The structural, electronic, and the optical properties of (LaN)$_n$/(ScN)$_n$ and (LaN)$_n$/(YN)$_n$ superlattices are investigated using the recent version of the first principles full potential linear muffin-tin orbitals method (FP-LMTO). The resemblances between LaN, ScN, and YN and their small lattice mismatch led us to perform investigations on rocksalt/rocksalt (LaN)$_n$/(ScN)$_n$, and (LaN)$_n$/(YN)$_n$ for $n = 1$, 2, and 3 monolayers. Our calculations performed for the band structure and density of states show indirect band gap superlattices for $n = 1$, 2, and 3. Details of the electronic structure and optical properties of the superlattices are discussed.

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I. INTRODUCTION

Superlattices (SLs) are structures that are produced by different growth methods by depositing alternately and periodically two bulk semiconductors, one that acts as a quantum well of width $L_w$ and the other acting as a quantum barrier of width $L_b$. The superlattice is thus a periodic structure with period $d = L_w + L_b$. The direction in which this deposition is made is called the growth axis. The artificial periodicity created in superlattices can lead to the tailoring of certain material properties for applications in fields such as optoelectronics [1, 2]. Since their invention superlattices quickly showed interesting qualities, such as the negative differential resistance and the quantum well laser with higher profits than a solid double heterojunction laser. Note also that the properties of superlattices change depending on whether their growth has been in one direction or another, although the bulk semiconductors have not changed. For example, The GaAs/AlGaAs superlattices display more interesting optical when the growth axis is taken in the [111] direction rather than in the [100] direction.
II. COMPUTATIONAL DETAILS

The calculations presented in this work were carried out using the full potential linear muffin-tin orbital method (FPLMTO) in which the non-overlapping muffin-tin spheres potential is Fourier transformed in the interstitial regions, and hence it treats the interstitial regions on the same footing with the core regions [3]. The exchange correlation energy of the electrons is described in both the local density approximation (LDA) [4, 5] and using the parameterisation of Perdew et al. [6, 7]. FPLMTO has been carried out using the Lmtart [3, 8] code. In the FPLMTO, the non-overlapping muffin-tin spheres MTS potential is expanded in spherical harmonics inside the spheres of radius RMTS. In the interstitial region, the s, p, and d basis functions are expanded in a number (NPLW) of plane waves determined automatically by the cut-off energies. The details of the calculations are as follows: the charge density and the potential are represented inside the muffin-tin (MT) spheres by spherical harmonics up to \( l_{\text{max}} = 6 \). The self-consistent calculations are considered to be converged when the total energy of the system is stable within \( 10^{-4} \text{ Ry} \). Accurate Brillouin integrations zone are performed using the tetrahedron method [9]. The corresponding integrating points over the irreducible BZ are 20 k-points for SLs(1,1), 30 k-points for SLs(2,2), and 56 k-points for SLs(3,3). In order to achieve energy eigenvalue convergence, the wave functions are expanded in plane waves up to 133.42 and 129.71 Ry for \((\text{LaN})_1/(\text{ScN})_1\) and \((\text{LaN})_1/(\text{YN})_1\), respectively, up to 134.49 and 127.43 Ry for \((\text{LaN})_2/(\text{ScN})_2\) and \((\text{LaN})_2/(\text{YN})_2\), respectively, and up to 133.79 and 131.88 Ry for \((\text{LaN})_3/(\text{ScN})_3\) and \((\text{LaN})_3/(\text{YN})_3\), respectively. The number of the planes waves is 10136, 20314, and 30548 for SLs(1,1), SLs(2,2), and SLs(3,3), respectively. To avoid the overlap of atomic spheres the MT radius for each atomic position is taken to be different for each case.

III. RESULTS

III-1. Structural Properties of SLs \((\text{LaN})_n/(\text{ScN})_n\) and \((\text{LaN})_n/(\text{YN})_n\)

