A comprehensive (S)TEM analysis of Zn_3P_2 suitability for green energy applications

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There has been an increasing demand for the development of innovative and sustainable energy conversion devices, aiming to replace conventional and often non-renewable or intermittent energy sources. The motivation for this drive lies in the quest for sophisticated devices, propelling efforts to discover innovative nanostructured materials pivotal in enhancing performance and safeguarding the environment. Understanding a material's compositional and structural traits at the nano and atomic levels, including the configuration of active atoms, crystalline phases, and defects, is paramount in establishing the structure-performance relationship crucial for designing new materials and enhancing existing ones. Transmission electron microscopy (TEM) is a valuable technique employed in characterizing functional nanomaterials, offering insights into crystal structures at a local scale. When combined with techniques like Electron Energy Loss Spectroscopy (EELS) and Energy-dispersive X-ray spectroscopy (EDS) it provides a comprehensive map of elemental information and atomic arrangements, facilitating insights into various promising applications. This work provides an overview of the benefits of utilizing these characterization tools for mapping layer growth, thickness, morphology, and defects of nanostructured Zinc Phosphide (Zn_3P_2) thin films and nanoislands grown by Molecular Beam Epitaxy (MBE) on substrates such as InP and 6H SiC/graphene, with a focus on solar energy applications. Atomic resolution HAADF STEM images of Zn_3P_2 thin films on InP substrates present homogeneous growth and epitaxial relationship between substrate and layer. GPA analysis displays misfit dislocations and rotated domains, and STEM EELS and XRD results indicate composition varying from 60-70% of Zn, in contrast to 30-40% of P. In the case of Zn_3P_2 nanoislands grown on 6H SiC/graphene, atomic resolution HAADF STEM images and GPA analysis reveal that some of the Zn_3P_2 grains are randomly oriented with respect to the 6H SiC/graphene substrate and also, between each other. Rotation maps reveal that, in some areas, there is a rotation of up to 1.6° of the Zn_3P_2 layer with respect to the substrate, which can be justified by the Van der Waals epitaxy between the Zn_3P_2 and graphene. These findings are corroborated by EBSD results, that indicate a most prominent orientation of the grains, and a potential small population of islands with different orientations. Rotated domains are observed, and STEM EDS attest the stoichiometry of the Zn_3P_2 grains. Samples of Zn_3P_2 on different substrates have been analysed to determine the ideal growth conditions for an effective final device. Atomic resolution STEM images have given powerful information on the crystallinity defects present on the samples. These results give the key for growth Zn_3P_2 in an optimal way and go beyond the state-of-the-art in the field of solar cells.

Keywords:

Solar cells;Zinc Phosphide(Zn3P2);HAADF STEM;Electron Microscopy.

Reference:

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