PCSI
Room Keahou I - Session PCSI-SuA2

Semiconductor Heterostructures: Growth, Nanostructures, & Interfaces I

Moderator: Kirstin Alberi, 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.

Work performed in collaboration with Cyrus Dreyer, Haochen Wang, Sai Mu, Nicholas Adamski, Suhyun Yoo, Darshana Wickramaratne, Mira Todorova, Jörg Neugebauer, and Simon Fichtner, and supported by DOE, SRC, and ARO.

5:00pm **PCSI-SuA2-31 Subsurface Nitrogen in Diamond (001)-2×1-H Studied by Density Functional Theory**, ***Shicai Wang***, Technion Israel Institute of Technology, China; *K. Huang,* Technion Israel Institute of Technology, Canada

To populate nitrogen centers in the near-surface region of diamond, there has been recent effort [1-3] of using activated dinitrogen to impact fully hydrogenated diamond surfaces as synthesized by chemical vapor deposition. There is implication [2-3] of nitrogen into the subsurface region (depth: 6 ± 5 Å) of the same diamond (001)-2x1-H by low energy N_2^+ ions. It remains, however, unclear about the atomistic understanding into the configuration and bonding of the nitrogen species in the subsurface region of diamond (001)-2×1-H. Here, we present studies into subsurface nitrogen in diamond (001)-2x1-H by density functional theory simulations, revealing in each case information regarding structure, energy and vibration that depend on the atomistic coordination as detailed below.

We have studied 10 configurations of a single interstitial nitrogen in the topmost 3 layers of diamond (001)-2x1-H. In all configurations, the carbon network is strongly distorted by an interstitial nitrogen atom, in which 2 carbon-carbon bonds are cleaved. The interstitial nitrogen is bound to 3 neighboring carbon atoms, of which one carbon becomes sp^2 hybridized. The stability of the interstitial configuration depends on the location of nitrogen and the direction of the formed C(sp^2)-N bond, exhibiting formation energies of +4.83 to +11.04 eV. The most characteristic mode of vibration arises from the C(sp^2)-N bond, i. e., stretch (1530 to 1901 cm^{-1}/ 189.7 to 235.8 meV) and swing (1101 to 1389 cm^{-1}/ 136.6 to 172.2 meV). Migration of nitrogen interstitial is also evaluated, involving a series of steps and intermediates; the rate determining step is of a barrier of 6.02 eV.

We have also evaluated 3 configurations of a single substitutional nitrogen in the topmost 3 layers of diamond (001)-2x1-H. In all configurations, the carbon network is largely preserved, giving formation energy of +2.79 to +3.41 eV. The substitutional nitrogen is bound to four neighboring carbons, and the formed C-N bond is larger than a typical C-N single bond, giving the characteristic C-N swing vibration of 844 to 979 cm^{-1} (105 to 121 meV).

We have finally evaluated 6 configurations of a pair of nitrogen atoms in the topmost 3 layers of diamond (001)-2x1-H. Our computations were restricted to the N_{2i} species that mimics the encounter of an interstitial N_i and a substitutional N_s species. The formation energy depends on the location of N_{2i} and the direction of the formed N_i-N_s bond, ranging from +4.12 to +9.71 eV. The most characteristic motions of vibration arise from N-N stretch mode of 1419 cm^{-1} (176.0 meV), C-N swing mode of 968 cm^{-1} (120 meV) and N-N swing mode of 471 cm^{-1} (58.5 meV).

5:05pm **PCSI-SuA2-32 Decay Dynamics of a Monolayer Silver Film on Si(001)**, ***Xiaohang Huang***, Guangdong Technion - Israel Institute of Technology, China; *K. Huang,* Guangdong Technion - Israel Institute of Technology, Canada

Under operando conditions, silicon-based semiconductor devices are subject to impulses from mechanical, thermal, electrical, and photonic excitations, leading inevitably to structural decay.[1–4]The dynamics associated with the decay process (e.g., rate, pathway and barrier) is of practical interest, because it is crucial for stability assessment, lifetime prediction, and performance optimization.

Here, we describe the decay dynamics of a monolayer silver film on Si(001). Extended in-situ monitors of the evolution of (2x2) Ag-film/Si(001), using ultra-high vacuum scanning tunneling microscopy between 245 K and 276 K, demonstrate the thermal decay of the silver film by successive detachment of silver tetramers at the edge of the film (shown in Figure S1a-b of the supplementary pages). Complementary measurements, using the "annealing/quenching" method, gave evidencethat the detached silver had transitioned into a mobile state, Ag(m), which is capable of migrating and aggregating into clusters on both bare and silver-covered silicon surfaces (as in Figure S1c of the supplementary pages). Based on these experimental findings, we propose a first-order kinetic model that centers on the reversible transition of silver between the (2x2) Ag-film and Ag(m). By applying this model to our experimental data, an excellent fit can be achieved, yielding an activation of 0.386 ± 0.010 eV for the (2x2) Ag-film to Ag(m) transition, and that of 0.332 ± 0.012 eV for the Ag(m) to the (2x2) Ag-film transition. The obtained pre-exponential factors are anomalouslylow, i.e. 2067 ± 877 s^{-1} for the (2x2) Ag-film to Ag(m) transition, and 90± 47 s^{-1} for the Ag(m) to the (2x2) Ag-film transition. Such low values of the pre-exponential factors are likely linked to an entropic effect, on which density functional theory simulations are underway to provide further insight.

5:10pm **PCSI-SuA2-33 Temperature-Dependent Recombination Rate Analysis of the Minority Carrier Lifetimes in Mid-Wave Infrared Antimonide based Materials**, ***Haley B. Woolf***, New Mexico State University; *R. Carrasco, P. Weber, A. Newell, A. Duchane, C. Morath, D. 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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