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Metal-induced gap states and Schottky barrier heights at nonreactive GaN/noble-metal interfaces

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We present *ab initio* local density FLAPW calculations on nonreactive N-terminated [001] ordered GaN/Ag and GaN/Au interfaces and compare the results (such as metal induced gap states and Schottky barrier heights) with those obtained for GaN/Al, in order to understand the dependence of the relevant electronic properties on the deposited metal. Our results show that the density-of-gap states is appreciable only in the first semiconductor layer close to the interface. The decay length of the gap states in the semiconductor side is about 2.0 ± 0.1 Å and is independent of the deposited metal, therefore being to a good extent a bulk property of GaN. Our calculated values of the Schottky barrier heights are $\Phi_{B_p}(\mathrm{GaN/Ag}) = 0.87$ eV and $\Phi_{B_p}(\mathrm{GaN/Au}) = 1.08$ eV; both values are smaller than the GaN/Al value $[\Phi_{B_p}(\mathrm{GaN/Al}) = 1.51\ \mathrm{eV}]$ and this quite large spread of values excludes the possibility of a Fermi-level pinning within the GaN band gap. Because of the low screening in GaN, the potential barrier at the junction is strongly affected by the structural arrangement of the first metal layer at the interface. This leads to quite large variations of the Schottky barrier height as a function of the metal, in contrast with the behavior of GaAs/metal interfaces.

I. INTRODUCTION

GaN has certainly been one of the most studied compounds in the last few years, mainly because of both interesting optical properties and remarkable thermal stability, which render this semiconductor particularly suitable for important technological applications. As is well known, however, device performances depend on good metallic contacts and so the study of Schottky barrier heights (SBH) in GaN/metal systems is of great relevance: as an example, the performance of GaN-based laser diodes is still limited by the difficulty in making low-resistance Ohmic contacts. In this regard, surface reactivity and the presence of interface states are also seen to play a relevant role in Schottky barrier formation.

In a previous work, we investigated the GaN/Al system, which is considered to be a *reactive* interface due to the Ga–Al exchange reaction driven by AlN formation at the immediate interface; we studied the ideal interface,[1] as well as the effects on the interface properties of some defects (such as atomic swap and $\mathrm{Ga}_x\mathrm{Al}_{1-x}\mathrm{N}$ intralayers[2]) at the initial stages of the SBH formation.[3]

In the present paper, we report results of *ab initio* calculations for GaN/M interfaces (with M = Ag, Au) which are considered to be nonreactive[4] and compare the results (such as metal induced gap states (MIGS) and SBH with those obtained for GaN/Al, in order to understand the dependence of the relevant electronic properties on the deposited metal. The interest in studying noble-metal contacts resides in understanding the effect of the *d* states on the Fermi-level position, which has been thought to be relevant in the case of GaAs interfaces.[5] Moreover, we investigate the role of the atomic positions in the interface region in determining the final SBH values: starting from GaN/Al, lineups differing by as much as 0.80 eV can be produced by changing the interface N-metal interplanar distance from its equilibrium value to that corresponding to the GaN-Ag interface; as a result, the Schottky barrier height is brought to a value very close to that obtained for GaN/Ag. This leads to the conclusion that strain effects, mainly affecting the magnitude of the interface dipole, play a major role in determining the final SBH at the GaN/metal interface.

II. TECHNICAL DETAILS

The calculations were performed using the all-electron full-potential linearized augmented plane wave (FLAPW)[6] method within density functional theory in the local density approximation (LDA). We used a basis set of plane waves with wave vector up to $K_{max} = 3.9$ a.u., leading to about 2200 basis functions and for the potential and the charge density we used an angular momentum expansion up to $l_{max} = 6$; tests performed by increasing l_{max} up to 8 showed changes in the Schottky barrier height of less than 0.03 eV. The Brillouin-zone sampling was performed using 10 special k points according to the Monkhorst-Pack scheme.[7] The muffin-tin radii R_{MT}, for Au and Ag were chosen equal to 2.1 a.u., while for Ga and N we used $R_{MT} = 1.96$ and 1.65 a.u., respectively. We have considered supercells containing 15 GaN layers (8 N and 7 Ga atoms) and 9 metal layers; tests

TABLE I. Interplanar distances (in Å) between the different atomic planes in the GaN/Al, GaN/Ag, and GaN/Au interfaces. Values in parentheses are taken from Ref. 1.

