ABSTRACT

Transition metal chalcogenides have attracted a lot of attention due to their potential application in the semiconductor industry. Crystalline pristine molybdenum disulphide (MoS_2), is also the basis of this study. The influence of defects in MoS_2 due to ion implantation on the material's electrical and optical properties are reported, the main aim being to enhance the capacity of electrode materials for use in energy storage devices; such as supercapacitors or supercapacitor batteries.

Both simulations and experimental studies were done. Simulations were formed using the Stopping and Range of Ions in Matter (SRIM) software, which was used to predict the depth of penetration of ions in the material. Density Functional Theory (DFT) and Boltzmann transport properties (BoltzTraP) codes were employed to study effects of defects on properties, including: electrical conductivity; thermal conductivity; magnetic susceptibility and band gaps.

Optical characterisation was done using Raman spectroscopy and photoluminescence spectroscopy (PL), using a green laser wavelength of 514.2 nm. Reported here are the Raman peaks shifts, due to damaged MoS_2 surfaces and PL showing quenching of photoluminescence peaks after ion implantation. Current-voltage (I-V) characterisation was done using silver paste contacts, which formed Ohmic contacts with both pristine and implanted MoS_2. Galvanostatic measurements were also performed and capacities for various electrode samples for both unimplanted and ion implanted MoS_2 were calculated. The constant current charge-discharge (CCCD) technique was used to evaluate specific capacities. Stability and retention tests were performed for 1000 cycles of charge and discharge with ion implanted electrode samples reporting higher than 98% retention capabilities. Electrochemical Impendance Spectroscopy (EIS) showing that after recycling, the electrodes were more stable. The electrode kinetics were evaluated using the standard rate constant (k_s) and it showed significant increase in all ion implanted electrodes compared to the unimplanted one, implying that faster equilibrium was attained with implanted electrodes.

The electrodes prepared from the synthesised and annealed MoS_2 powder gave the highest specific capacitance of 15.63 $F{\cdot}g^{-1}$ while the as-synthesised MoS_2 powder had specific capacitance of 10.43 $F{\cdot}g^{-1}$. These values were one order magnitude higher than what was measured from the electrodes made from the cyrstalline bulk MoS_2. However, electrodes made from the same powders and ion-implanted with either Mo or W ions shown suppressed capacitances, attributed to blockage of the pores as a result of ion irradiation.