Sujet thèse / PhD subject 2024

Titre Thèse	GaSe/InSe heterostructures for microelectronics and optoelectronics applications	
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Projet phare (principal)	Materials	
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Résumé du sujet :

III-V semiconductors have demonstrated their superiority for high frequency electronics and photonic devices, with applications in many areas as telecommunications, sensing, defense or solar energy. The related technologies make use of expensive Ga or In-based substrates and of a large amount of gallium and indium in their active layers. However, besides environmental issues linked to their production, both gallium and indium face serious sourcing problems either from a reserve viewpoint or from a geopolitical one. This motivates the search for new active materials that could be grown on standard III-V-material-free substrates and with sparing use of indium and gallium in the active layer.

Two-dimensional materials (2DMs) offer unique properties mainly related to their crystallographic structure composed of weakly coupled layers consisting of a few atomic planes (1 to 4) in which the atoms are covalently bonded. This peculiar structure leads to the absence of surface dangling bonds and favours strain free integration within heterostructures without lattice-matching requirement. Among the 2DMs, chalcogenides associating a metal atom and a chalcogen one (S, Se or Te) are particularly interesting because, unlike graphene, they have significant bandgaps in the range of 0.5 to 3 eV and offer a variety of band alignments. In addition, their band gap can change in nature and can be modulated according to the thickness. These properties make chalcogenides promising candidates for many applications, including electronic and photonic devices, spintronics, energy harvesting, and quantum sources[1]. This is evidenced by the large amount of studies related to the fabrication of devices based on transition metal dichalcogenides (TMDs) in the last decade with a strong focus on MoS_2, $MoSe_2$, WS_2 and WSe_2[2]. However, for optoelectronic applications, it turns out that TMDs exhibit direct band gap only at the monolayer limit, which makes processing very tricky. More, the growth of homogeneous crystalline TMD layers requires rather high temperatures and is not possible directly on silicon substrates. Therefore, the current process involves the growth on a specific substrate (sapphire for instance) before a subsequent transfer step on a host substrate (in most cases silicon) which makes the overall processing even more complex.

To go beyond these technological locks is possible considering the GaSe and InSe monochalcogenides. Indeed, starting from indirect band gaps of 3.5 eV (GaSe) and 2.11 eV (InSe), these materials exhibit a transition to direct band gaps for a few monolayer thickness, which can be further modulated towards the bulk value of 2.0 eV (GaSe) and 1.26 eV (InSe). These values allows covering a spectral range extending from the near infrared to the UV and make GaSe and InSe promising candidates for numerous optoelectronics applications[3]. For microelectronics devices, InSe

exhibits one of the highest electron mobility among the 2DMs, exceeding 10^3 cm^2/Vs and 10^4 cm^2/Vs at room and liquid-helium temperatures[4] and an I_{ON}/I_{OFF} ratio of 10^8 was achieved on a field effect transistor[5], making it a candidate of choice for transistor manufacturing. Indeed, the use of a 2DM, free of surface dangling bonds, as channel material allows a strong reduction of the surface scattering suffered by the charge carriers in thin channels. Therefore, the charge carrier mobility remains high even at the atomic thickness limit. Finally, until now, most devices have been fabricated from exfoliated flakes and a scalable elaboration method is clearly needed to take full advantage of these materials.

The objective of the proposed work is then to explore the growth and characterization of crystalline GaSe, InSe and the associated heterostructures on silicon substrate by Molecular Beam epitaxy (MBE). MBE growth will be performed in a dedicated chalcogenide reactor installed at IEMN, equipped with Ga, In and Se cells and fully operational for the proposed project. The IEMN epitaxy team will benefit from the experience gained during the recent past years in the growth of 2DM selenides. The epitaxy will be performed on Si(111) substrates after thermal deoxidation of the surface. The surface preparation will take advantage of an atomic hydrogen plasma cell fitted on the reactor, allowing the efficient cleaning of the residual carbon contamination. The work will aim to extend the published results on the epitaxial growth of GaSe on silicon[6] to InSe. Particular emphasis will be placed on the crystal quality and phase purity of the grown layers and interfaces according to the growing conditions. Different strategies will be considered including selective area growth (SAG) on patterned silicon substrate to improve the crystalline quality, benefitting from the strong experience of the Epiphy team in the SAG of III-V semiconductors[7]. The layer composition and interface chemistry will be studied *in-situ* by X-ray and UV photoelectron spectroscopies, thanks to a surface analysis chamber connected under ultra-high vacuum to the growth chamber. Their surface morphology will be examined by atomic force microscopy (AFM) and scanning electron microscopy (SEM) whereas their structural quality will be assessed by X-ray diffraction either on the IEMN equipment or through a collaboration with the Chevreul platform. Optical properties will be investigated by photoluminescence and Raman spectroscopy. For some samples, a deeper structural characterization will be performed by transmission electron microscopy (TEM) through a collaboration with the C2N laboratory to explore the possible epitaxial relationship and to check the sharpness of the grown van der Waals heterostructures at the atomic resolution.

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