	$d_{int}^{\mathrm{Ga}-N}$	d_{int}^{N-M}	d_{int}^{M-M}	d_{bulk}^{M-M}	d_{MTE}^{M-M}
GaN/Al	1.11 (1.12)	1.11 (1.15)	1.88 (1.94)	1.64 (1.94)	1.78
GaN/Au	1.10	1.34	1.77	1.68	1.70
GaN/Ag	1.07	1.32	1.60	1.64	1.75

performed on the cell dimensions have shown that bulk conditions are well recovered far from the interface using this $15+9$ layer cell size (see discussion below).

III. STRUCTURAL PROPERTIES

GaN is well known to show polytypism between the zinc blende and the wurtzite phase, so that either one can be easily stabilized; we therefore concentrate on [001] ordered N-terminated zinc blende interfaces in order to avoid the contribution of spontaneous polarization effects inside GaN that might contribute to the Schottky barrier height. Our goal is in fact to investigate the role played by the different metals in determining the position of the Fermi level within the semiconductor band gap. We considered the metal as grown epitaxially on a GaN substrate ($a_{subs}=a_{GaN}=4.482$ Å). Given the bulk lattice constants of the three metals, $a_{\mathrm{Al}}=4.05$ Å, $a_{\mathrm{Ag}}=4.09$ Å, and $a_{\mathrm{Au}}=4.08$ Å, all the metals considered show a quite large mismatch with the GaN substrate, ranging from 8.8% in the case of fcc-Ag up to 9.6% in the case of fcc-Al. In all cases, their lattice constants are smaller than that of the substrate, which implies that appreciable bond-length relaxations are expected for the metal overlayers. We calculated the most stable structures, assuming pseudomorphic growth conditions (an assumption common to all *first principles* approaches to these problems, since it is the only one that allows calculations to be performed) and a geometry in which the metal atoms simply replace the Ga atoms on their fcc sites, using total-energy minimization and the *ab initio* forces calculated on each atomic site to find the equilibrium values of the interface Ga-N, N-M, and M-M interplanar distances. In-plane relaxations, as well as the possibility of in-plane reconstruction of the GaN surface, before or during metal deposition, were neglected. Of course, the occurrence of such effects may strongly modify the calculated values of the Schottky barrier heights which, as we will show, are very sensitive to the details of the interface morphology. In this paper, however, we are interested mostly in studying the effect of the metal overlayer on the interface GaN/M electronic properties rather than determining the structural configurations that may occur experimentally.

Our structural data are reported in Table I. Due to a refinement[8] of our previous calculations on the GaN/Al system, the data listed in Table I for this system differ from those already published;[1] the largest change occurs for the Al-Al bulk interplanar distance. For clarity, we report our previous results in parenthesis in this same table. Let us focus on the structural rearrangement of Al, Ag, and Au on the GaN substrate and consider some relevant interplanar distances (i.e., distances between atomic planes along the [001] growth direction). A comparison between the free-electronlike case of Al and the behavior of noble metals shows that none of the metals considered seems to alter appreciably the bond length at the interface semiconductor layer so that the interplanar distance remains close to its bulk value (1.12 Å); the larger deviation, found in the case of Ag, still gives a reduction of the Ga-N interface distance by less than 5%. A larger difference is found for the interface nitrogen-metal interplanar distance: the N-Al distance is smaller than those corresponding to the Ag and Au structures by about 20%. This can be related to the different bonding at the interface in the different cases—as will be further discussed later on. For both Al and Au we find that the interplanar metal-metal distance d_{int}^{M-M}, increases compared to the bulk, leading to a bondlength larger than equilibrium just at the interface layer. This effect is far more evident in the case of Al and can be related to a weakening of the *s*-type metallic Al-Al bond due to a partial *s-p* hybridization of the interface aluminum in the Al-N covalent bond. We find that already in the subinterface layers, the forces are very small, thereby indicating that the metals recover quickly their strained bulk-tetragonal bondlengths.

In the last column of Table I, we report the interplanar distances calculated according to the macroscopic theory of elasticity (MTE)[9] for the tetragonal metal strained to match the GaN substrate, using the bulk elastic constants[10] and the equilibrium bondlengths[11] as input parameters. We recall that in all cases considered, the mismatch is pretty large (about 9%) so that we might probably be out of the range of validity of the MTE. In fact, the discrepancies between the optimized interplanar distances within the bulk regions (namely, d_{bulk}^{M-M}) and those predicted by the MTE range between 1% in the case of Au to up to 8% in the Al case. As expected, the bond-length distances in the metal bulk side are very similar for all the metals considered, seeing that their equilibrium lattice constants are very close.

