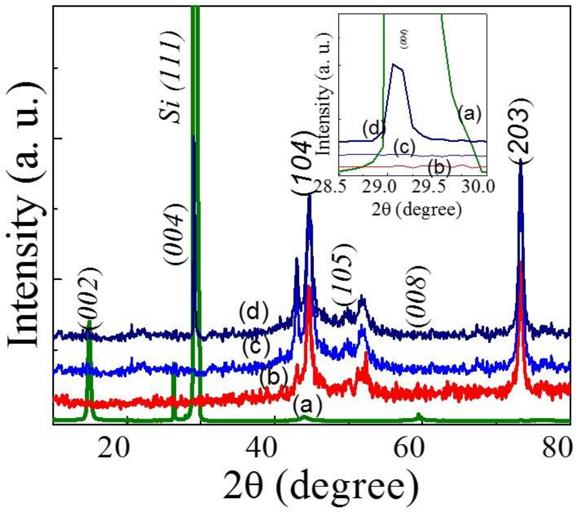

Fig.1 Shows the XRD patterns recorded on the MoS_2 coated Si wafers: (a) Si (111) wafer coated by thermal evaporation (60 nm layer) (b) CAST wafer deposited by thermal deposition (60 nm), (c) CAST wafer coated by dip coating and (d) Si (111) wafer coated by dip coating. The inset shows the expanded view of the intense diffraction peak at 29.03^{o} (corresponding to MoS_2 (004 reflection) which lies close to the Si (111) reflection. The reflections are indexed and fitted with the JCPD standard (77-1716).

The XRD patterns obtained on commercial Si(111) and CAST wafers coated by MoS_2 using different methods described above are given in Fig. 1. It is seen that a strong (002) andmore intense (004) reflections corresponding to $MoS_2$are observed in the case of the Si (111) wafer deposited with a 60 nm layer of MoS_2 indicating single crystalline nature of the films. The thickness of the film could be measured in this case and not in other methods. The CAST wafer deposited along with the Si (111) wafer shows a powder like pattern. All the reflections are indexed to the JCPD standard (77-1716). Intense (004) reflection is observed in thedip coated Si (111) sample(Fig. 1(d)) in addition to a powder pattern. It is likely that this corresponds to the Si (111) reflection. But it was shown that the intense peak at 29.03^{o}does not belong to the Si (111) reflection in case of the commercial wafer [18]. The CAST wafer surface is not uniformly flat (even though oriented in either (111) or (220) directions [18]) and the deposited films give the appearance of a powder like pattern in both cases due to random deposition.Theabove results indicate that the films deposited on all the wafers by different methods represent MoS_2.

3.2 Scanning electron Microscopy and Energy Dispersive x-ray Spectroscopy.

In order to assess the quality of the films SEM in conjunction with EDX was used.

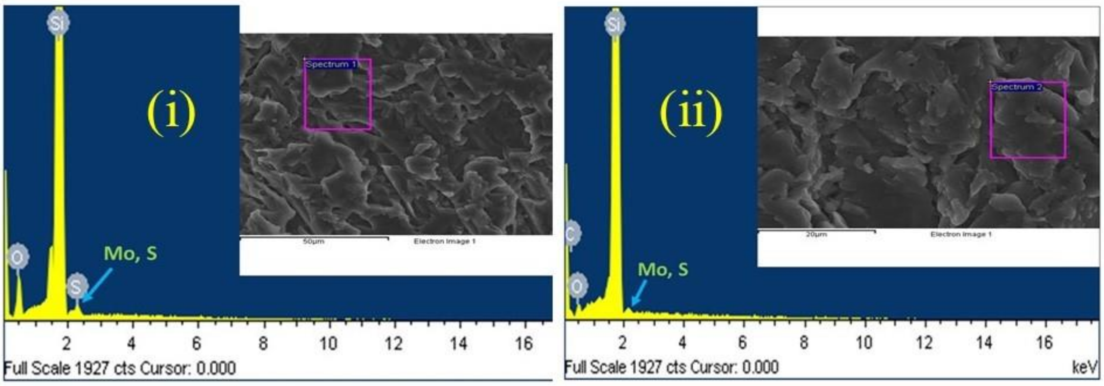

Fig. 2 shows the SEM micrographs of (a) Si (111) wafer and (b) CAST mc-Si wafer.

Fig. 2 SEM micrographs of MoS_2 coated Si(111) wafer (i) and Si (CAST) wafer (ii). The EDX spectra indicate the presence of MoS_2 next to a strong Si peak indicated by arrow. While large ordered features are observed in the Si (111) wafer randomly deposited film is seen on the dip coated wafer.

EDX and SEM images of MoS_2 coated Si (111) wafer (i) and Si (CAST) wafer (ii) are given in Fig. 2 SEM micrographs. The EDX spectra indicate the presence of MoS_2 next to a strong Si peak. While large ordered triangular growth features are observed (indicating an epitaxial growth) in the Si (111) wafer randomly deposited film is seen on the dip coated wafer. This is in conformity with the XRD results of Fig. 1.

