Effect of MoS_2(00l)/MoO_2(0kl), (h00) crystal plane orientation of horizontal and vertical sheets on thermoelectric properties of MoS_2/MoO_2 hierarchical thin film

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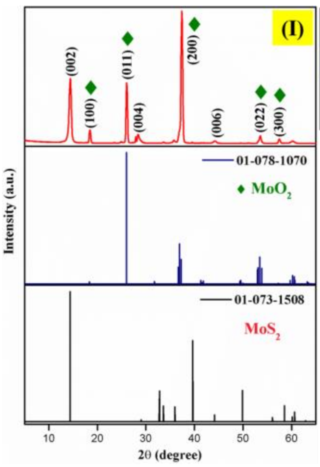
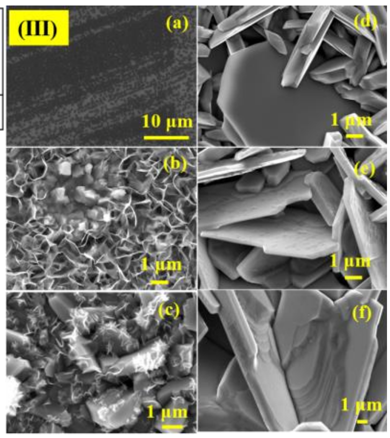
Thermoelectricity, architecting a highly efficient thermoelectric material will give a way to the future electrical energy sources by direct conversion between thermal and electrical energy. The efficiency of thermoelectric material can be quantified as a figure of merit, $zT = [S^2\sigma/k]\ T$ which has interdependent parameters of S, σ, k. In search of better thermoelectric performance, 2D materials showed the good results. The ability to achieve high zT, MoS_2 nanosheets can be a promising candidate due to its strong thermoelectric properties such as large effective mass, large anharmonicity, high chemical potential (2D nanosheets), valley degeneracies, anisotropy. We report thermoelectric properties of chemical vapor deposition (CVD) based growth of 2D MoS_2 nanostructures and its thermoelectric behavior. XRD pattern *(figure. I)* confirms the formation of MoS_2/MoO_2 hierarchical thin film with crystal plane orientations MoS_2 (00l) and MoO_2 (0kl) and (h00), *(figure. d)*. The Hall measurement *(figure. II)* suggest that fabricated film is p-type carrier concentration and the carrier concentration is consistent with the good thermoelectric material on the order of ~ 10^{16} cm^{-3} with carrier mobility of 11.7 $cm^2V^{-1}s^{-1}$. Vertical growth of MoS_2 is achieved by large supersaturation of S: MoO_3 ratio using large growth time of 30 min. Mechanistic understanding of MoS_2 growth and alignment has been developed with the aid of FESEM observations *(figure. III)*. The gradual growth of vertical nanosheets *(figure. III. b)* evolution from horizontal nanosheets *(figure. III. a)* is noticed. The sheet thickness is increased by overgrowth of MoS_2 on vertical nanosheets *(figure. III. c)* and very smooth surfaced nanosheets also observed *(figure. III. d)*. But anchoring of MoO_2 particles over MoS_2 nanosheets *(figure. III. e)* along with step-like layered nanosheets has been obtained *(figure. III. f)*. The possible mechanism is shown *(figure. IV)* and anchoring of MoO_2 particles on MoS_2 sheets *(figure. IV. c)* are demonstrated.



(II)

Parameters	Carrier mobility ($cm^2V^{-1}S^{-1}$)	Carrier concentration (cm^{-3})	Carrier type
Magnitude	11.7	2.16 x 10^{16}	p



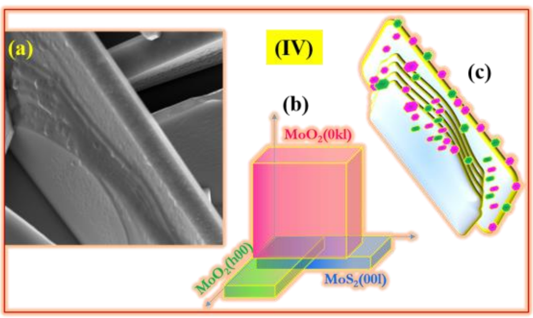


Figure. XRD (I), Hall results (II), FESEM (III), Schematic illustrations (IV).