IV. MIGS: THE NOBLE-METAL CASE AND COMPARISON WITH THE GaN/Al SYSTEM

We compare in Fig. 1 the atomic site-projected partial density-of-states (PDOS) for the GaN/Au and GaN/Al interfaces and inner N and M atoms, taking the valence-band maximum (VBM) of the inner N PDOS as the zero of the energy scale (vertical arrows denote the position of E_F). The GaN/Ag PDOS is very similar to that of GaN/Au, and are therefore not shown. In order to demonstrate the presence of the MIGS and the strong effect of the metal deposition on the interface semiconducting atoms, we show as a reference the PDOS of the same atoms (N and metal) in the corresponding bulk compounds (i.e., zinc blende GaN and bulk metal). The PDOS for the interface N and Au atoms—essentially due to *p* and *d* states, respectively [Figs. 1(c) and 1(d)] show peaks with a quite high-density-of-states in the GaN band-gap en-

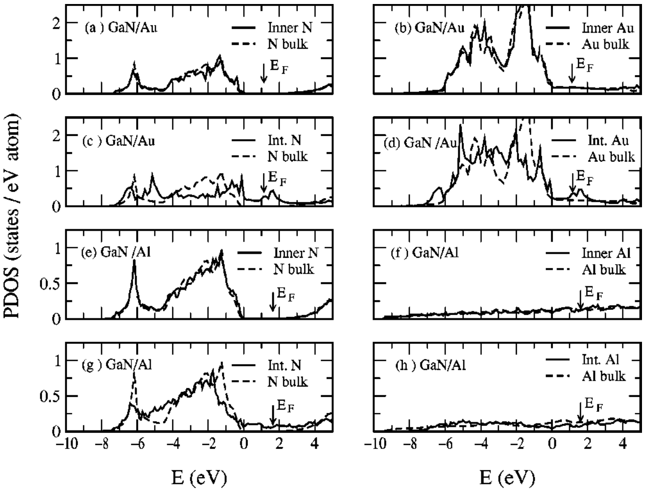

FIG. 1. Inner [panels (a) and (e)] and interface [panels (c) and (g)] N atom PDOS in the GaN/Au and GaN/Al systems, respectively. Panels (b), (f) and (d), (h) show the PDOS for the inner and interface Au (Al) atoms, respectively. In all panels, dashed lines indicate the corresponding atomic contribution in the bulk materials. The GaN VBM is taken as zero of the energy scale. Vertical arrows indicate E_F with respect to the semiconductor VBM.

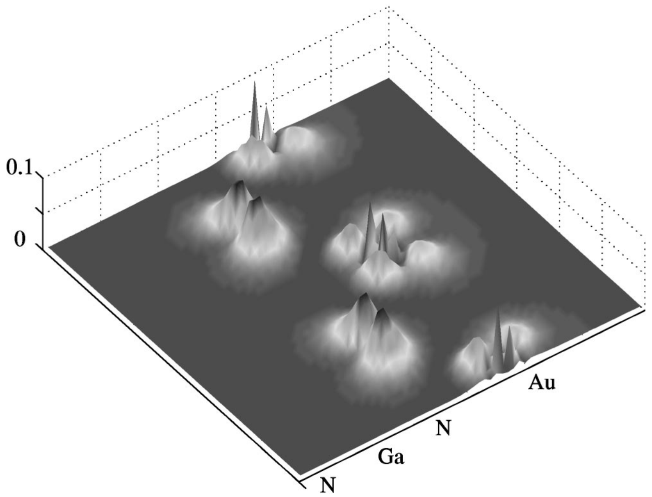

FIG. 2. Three-dimensional plot of the GaN/Au MIGS charge density due to the density-of-states (DOS) peak in proximity to E_F projected on a plane that cuts the N-Au interface bond. Values on the z axis in electrons/cell.

ergy region (i.e., between 0 and 1.8 eV). We recall here that LDA strongly underestimates the GaN band gap whose experimental value is $E_{gap}^{expt}=3.39$ eV;[12,13] these states are seen to disappear in the inner bulk atom [Figs. 1(a) and 1(b)]. Therefore, the presence of the metal affects only the semiconductor layers closer to the interface; already in the second layer (not shown) the MIGS decrease appreciably and the DOS gets very close to their bulk shape. Bulk conditions are perfectly recovered in the inner layers [see the practically overlapping lines in Figs. 1(a) and 1(e)], showing that the supercell dimensions are sufficient for our purposes. In particular, we notice that the LDA GaN gap is recovered in the PDOS of the inner N atoms.