The investigated structures consist of ideal quantum well superlattices SL\((n, n)\) made of a periodical sequence of \(n\) monolayers of LaN atoms and \(n\) other monolayers of YN or ScN atoms (a monolayer contains two atoms, one anion and one cation). These SLs have tetragonal symmetry. In Figure 1, we show an example of a direct lattice of a [001] growth axis SL\((1,1)\). The link between the bulk and the SL direct lattices is clear in the figure in which aSL and a0 represent the SL and the binary lattice constants, respectively. Fig. 2 represents the reciprocal lattice of the [001] growth axis SL\((n, n)\), and the high symmetry points are also shown. For the SLs \((\text{LaN})_n/(\text{YN})_n\) calculation, we have supposed the lattice constant to be the mean value of that of LaN (5.182 Å) [10] and YN (4.8448 Å) [11], and we have made the same approximation for SLs \((\text{LaN})_n/(\text{ScN})_n\), for which we have considered the equilibrium lattice constant of ScN (4.877 Å) [12]. In order to calculate the ground state properties of SL\((n, n)\), the total energies are calculated for superlattices for different volumes around the equilibrium volume \(V_0\). The calculated total energies are then fitted to
the Birch-Murnaghan equation of state [13] to determine the ground state properties. The calculated equilibrium parameters \((a, B, \text{ and } B')\) in the superlattices are given in Table I.

FIG. 1: The direct lattice of a [001] growth axis SL(1,1). Its delimitations are shown with bold gray lines. Each monolayer is represented with spherical atoms of a different color (white and black).

We found that \(a_{1,1}, a_{2,2}\) and \(a_{3,3}\) are very close, the difference not exceeding 0.01 Å for \((\La\Na)n/(\Sc\Na)n\) and 0.04 Å for \((\La\Na)n/(\Y\Na)n\). From Table I, one can remark that the bulk modulus increases with the enhancement of the number of the monolayers \(n\) for \((\La\Na)n/(\Y\Na)n\), indicating that SL\(_{3,3}\) is harder than SL\(_{2,2}\) and SL\(_{1,1}\). For \((\La\Na)n/(\Sc\Na)n\), the bulk modulus decreases with the enhancement of the number of monolayers \(n\), indicating that SL\(_{1,1}\) is harder than SL\(_{2,2}\) and SL\(_{3,3}\).
TABLE I: Calculated lattice parameter $a$, the bulk modulus $B$ and its pressure derivative $B'$ for the superlattices $(\text{LaN})_n/(\text{ScN})_n$ and $(\text{LaN})_n/(\text{YN})_n$ ($n$, the number of monolayers: $n = 1, 2, \text{ and } 3$).

<table>
<thead>
<tr>
<th></th>
<th>$a$ (Å)</th>
<th>$B$ (GPa)</th>
<th>$B'$</th>
</tr>
</thead>
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<tr>
<td>$(\text{LaN})_1/(\text{YN})_1$</td>
<td>3.50</td>
<td>124.523</td>
<td>4.80</td>
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<tr>
<td>$(\text{LaN})_2/(\text{YN})_2$</td>
<td>3.54</td>
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<td>1.67</td>
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<tr>
<td>$(\text{LaN})_3/(\text{YN})_3$</td>
<td>3.51</td>
<td>236.536</td>
<td>3.84</td>
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<tr>
<td>$(\text{LaN})_1/(\text{ScN})_1$</td>
<td>3.46</td>
<td>195.496</td>
<td>3.79</td>
</tr>
<tr>
<td>$(\text{LaN})_2/(\text{ScN})_2$</td>
<td>3.45</td>
<td>179.756</td>
<td>4.30</td>
</tr>
<tr>
<td>$(\text{LaN})_3/(\text{ScN})_3$</td>
<td>3.46</td>
<td>171.2244</td>
<td>3.69</td>
</tr>
</tbody>
</table>

III-2. Electronic Properties of SLs $(\text{LaN})_n/(\text{ScN})_n$ and $(\text{LaN})_n/(\text{YN})_n$

In the present work, we have calculated the band structures for $(\text{LaN})_n/(\text{ScN})_n$ and $(\text{LaN})_n/(\text{YN})_n$ superlattices ($n = 1, 2, \text{ and } 3$) at their respective equilibrium volumes, with the binaries crystallizing in the rocksalt structure (Figure 3). All SLs were found to display negative indirect gaps: $-0.51$ eV for $(\text{LaN})_1/(\text{ScN})_1$ with the top of the valence band (VB) at A and the bottom of the conduction band (CB) lying between Γ and Z, $-0.86$ eV for $(\text{LaN})_2/(\text{ScN})_2$ with the top of the VB at A and the bottom of the CB at Z, $-0.74$ eV for $(\text{LaN})_3/(\text{ScN})_3$ with the top of the VB lying between A and Z and the bottom of the CB lying between Z and R, $-0.4$ eV for $(\text{LaN})_1/(\text{YN})_1$ with the top of the VB at A and the bottom of the CB lying between Γ and Z, $-0.64$ eV for $(\text{LaN})_2/(\text{YN})_2$ with the top of the VB at A and the bottom of the CB lying between Γ and Z, and $-0.67$ eV for $(\text{LaN})_3/(\text{YN})_3$ with the top of the VB lying between A and Z and the bottom of the CB at Z. We remark that the top of the VB is always at A while the bottom of the CB is always located in a direction including Z. Speaking in terms of zone folding, this is probably due to the fact that the top of the VB is derived from LaN bands, while the bottom of the CB is expected to be derived from the YN and ScN bands. It is well known that the LDA underestimates the gaps. The problems of self-interaction and of the discontinuity of the exchange correlation potential limit its ability to predict the gaps of semiconductors and insulators correctly. On the other hand, and since the obtained mixing between conduction and valence bands of our SLs is not severe and the negative gaps are not very important, we think that there is a reasonable possibility for these SLs to be semiconductors.