The SEM micrographs of Fig. 2 show thatin case of the Si (111) single crystal wafer, the surface features are oriented in the same direction indicting a single crystalline epitaxial film. These ordered figures are not seen in case of the multi-crystalline CAST wafers meaning the polycrystalline nature of these films. The XRD patterns above confirm this observation. The influence of Si is seen in both cases.

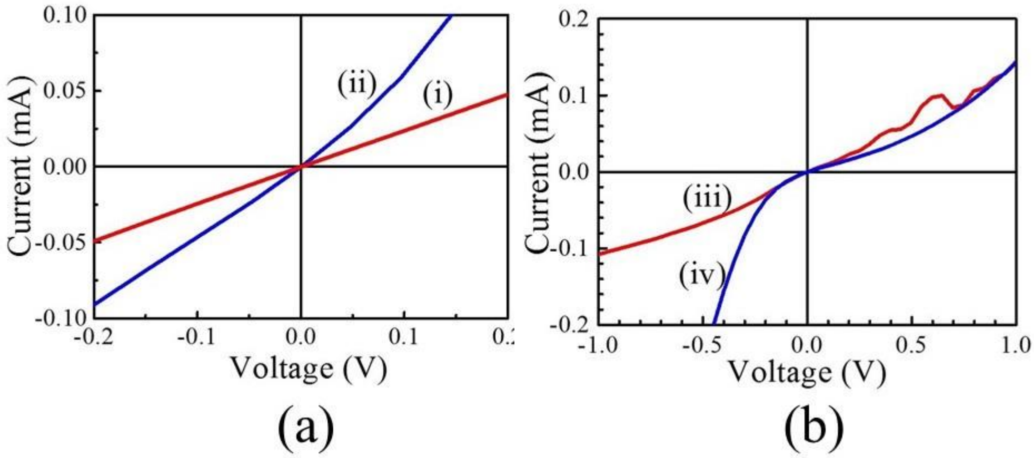

Fig. 3 The I-V plots recorded on (a) vacuum thermal deposition of MoS_2 on Si (111) wafer (i) and CAST wafer (ii); (b) dip coated MoS_2 on Si (111) wafer (iii) and CAST wafer (iv).

The influence of the MoS_2surface coating by thermal vapor deposition on the I-V characteristics are shown in Fig. 3(a). While linear variation is seen in the case of the Si (111) wafer a nonlinear variation is seen in the CAST wafer. Nonlinearity is attributed to the multi-crystalline nature of the films which was found to increase with increasing dislocation density in case of the CAST wafers [19]. Since the measurements were made on the MoS_2 films, the curves reflect the property of this film as influenced by the substrate.

After dip coating samples were subjected to the thermal annealing at 400 ^oC (as mentioned above) which might result in a shallow diffusion of MoS_2 in the Si wafers. Fig. 3(b) gives the I-V characteristics of the dip coated MoS_2 films deposited on (iii) p-Si (111) and (iv) CAST n-Si wafers. I-V characteristics exhibit pseudo rectifying behavior in case of the CAST n-Si wafer and nonlinearity in case of the p-Si (111) wafer. This may be attributed to the annealing of MoS_2 coated n-type CAST Si wafers which leads to the formation of a heterojunction with a small Schottky barrier height ~ 0.05 eV determined from the difference between electron affinity χ of n type CAST Si and MoS_2 layer 4.05 eV and 4.0 eV, respectively [22]. This marginal difference in electron affinities is probably responsible for the pseudo nature of rectification at the interface of CAST n-Si and MoS_2. For p-Si (111), the difference in electron affinities 0.05 eV produces a small band bending which may not be effective for carrier transportation across the interface to make ohmic contact. This resulted in non- linear I-V characteristics. The major difference in I-V characteristics for dip coated-Si (111) and n-Si CAST was observed under reverse bias condition. This could be due to relatively low fermi level difference for p-Si (100)/MoS_2 that resulted in the weak electric field generation at interface in comparison to n-Si (CAST)/MoS_2 [22,23]. It is interesting to see that rectification behavior is observed in the present work without the use of a graphene layer as reported by Tsuboi et al. [22]. Both the procedure of deposition of the films as well as the I-V characteristics were reproducible. Thus this method may offer a low cost alternative for making sensitive photodetectors. More work on the preparation procedure, measuring properties of the films and methods of charge collection are in progress and will be reported separately.

4. CONCLUSIONS

MoS_2 films deposited on well characterized Si wafers have been investigated and found to take the structure of the depositing Si surface namely epitaxial in the case of a single crystal and powder like on a multi-crystalline surface. The resistivity of the MoS_2 films deposited by vacuum thermal evaporation shows a linear variation where as a heterojunction like behavior is seen in the n-type dip coated samples. This is attributed to the formation of a pseudo rectifying junction due to the annealing of the dip coated sample at 400^{o}C.

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