Apart from the presence of MIGS, the PDOS for both the N and Au interface atoms shows strong differences relative to the bulk, much larger than in the GaN/Al case, where the most relevant difference consists in the general modulation that brings the Al PDOS from the free-electron square-root-like behavior closer to the PDOS of bulk AlN. The reason for this behavior is that in GaN/Au, the Au $3d$ states are occupied and interact strongly with the N p states, which are also filled. As a result, the antibonding states rise in energy above the semiconductor VBM and form the peaks at around 1.5 eV, just in proximity to E_F. Such features are absent in the GaN/Al case [Fig. 1(g)] and are present in the PDOS of the interface N and Au atoms [Fig. 1(c)], completely disappearing on atoms far from the junction inside GaN. The presence of a peak at E_F might indicate a tendency to an instability, probably leading to in-plane reconstruction with the possible introduction of defects. The spatial location of the charge density corresponding to the peak around E_F is shown in Fig. 2: these states, which have a clear antibonding character between N and Au, are mainly localized in the interface region with a resonant behavior inside the Au region (not shown) and a negligible charge density in the GaN region. A similar situation occurs in the GaN/Ag system (not shown) and was also reported for a [110] GaAs/Ag interface,[14] whereas it is completely absent in GaN/Al-type structures due to the lack of d states in this system.

The overall shape of the interface N PDOS shows a depletion of states in the region from -4 to -1 eV, and a peak around -5 eV, presumably representing the bonding partners of the structures around E_F and around the GaN VBM. This corresponds to a degradation of the sp^3 bonding environment around the interface N. On the basis of this discussion, we can try to give an explanation for the much larger distances d_{int}^{N-Au} and d_{int}^{N-Ag}, compared with the Al case. In fact, the N-Al interface bond is similar to the one in bulk AlN that provides its stability. The N-Au bond, on the other hand, mixes together filled states and pushes towards higher energies the antibonding combinations [with a large anion (N) contribution] around E_F (but mostly below it). This is consistent with the smaller amount of charge present inside the interface N atom, to be discussed later. In this scenario, decreasing the N-Au (Ag) distances, would not further stabilize the structure.

In order to investigate the spatial dispersion of the occupied gap states, we show in Fig. 3 the macroscopic[15] average of the MIGS charge density in GaN/Al (solid line), GaN/Au

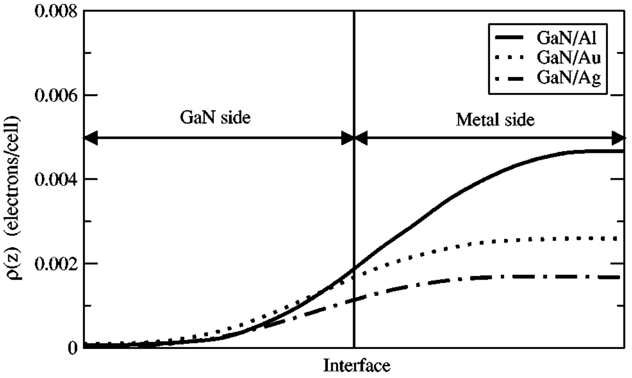

FIG. 3. Planar macroscopic average of the MIGS charge density for the GaN/Al (solid line), GaN/Au (dotted line), and GaN/Ag (dot-dashed line) interfaces.

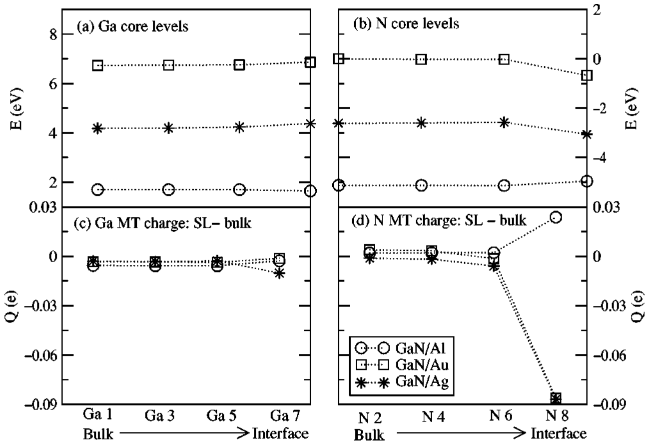

FIG. 4. Panels (a) and (b): core energy levels of Ga and N atoms, respectively, for the GaN/Ag (stars), GaN/Au (squares), and GaN/Al (circles) systems as a function of the distance from the interface. Binding energies (in eV) are referred to the Fermi levels in the different systems and were shifted by 10 190.74 and 353.75 eV in the Ga and N case, respectively. Panels (c) and (d): difference between MT charges in GaN/metal superlattices (SL) and in GaN bulk for Ga and N atoms, respectively, as a function of the distance from the interface. Symbols as in panels (a) and (b).

