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Impact of surface passivation of III-V elements on Si (001) substrate based on absolute surface and barrier energy calculations



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Introduction

Integrating III-V compound semiconductors on (001) Si substrates is a long-standing challenge, which has driven many researches for the past 40 years. A large portfolio of passive photonic devices and their mature fabrication technology are available on the Si platform. This gives greater flexibility to design photonics integrated circuits (PICs) as compared to the pure III-V technologies and opens a number of possibilities for e.g. lasers, photovoltaic energy production, or energy storage via solar hydrogen production.

Active photonics

- Direct bandgap in III-V materials for integrated lasers
- High carrier mobilities in III-V materials for advanced CMOS concepts

Electronics

- High carrier mobilities in III-V materials for advanced CMOS concepts

Passive photonics

- Non-linear properties of III-V materials for integrated passive devices (frequency converters)

Water splitting

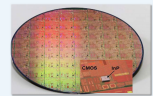
- High efficiency III-V photo-catalysts for solar hydrogen production

Photovoltaics

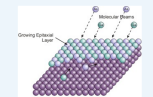
- Bandgap engineering in III-Vs for high efficiency multijunction architectures

III-V/Si co-integration

Bonding strategies



Monolithic integration



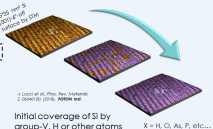
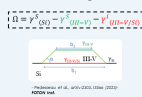
III-V/Si crystal growth by MBE



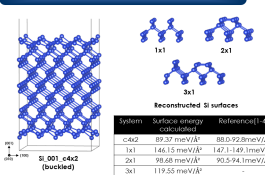
Experiments



Wetting



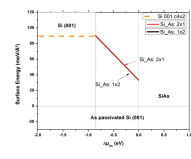
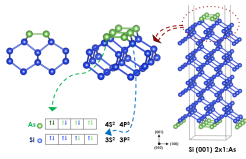
Surface



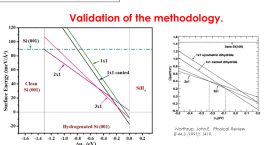
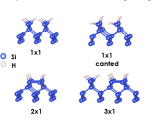
Surface Energy

$$E_{\text{surf}} = E_{\text{slab}} - N_{\text{atoms}} \cdot E_{\text{atom}}$$

Group V passivation on Si (001)

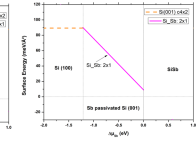
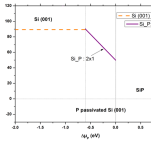


H passivation on Si (001)

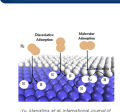


"Adapted similar technique for other group V elements"

"First results of surface passivation diagrams of group V elements on Si (001) substrate in terms of chemical potential"

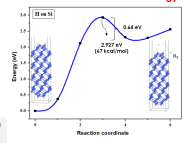


Energy barrier



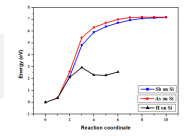
Nudged Elastic Band Method

Validation of the methodology.



"As desorption on Si (001) behaves like molecular adsorption not dissociative adsorption for H on Si"

"The first results show that group V elements on Si (001) substrate are more stable than H"



Conclusions

- Absolute surface energies of Si (001) surfaces with mono or sub-atomic layers of H and group V elements.
- Energy barrier calculation to study the desorption of different passivating elements from the Si surface.

Prospects

- The surface and interface energies calculations for III-V/Si.
- The influence of dislocations and antiphase boundaries.

Acknowledgements

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