The calculated total and partial densities of states (DOS) of these superlattices (Figures 4, 5) show a resemblance with some difference in details for each system, $(\text{LaN})_n/(\text{ScN})_n$ or $(\text{LaN})_n/(\text{YN})_n$. One can see that the contribution of different orbitals is proportional to the number of monolayers of the two constituents of the superlattice. For the $(\text{LaN})_n/(\text{ScN})_n$, the valence band consists entirely of N-2p states with a few contribution of the Sc-4p states. The conduction band is essentially dominated by La-4f states with a admixture of Sc-4p, N-2p, and La-5d states. For the $(\text{LaN})_n/(\text{YN})_n$, the valence band is formed by a mixture of N-2p states and Y-4d states in the low region, while the
FIG. 3: The band structure of $(\text{LaN})_n/(\text{ScN})_n$ (a, b, and c) and $(\text{LaN})_n/(\text{YN})_n$ (d, e, and f) superlattices ($n = 1, 2, \text{ and } 3$) calculated within the FPLMTO+LDA in the rocksalt (B1) phase.

The conduction band is mainly due to the La-4f states mixed with Y-4d and La-5d states. These contributions are formed by hybridization of the s, p, d, and f states of the four atoms.

III-3. Optical Properties of SLs $(\text{LaN})_n/(\text{ScN})_n$ and $(\text{LaN})_n/(\text{YN})_n$

The frequency dependent complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is known to describe the linear response of a system to an external electromagnetic field. Two kinds of contributions to $\varepsilon(\omega)$ are usually distinguished, namely intraband and inter-band
FIG. 4: Total density of states (DOS) and partial DOS of $(\text{LaN})_n/(\text{ScN})_n$ ($n = 1, 2, \text{ and } 3$).
FIG. 5: Total density of states (DOS) and partial DOS of (LaN)$_n$/(YN)$_n$ ($n = 1, 2, \text{ and } 3$).
electronic excitations. Intraband transitions are not present in semiconductors, as they are important only for metals and semimetals. The dispersion of the imaginary part of the dielectric function $\varepsilon_2(\omega)$ can be calculated from the momentum matrix elements between the occupied and unoccupied wave functions, giving rise to the selection rules. The real part $\varepsilon_1(\omega)$ of the dielectric function can be evaluated from the imaginary part $\varepsilon_2(\omega)$ by the Kramers-Kronig relationship. A full detailed description of the calculation of the optical properties is given by Ambrosch-Draxl and Sofo [14]. As shown in Figure 6, we can see that for $\varepsilon_1(\omega)$ the spectrum does not vary greatly from SL(1,1), SL(2,2), to SL(3,3). This is attributed to the fact that the conduction band features and the symmetries of the wave
functions, which dictate the selection rules and are fully reflected in the matrix moment
elements, are somewhat similar. One can also remark that the spectra are shifted towards
higher energies in going from SL(1,1) to SL(3,3). This is a consequence to the increase of
the indirect band gaps.

IV. CONCLUSION

In this paper, we have studied the structural, electronic and optical properties of
(LaN)$_n$/(ScN)$_n$ and (LaN)$_n$/(YN)$_n$ Superlattices ($n = 1, 2, and 3$), by employing the FP-
LMTO method with the LDA approximation. The main conclusion for our results are as
follows:

1. We found that $a_{1,1}$, $a_{2,2}$, and $a_{3,3}$ are very close, the difference not exceeding 0.01 Å
   for (LaN)$_n$/(ScN)$_n$ and 0.04 Å for (LaN)$_n$/(YN)$_n$.

2. All SLs were found to display negative indirect gaps; we think that there is a reasonable
   possibility for these SLs to be semiconductors.

3. Alternating atomic layers of bulk LaN, ScN, and YN semiconductors significantly
decreases the static dielectric constants.

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