(dotted line), and GaN/Ag (dot-dashed line). As already pointed out for GaN/Al,[1] the presence of the metal affects almost exclusively the interface semiconductor layer; the MIGS decay exponentially, approaching zero inside the semiconductor. Due to the different density-of-states distribution of Al and Au (or Ag) for energies close to E_F and the consequent different positions of E_F with respect to the GaN VBM, the total integrated MIGS charge in the whole cell (metal side included) is larger in the free-electron metal-like case; however, the behavior of these states as a function of the distance from the junction in the three interfaces is overall very similar. Actually, we find from Fig. 3 a very similar behavior, which can be extrapolated with an exponential, leading to the same decay length (see Ref. 1 for details) for both GaN/Au and GaN/Ag estimated to be $\lambda = 2.0 \pm 0.1$ Å, which is close to the value obtained for the GaN/Al system ($\lambda \approx 1.9$ Å).[1] Therefore, even though the energy dispersion of the MIGS is somewhat different in the free-electron-like and noble metal interfaces (see Fig. 1), they are equally screened in the semiconductor side within one to two layers, thus showing that, within a good approximation, λ is a GaN bulk property.

We plot in Fig. 4 the binding energies of 1s core levels, with respect to the E_F of Ga and N [panels (a) and (b), respectively] and the difference between MT charges in the GaN/M superlattices (SL) and in GaN bulk [Fig. 4(c) and 4(d) for the Ga and N atoms, respectively] as a function of the distance from the interface. As already discussed in Ref. 1, it is clear that in the Al case the charge rearrangement at the interface causes a small effect (about 0.15 eV) on the interface N core level and negligible effects on the other semiconductor atoms. On the other hand, in the noble metals case, the interface effect is much stronger: the GaN interface layer shows core-level binding energies differing by about 0.4 (0.5) eV for Ag (Au), from the values of the inner bulk-like atoms. Moreover, the core levels *bending* in going from the bulk towards the interface follows an opposite trend in the noble and free-electron-like metals. This behavior is consistent with the trend of the valence charge inside atomic spheres: the interface nitrogen atom shows a charge depletion (enhancement) with respect to the bulk atoms in the noble metal (Al) case. As discussed above, the presence of a peak (see Fig. 1) in the GaN gap energy region, with antibonding N p-Au d character, might be the cause of this charge rearrangement and the resulting chemical shift observed on the core-level profiles.

TABLE II. Schottky barriers (in eV) at the GaN/Al, GaN/Ag, and GaN/Au interfaces.

	GaN/Al	GaN/Au	GaN/Ag
Φ_B	1.51	1.08	0.87

V. SCHOTTKY BARRIER HEIGHTS

To calculate the values of the SBH, we adopt the usual procedure[16,17] that takes core levels as reference energies. In particular, the potential discontinuity can be expressed as the sum of two terms: $\Phi_B = \Delta b + \Delta E_b$, where Δb and ΔE_b denote an *interface* and *bulk* contribution, respectively. We evaluate Δb taking the difference of Ga 1s and the noble-metal 1s core-level energies in the superlattice: $\Delta b = E_{1s}^{Ga} - E_{1s}^{NM}$. On the other hand, the *bulk* contribution can be evaluated from separate calculations for bulk GaN and noble metal and calculating the difference between the binding energies of the same 1s levels considered above: $\Delta E_b = (E_{VBM}^{GaN} - E_{1s}^{Ga}) - (E_F^{NM} - E_{1s}^{NM})$.

