PCSI
Room Keahou I - Session PCSI-SuA2

Semiconductor Heterostructures: Growth, Nanostructures, & Interfaces I

Moderator: Stephan Lany, National Renewable Energy Laboratory

4:20pm **PCSI-SuA2-23 Correct Treatment of Spontaneous Polarization at Polar Wurtzite Interfaces*, Chris Van de Walle,*** University of California Santa Barbara **INVITED**

Herbert Kroemer's famous statement, "the interface is the device," also applies to polar interfaces in nitride-based devices; but in wurtzite-structure materials we additionally have to reckon with polarization fields. Sometimes these fields are a nuisance, suppressing efficiency of light emitters, sometimes they provide functional enhancement, by increasing the density of two-dimensional carrier gases in transistors. Accurate knowledge of polarization constants is critical for analysis of experiments and for device design. Some time ago we identified deficiencies in the calculation of polarization fields in simulation tools, related to the choice of the zinc-blende phase as a reference for the spontaneous polarization of wurtzite. However, since the current implementations contain *two* errors that to some extent cancel, most modeling has continued to use the zinc-blende-referenced approach.This has, unfortunately, led to major confusion in the analysis of polarization in AlScN alloys. Correct referencing of spontaneous polarization (relative to a layered-hexagonal phase) is essential for consistent interpretation of ferroelectricity.

Correct referencing of polarization also allows for an intuitive visualization of the origins of polarization, in which the electron cloud within the unit cell is shifted relative to the positive ionic cores. Different shifts in GaN and (strained) AlN then produce the polarization discontinuity at the interface, and lead to the insight that the electrons in the two-dimensional electron gas (2DEG) at a GaN/AlN [0001] heterojunction are *intrinsic* to the interface; i.e., they do not need to be provided by doping or surface states. The surface actually acts as a *sink* for electrons; proper surface engineering should prevent interfacial carriers from leaking away to the surface. The majority of the compensation charge on the surface is provided by fixed charge. This is consistent with the observation that the density of surface states (containing mobile charge) is much lower than the 2DEG density. All these considerations also apply, *mutatis mutandis*, to hole gases at GaN/AlN [000-1] junctions.

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5:00pm **PCSI-SuA2-31 Temperature-Dependent Recombination Rate Analysis of the Minority Carrier Lifetimes in Mid-Wave Infrared Antimonide based Materials*, Haley B. Woolf,*** New Mexico State University*; Rigo A. Carrasco, Preston T. Weber, Alexander T. Newell, Alexander W. Duchane, Christian P. Morath, Diana Maestas,* Air Force Research Laboratory

Various mid-wave infrared III-V materials (lattice-matched InAsSb, GaInAsSbBi on GaSb, strain-balanced InAs/InAsSb and InGaAs/InAsSb superlattice on GaSb) are characterized by time-resolved photoluminescence over temperatures ranging from 4 to 295 K. The samples are excited to low-excitation conditions, injections between 1015-1016 electron-hole pairs/cm3 per pulse, which yields single exponential decay of the time-resolved photoluminescence where the minority carrier lifetime can be evaluated. The temperature dependent lifetime is analyzed using a recombination rate model to determine the temperature-dependent Shockley-Read-Hall (SRH), radiative, and Auger recombination rates. The SRH and Auger recombination rates effectively model the lifetime data above 100 K in all samples, and provide evaluations of the defect energy level, capture cross section defect concentration product, carrier concentration, and Bloch overlap parameter in each sample.

Below 100 K, the lifetime's temperature dependence is complicated by additional factors. Samples with lifetimes on the order of 1-2 µs or less exhibit an SRH-limited temperature dependence down to 4 K that is largely constant or slightly increasing with decreasing temperature due to the thermal velocity term in the SRH recombination rate. On the other hand, undoped lattice-matched InAsSb and strain-balanced InAs/InAsSb superlattice samples with longer lifetimes around 6-7 µs exhibit markedly different behavior. In the lattice-matched InAsSb sample, the lifetime begins to decrease with decreasing temperature, consistent with radiative recombination becoming increasingly dominant as temperature approaches zero. There is no indication of radiative recombination in the 6-7 µs lifetime strain-balanced InAs/InAsSb superlattice, however, which, remains constant with decreasing temperature. This may be a consequence of the non-unity wavefunction overlap in the superlattice that would increase the radiative lifetime. The GaInAsSbBi sample exhibits a rapidly increasing lifetime with decreasing temperature from ~0.3 µs at 100 K to 4 µs at 4 K, which may indicate that localization in this alloy is suppressing SRH at lower temperatures. These conclusions will be explored in the context of how well the recombination rate model predicts them and potential improvements to it.

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