Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Band Gap Engineering of PbI2 by Incommensurate Van der Waals Epitaxy YIPING WANG, JIAN SHI, Department of Material Science and Engineering, Rensselaer Polytechnic Institute — Van der Waals epitaxial growth had been thought to have trivial contribution on inducing substantial epitaxial strain in thin films due to its weak nature of Van der Waals interfacial energy. Due to this, electrical and optical structure engineering via Van der Waals epitaxial strain has been rarely studied. However, by appropriate film-substrate selection, we show that significant band structure engineering could be achieved in a soft thin film material PbI2 via Van der Waals epitaxy. The thickness dependent photoluminescence of single crystal PbI2 flakes was studied and attributed to the substrate-film coupling effect via incommensurate Van der Waals epitaxy. It is proposed that the Van der Waals strain is resulted from the soft nature of PbI2 and large Van der Waals interaction due to the involvement of heavy elements. Such strain plays vital roles in modifying the band gap of PbI2. The deformation potential theory is used to quantitatively unveil the correlation between thickness, strain and band gap change. Our hypothesis is confirmed by the subsequent mechanical bending test and Raman characterization.

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Date submitted: 06 Nov 2015 Electronic form version 1.4