The p type SBH values obtained, shown in Table II, include a spin-orbit perturbation $\Delta_{SO}^{GaN} \approx 0.1$ eV, but do not include quasiparticle corrections. Note that, as already pointed out, this refinement in the calculation of the GaN/Al system[8] gives a 4% difference in the N-Al interface distance (which changes the core-level alignment at the interface) and a large difference in the tetragonal bulk Al interplanar distance. This last quantity affects the Al core-level binding energies used in the evaluation of the final SBH, changing considerably the *bulk* contribution, essentially related to the absolute deformation potential of the Fermi level in bulk Al. As a result, we obtain a SBH value different from the one previously published[1] ($\Phi_B = 1.12$ eV). The values shown in Table II are in good agreement (within 0.1–0.2 eV) with those calculated from the density-of-states, obtained by considering the SBH as the energy distance between E_F (see vertical arrows in Fig. 1) and the top of the valence band of the PDOS corresponding to the inner semiconductor layer inside the bulk region of the superlattice (the energy zero in Fig. 1).

We note that the SBH values in the noble-metal case are lower than the SBH in the GaN/Al interface [Φ_{B_p}(GaN/Al) $= 1.51$ eV]. To better understand this result, we should consider that the Al and noble-metal interfaces differ in two main aspects: (i) different chemical species of the metal overlayer and (ii) different structural properties, i.e., different bondlengths at the interface that comprise, in all respects, an interfacial strain contribution. In particular, from inspection of Table I it is evident that the Ag and Au structures show

TABLE III. Interplanar distances (in Å) between the different atomic planes in the GaN/Al, GaN/Ag, and GaN/Au interfaces (first three columns) and Schottky barrier heights (in eV—last column).

	$d_{int}^{\mathrm{Ga}-N}$	d_{int}^{N-M}	d_{int}^{M-M}	Φ_B
GaN/Al	1.11	1.11	1.88	1.51
Step I	1.11	1.32	1.88	0.76
Step II	1.11	1.32	1.60	0.80
Step III	1.07	1.32	1.60	0.71
GaN/Ag	1.07	1.32	1.60	0.87

very similar d_{int}^{N-M} and d_{int}^{M-M} interplanar distances, which are at variance with those with Al. In order to separate the chemical from the strain contribution, we evaluate the SBH for three different structures that can be regarded as intermediate steps necessary to bring the GaN/Al structure to match perfectly the GaN/Ag one. We show in Table III the interface interplanar distances and final SBH values for the equilibrium GaN/Al and GaN/Ag systems and for the three intermediate interfaces. In the first structure (step I), the interplanar d_{int}^{N-M} distance of the GaN/Al SL is taken equal to that minimized for the GaN/Ag SL ($d_{int}^{N-M}=1.32\,\text{Å}$): the SBH is reduced from 1.5 to 0.76 eV (this surprising result will be discussed in detail later on).

As a second step (step II), we change d_{int}^{M-M} to recover that calculated for the GaN/Ag structure: $d_{int}^{M-M}=1.60\,\text{Å}$. The SBH is remarkably less sensitive to this parameter, giving only a 0.04 eV change in the potential barrier, which brings the SBH to about 0.80 eV. This is expected since the metal efficiently screens out the perturbation generated by atomic displacements: actually, the dynamical effective charge, related to the dipole induced by a unit displacement of atoms, is zero inside a metal.

In the third structure (step III), the Ga–N interface distance is brought to its value in the GaN/Ag superlattice, $d_{int}^{Ga-N}=1.07\,\text{Å}$, and we have a system where Al atoms perfectly replace Ag in GaN/Ag. Although this last structural change is very small (about 4%), this interplanar distance turns out to be very important for the final potential lineup, due to the incomplete screening in the semiconductor side and the large N effective charge. As a result, the SBH changes appreciably ($\Phi_B=0.71\,\text{eV}$). This final result is quite close (within 0.2 eV) to the value found for the real GaN/Ag interface, showing that apparently the interface strain plays a more important role than the bare chemical contribution.

Perhaps the most surprising result of our tests is the very strong dependence of the SBH on the interface N-Al distance, whose variation represents the larger contribution to the difference between GaN/Al and GaN/Ag (Au) SBH's. Test calculations have shown an almost perfect linear behavior of Φ_B against d_{int}^{N-Al}, leading to an Al effective charge $Z_L^*=0.08$, ($Z_L^*=Z_T^*/\epsilon_\infty$, where Z_T^* is the Born dynamical charge and ϵ_∞ is the electronic static dielectric constant). This result is in sharp contrast with the case of GaAs/Al,[18] where no significant changes were found for small elongations of the As-metal interface distance, therefore, resulting in $Z_L^*\sim 0$—an almost perfect metallic behavior. As a further test, we performed calculations on GaAs/Al, similar to those of Ruini *et al.*,[18] confirming their results both in terms of the SBH values, and of their behavior as a function of $d_{int}^{\text{As-Al}}$.

