

Theory of the optical properties of segregated (InAs)/(GaSb) superlattices

Rita Magri¹ and Alex Zunger²

¹Dipartimento di Fisica, Università di Modena e Reggio Emilia and INFN, Via Campi 213/A,
I-41100 Modena, Italy

²National Renewable Energy Laboratory, Golden, CO, 80401, USA

The differences in surface energies of various materials necessarily lead to a structural and chemical asymmetry of composition profiles of quantum wells and superlattices. The segregation induced structural asymmetry affects the electronic and optical properties. Segregation effects are particularly interesting in a system where both anion and cation segregation occurs. Here we focus on the infrared laser and detector material GaSb/InAs grown along the [001] direction. Since the binary components do not share a common element, the two interfaces of an ideal quantum well have chemically distinct bonds that do not appear in the respective end-point materials: the growth of InAs-on-GaSb (normal interface) has interfacial Ga-As bonds whereas the growth of GaSb-on-InAs (inverted interface) has interfacial In-Sb bonds. Segregation profiles which are different at the two interfaces modify this bonding configuration, thus, the optical properties of these systems are particularly susceptible to segregation.

In this paper we discuss:

- (1) the effects of the different interfacial bonding configurations on the electronic and optical properties;
- (2) the segregation profiles at the normal and inverted interfaces;
- (3) how the structural disorder at the interfaces due to atomic segregation affects the optical properties of (InAs)/(GaSb) superlattices.

To generate realistic composition profiles we used a kinetic model for MBE growth[1] that we have extended to treat simultaneously segregation of both group III and group V species. The model of segregation considers a layer by layer growth. Atomic exchanges involve the barrier energies $E_{\text{In/Ga}}^1$ ($E_{\text{As/Sb}}^1$) associated with the process in which a subsurface In (As) atom undergoes an exchange with a Ga (Sb) atom originally at the surface. The inverse process requires energies $E_{\text{In/Ga}}^2$ ($E_{\text{As/Sb}}^2$). For the cation segregation energies we have used the values proposed in previous papers[1] $E^1 = 1.8$ eV and $E^2 = 2.0$ eV, whereas for anions we have adjusted the atomic segregation energies of Sb and As so as to fit the detailed segregation profile measured by cross-sectional STM for GaInSb/InAs[2]. We obtained $E^1 = 1.750$ eV and $E^2 = 1.680$ eV, with an excellent fit to the X-STM profile.

Having determined the composition profiles along the growth direction we model the atomistic structure of the superlattices and apply the empirical pseudopotential electronic structure calculation method, finding the energy levels, wavefunctions, transition probabilities, thus directly establishing the effect of segregation on the electronic properties.

References

- [1] O. Dehaese et al., Appl. Phys. Lett. 66, 52 (1995).
- [2] J. Steinshnider et al., Phys. Rev. Lett. 85, 4562 (2000).