The correlation between the microstructure and the optoelectronic properties of Zn_3P_2 grown by Selective Area Epitaxy

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Zinc phosphide (Zn_3P_2) is a promising material for low-cost photovoltaics made of earth-abundant elements. Its direct band gap of 1.5 eV makes it ideal for efficient photovoltaics. However, the record efficiency of 6% for a Zn_3P_2 solar cell achieved in the 1970s has never been outperformed ever since [1]. The main obstacle is the synthesis of Zn_3P_2 with high crystal quality and controllable properties. We have previously reported the growth of monocrystalline Zn_3P_2 on InP by Molecular Beam Epitaxy (MBE) [2]. Furthermore, we showed that the hole concentration can be controlled by tuning the Zn:P stoichiometry [3]. Nevertheless, the high lattice mismatch with the substrate induces strain in the layer with consequent formation of defects that limit the mobility. In this work, we explore selective area epitaxy (SAE) to improve the carrier transport by reducing the defect density [4]. The idea is to grow the thin film starting from a nanoscale pattern enabling Zn_3P_2 pyramidal growth and subsequent merging.

Here, we report on the combination of Hall Measurements and Photoluminescence Measurements on thin films grown by Selective Area Epitaxy. The highest hole mobility ever measured for Zn_3P_2 (520 cm^2/Vs) was obtained from high-quality thin films. Furthermore, Transmission Electron Microscopy (TEM) is used to characterize the microstructure of the samples. We determined which defects have the greatest impact on the optoelectronic properties of the films. The investigation extends to the effect of the hole size and the pitch size on the structure and, on the optoelectronic properties (see Figure 1 and 2).

a) b) c)

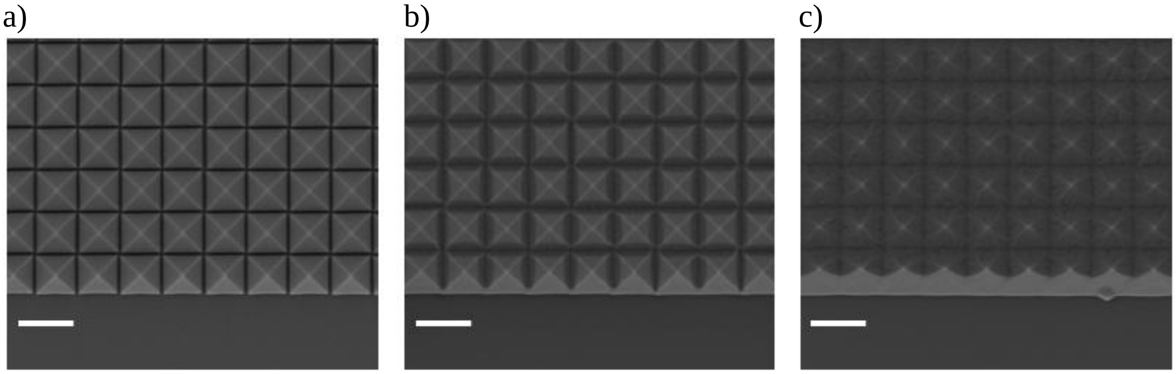

Figure 1: SEM images of Zn_3P_2 grown by SAE on InP (scale bar=500nm). (a) 40/400. (b) 75/400. (c) 120/400 (hole radius in nm/hole pitch in nm).

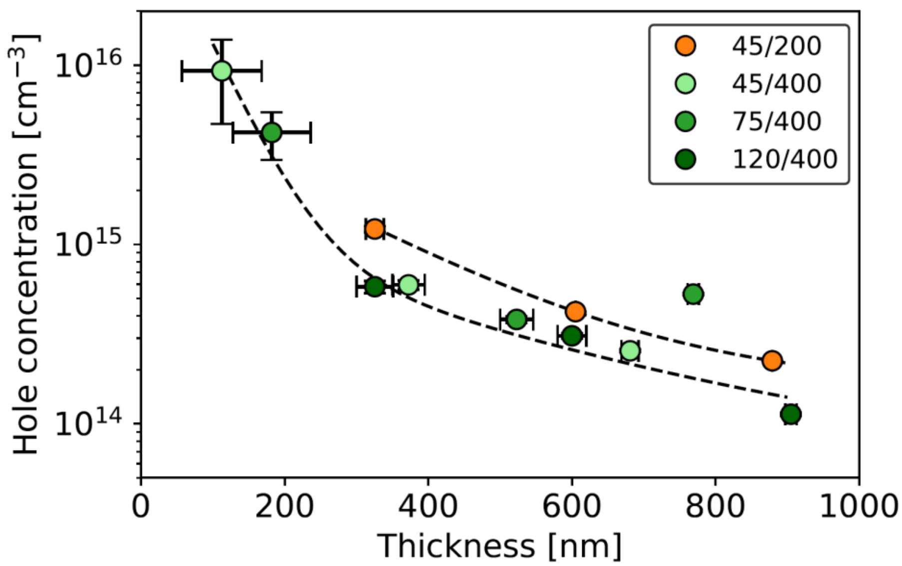

Figure 2: Evolution of the carrier concentration with the thickness for thin films grown from different patterns (hole radius in nm/hole pitch in nm).

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