A possible explanation of the striking difference between the GaN/Al and GaAs/Al systems can be provided by an analysis of the relevant physical parameters involved. The MIGS decay length is larger for GaAs/Al ($\lambda_{\mathrm{GaN}}\approx 2$ Å and $\lambda_{\mathrm{GaAs}}\approx 3$ Å)[19,20] therefore providing a more extended region with metallic behavior inside the semiconductor; in addition, the density-of-states at the Fermi level $N(E_F)$ is larger for GaAs/Al (see Fig. 5), giving rise to a smaller (by a factor of ≈ 1.5) Thomas-Fermi screening length λ_{TF} in this system. Still, the values of the MIGS decay length and of $N(E_F)$ are not *very* different between GaAs and GaN, so that it is not at all obvious to expect such a behavior of the SBH in the two compounds.

To understand these results, we can use elementary electrostatics arguments. If we make a few rough assumptions such as a simple Yukawa-like screened potential and consider a metallic behavior inside the semiconductor up to distances of the order of λ, the MIGS decay length, we find that the potential difference across the metal/semiconductor junction induced by displacements of the Al interface atom, scales with the factor $e^{-k_{TF}\lambda}$. If we now estimate the values of the Thomas-Fermi screening lengths k_{TF}, using the GaN/Al and GaAs/Al superlattice value of $N(E_F)$, we are led to the conclusion that a unit displacement of the interface Al atoms produces a potential change across the interface that is roughly seven times larger in GaN/Al than in GaAs/Al. Considering the crudeness of this model, such an estimate is in satisfactory agreement with the first-principles results, which indicate a factor of ≈ 10 for the same ratio. In other words, GaAs screens out almost perfectly all the struc-

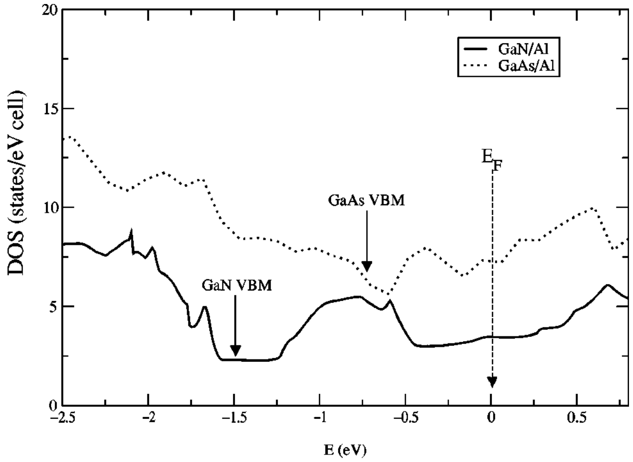

FIG. 5. Total DOS of GaN/Al (solid line) and of GaAs/Al (dotted line) in proximity to E_F (taken as zero of the energy scale). Vertical arrows denote the position of the semiconductor VBM.

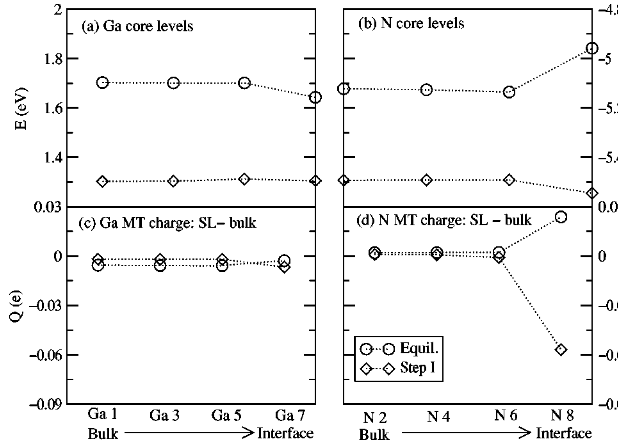

FIG. 6. Panels (a) and (b): core energy levels of Ga and N atoms, respectively, for the GaN/Al equilibrium (circles) and Step I (diamonds) systems as a function of distance from the interface. Binding energies (in eV) are referred to the E_F. Panels (c) and (d): difference between MT charges in GaN/metal SL and in GaN bulk for Ga and N atoms, respectively, as a function of the distance from the interface. Symbols as in panels (a) and (b).

tural changes in the interface region (namely, displacements of the interface Al atoms), while the same is not true for GaN.

