Bandgap engineering of III/V semiconductors on silicon for solar hydrogen production

M. Piriyev¹, L. Chen¹, Y. Léger¹, C. Levallois¹ T. Rohel¹, A. Létoublon¹, G. Loget², B. Fabre², N.

Bertru¹ and C. Cornet¹

¹ Univ Rennes, INSA Rennes, CNRS, Institut FOTON – UMR 6082, F-35000 Rennes, France

² Univ Rennes, CNRS, ISCR – UMR6226, F-35000 Rennes, France

mekan.piriyev@insa-rennes.fr

One of the appealing approaches to convert solar energy into hydrogen fuel is solar water splitting with photoelectrochemical (PEC) cells in which photoelectrodes are used to drive the solar to hydrogen conversion at the electrolyte level. The semiconductor materials used as photoelectrodes with suitable bandgap for maximum solar light absorption and adapted band-lineups play a crucial role in determining the overall solar-to-hydrogen (STH) efficiency [1]. The direct bandgap III–V semiconductors are promising candidate, as they can provide STH efficiencies much higher than those of metal oxide semiconductors [2]. The pioneering work of Khalesev and Turner with multijonction Pt/GaInP₂/GaAs photoelectrode confirmed the advantages of using III-V semiconductors to reach high STH efficiency [3]. While many PEC studies were proposed using high cost commercial wafers with binary III-V semiconductors, [2-3] the development of III-V ternary alloys enabling bandgap engineering for PEC cells was explored only very recently [4 - 5].

In this contribution, we show the potentials of GaAs and its alloys with phosphorus (P) epitaxially grown on the low cost silicon substrate for the development of efficient photoelectrodes for solar hydrogen production. Based on a combination of structural, optical and PEC characterizations, we clarify the influence of the As content (Fig. 1a) on the performances of $GaAs_xP_{1-x}$ /Si:n photoelectrodes. We especially demonstrate how photocurrent similar to the commercial GaAs:n wafer is achieved with epitaxial grown GaAs on Si:n (Fig. 1b)



Fig. 1 (a-top) Net photocurrent density obtained at 1.23V vs RHE, (a-bottom) Band alignment of Γ , L and X valleys of GaAs_xP_{1-x} and indirect bandgap of Si; (b) I(V) curves of the epitaxial grown GaAs/Si and commercial n:GaAs wafer. (electrolyte pH=1)

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