In order to further investigate the effects of the d_{int}^{N-M} change, we compare the core levels and MT charges for the equilibrium GaN/Al interface and the step I system. Recall that these systems are exactly equal, except for the difference in the interface nitrogen-metal distance: $d_{int}^{N-M}=1.11$ Å and $d_{int}^{N-M}=1.32$ Å, for the equilibrium and step I structures, respectively. As in Fig. 4, we show in Fig. 6 the trends for the core-level binding energies [panels (a) and (b) for Ga and N atoms, respectively] and the difference between the MT charges compared to their values in the bulk compounds [panels (c) and (d) for Ga and N atoms, respectively], as a function of the atomic distance from the interface. In terms of core levels and charge transfer within the MT, a comparison with Fig. 4 shows that the step I system behaves very closely to the GaN/Ag structure but very differently from the equilibrium GaN/Al interface. Therefore, the electronic charge distribution around the interface N and Al atoms has a strong dependence on the interplanar distance and is able to reduce the SBH by as much as 0.75 eV, bringing a GaN/Al step I SBH within only 0.16 eV from the GaN/Ag SBH.

The dispersion of the SBH values seems to exclude a *Fermi-level pinning* in the GaN case, as experimentally confirmed by the large spread of values reported in the literature for the SBH between GaN and different metals. In particular, let us recall those obtained for *n*-GaN/Ag and *n*-GaN/Au: $\Phi_{B_p}^{expt}(n-\mathrm{GaN/Ag})=2.7\,\mathrm{eV}$ (Ref. 21) and $\Phi_{B_p}^{expt}(n-\mathrm{GaN/Au})\approx 2.4\,\mathrm{eV}$ (Ref. 22) and 2.2 eV.[23,24] On the other hand, recent photoemission measurements[24] performed for Au deposited on *p*-type GaN show that the Fermi level is stabilized around 1 eV above the *p*-GaN VBM, in apparent good agreement with our calculated value ($\Phi_B=1.08\,\mathrm{eV}$). The disagreement between some of these values and our calculated ones are certainly related to the different conditions of the GaN surface (which is ideal in our calculations and subject to different preparations in the experimental case); moreover, we considered the GaN zinc blende structure and [001] oriented interfaces, whereas all the experimental samples are grown on [0001] wurtzite Ga.[25]

We note finally that the spread of experimental values for GaN/metal interfaces has not been found for the GaAs/metal systems, where a Fermi-level pinning was experimentally observed.[26] This can be understood in terms of the much more efficient screening provided by GaAs with respect to GaN, as discussed above. In fact, the main difference between the noble metal and Al systems is the length of the anion-metal bond that gives rise to large variations of the interface dipole: this electrostatic contribution is poorly screened in GaN and therefore contributes considerably to the final SBH value. In addition, it has to be observed that GaAs matches better (within 2%) the Au, Ag, and Al lattice constants so that the interface strain does not play a crucial role in this case.

VI. CONCLUSIONS

We have performed FLAPW calculations for [001] ordered GaN/Ag and GaN/Au interfaces, mainly focusing on the electronic properties and comparing our results with those obtained from previous calculations for the GaN/Al interface. Our calculations show that there is an appreciable density of MIGS in the noble-metal interfaces considered (even higher than in the GaN/Al case); however, the presence of the gap states is relevant in the interface layer only, being strongly reduced already in the subinterface layer. We estimate the MIGS decay length to be $\lambda\approx 2.0$ Å, for all the metals considered (Al, Ag, and Au). The SBH values $[\Phi_{B_p}(\mathrm{GaN/Ag})=0.87\,\mathrm{eV}$ and $\Phi_{B_p}(\mathrm{GaN/Au})=1.08\,\mathrm{eV}]$ are significantly smaller than the value obtained in the GaN/Al case $[\Phi_{B_p}(\mathrm{GaN/Al})=1.51\,\mathrm{eV}]$; we demonstrated that the appreciable SBH reduction in going from the free-electron to the noble-metal case is mostly due to structural effects. In particular, the distance between the last N and the first metal layer plays a critical role in dictating the final SBH value, in contrast with that found in GaAs/Al, where previous,[18] as well as our present, calculations showed negligible effects of this same structural parameter. We found that the largest structural differences between the various GaN/M interfaces considered are related to this distance, mainly determined by the different bonding nature between N and free-electron-like or noble metals. Finally, we were able to show, at least for our perfectly ordered abrupt interfaces, that the lack of Fermi-level pinning in GaN can be understood in terms of electrostatic effects related to variations of the interface anion-metal dipole: these effects are not properly screened in GaN, so that they contribute considerably to the final potential lineup at the interface.

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