Materials Science in Semiconductor Processing 19 (2014) 179–185

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

Structural stability, elastic and electronic properties of zincblende $(GaN)_1/(ZnO)_1$ superlattice: Modified Becke–Johnson exchange potential

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ARTICLE INFO

Available online 9 January 2014

Keywords:
Ab initio
FP-LAPW
LCPAO
MBJ-(LDA,GGA)
GaN/ZnO superlattice
Structural stability
Electronic structure
Effective mass

ABSTRACT

The structural stability, elastic and electronic properties of hypothetical zincblende $(GaN)_1/(ZnO)_1$ superlattice structure have been investigated using two different theoretical techniques: the full potential-linearized augmented plane wave method and the linear combination of localized pseudo-atomic orbital. The new modified Becke–Johnson exchange potential is chosen to improve the bandgap and the effective masses of the studied superlattice. The bandgap is found to be slightly indirect and reduced than those of pure GaN and ZnO. The origin of this reduction is attributed to the *p–d* repulsion of the Zn–N interface and the presence of the O *p* electron. The electron effective mass is found to be isotropic.

1. Introduction

The $(GaN)_1/(ZnO)_1$ superlattice is an ordered form of a pseudobinary semiconductor alloy discovered in these last few years [1,2]. This later represents a new class of alloys typed as III–V/II–VI, strongly different from classical isovalent semiconductor alloys (i.e., III–V/III–V, II–VI/II–VI). From technological aspect, the growth of ZnO on GaN heterostructure was realized using the vapor cooling condensation system, thus the related heterojunctions light-emitting diodes LEDs are fabricated [3]. An other important technological application is the hydrogen generation from water photosplitting through the photoelectrochemical cell (PEC). In fact, under visible light, the GaNZnO alloy has a much higher water splitting efficiency compared to other oxides [4]. The spectacular feature of this characteristic is attributed partly to the lower bandgap of this alloy and in particular of its heterostructure form compared to its parent elements (GaN and ZnO). Few theoretical and experimental studies, estimating the optical bowing parameter, have been reported [5–7]. Large difference in the estimated values was then observed. The recent calculation of Wang and Wang [7] shows that the ordering plays an important role in the reduction of the bowing parameter.

On the other hand, there has been a particular interest in this decade in the growth and characterization of GaN and ZnO in the metastable zincblende (ZB) structure [8,9] using molecular beam epitaxy. The zincblende phase is obtained now with high quality [9]. The motivation for this interest is that the zincblende phase may solve the challenge of controlling p-type conductivity in the optoelectronic devices [8]. Despite that the superlattice formed between GaN and ZnO exists actually only in the wurtzite structure (W), and the growth of the superlattice in the zincblende structure is not a simple task, nevertheless, it would be an interesting choice for research purposes. In this light, we are motivated by a predictive study of this $(GaN)_1/(ZnO)_1$ superlattice in this structural phase. Indeed, the lattice constants of GaN and ZnO are nearly identical and therefore, from theoretical point of view, there is a

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http://dx.doi.org/10.1016/j.mssp.2013.12.022

possibility to have a growth of this superlattice in the zincblende structure. It is necessary then, in the beginning of the study, to verify if this phase can be stable or not. Thus, we examined the mechanical stability via the elastic constants and investigated the comparison with the stable wurtzite structure taken as reference. Regarding the electronic properties from theoretical framework, the problem of the underestimation of the bandgap using the local density and the generalized gradient approximations (LDA and GGA) of the density functional theory (DFT) is, in particular, very remarkable for ZnO. Recent works have predicted the values of 0.710 eV [10] for ZnO and 1.811 eV [11] for GaN, which are lowered than the experimental ones by 78% and 45% respectively. Consequently, this error affects considerably the value of the large bandgap discontinuity at the heterointerface for $(GaN)_1/(ZnO)_1$ layered structure. In order to overcome this problem and improve the bandgap of the superlattice we used the most recent proposed approximation called modified Becke–Johnson (mBJ) exchange potential [12]. This technique is capable to describe with high accuracy the electronic structure of semiconductors and insulators giving rise to a significantly improved bandgap values to be much closer to the experimental ones. Because of the lack of data for structural and electronic properties of the studied superlattice, we used two different ab initio techniques FP-LAPW and LCPAO in order to help understanding the related properties and consolidate our results.

The present investigations are organized as follows. In Section 2, we describe the computational methods used in this work. Theoretical results are compared and discussed in Section 3. Section 4 presents a summary of our results and conclusions.

2. Computational details

The simulation of the $(GaN)_1/(ZnO)_1$ structure in the (001) direction is achieved with $1 \times 1 \times 1$ zincblende supercell containing 8 atoms (Fig. 1(a)), while the $1 \times 1 \times 2$ wurtzite structure of the superlattice is modeled for two possible configurations $(GaN)_n/(ZnO)_n$ ($n=1,2$) (Fig. 1(b), (c)) in order to achieve more stability between them. The calculation of structural and electronic properties was performed using both full potential-linearized augmented plane wave (FP-LAPW) and linear combination of localized pseudo-atomic orbital (LCPAO) methods, based on the density functional theory (DFT) [13,14]. Although the LAPW method with mBJ is sufficient and gives accurate values, the use of another method such as LCPAO to solve the Kohn–Sham equations is beneficial in order to better understand the predicted values according to different chosen approximations. The description of the specific parameters corresponding to each technique is given as follows.

2.1. FP-LAPW

We used the full-potential linear augmented plane-wave method (FP-LAPW) implemented in the Wien2k code [15] which self-consistently finds the eigenvalues and eigenfunctions of the Kohn–Sham equations for the system [13,14]. We used both the Generalized Gradient Approximation (GGA) as parameterized by Perdew et al. [16], which includes the second order gradient components, and the Local Density Approximation (LDA) coupled with the modified Becke–Johnson exchange potential (mBJ). The core states of Ga, N, Zn and O atoms are self-consistently treated and relativistically relaxed in a spherical approximation, whereas the valence states are treated self-consistently within the semi-relativistic approximation (spin–orbit coupling excluded). The valence electron configurations used in the calculations are Ga ($3d^{10}4s^24p^1$), N ($2s^22p^3$), Zn ($3d^{10}4s^2$) and O ($2s^22p^4$). The wave function, charge density and potential are expanded by spherical harmonic functions inside non-overlapping spheres surrounding the atomic sites (muffin-tin spheres) and by a

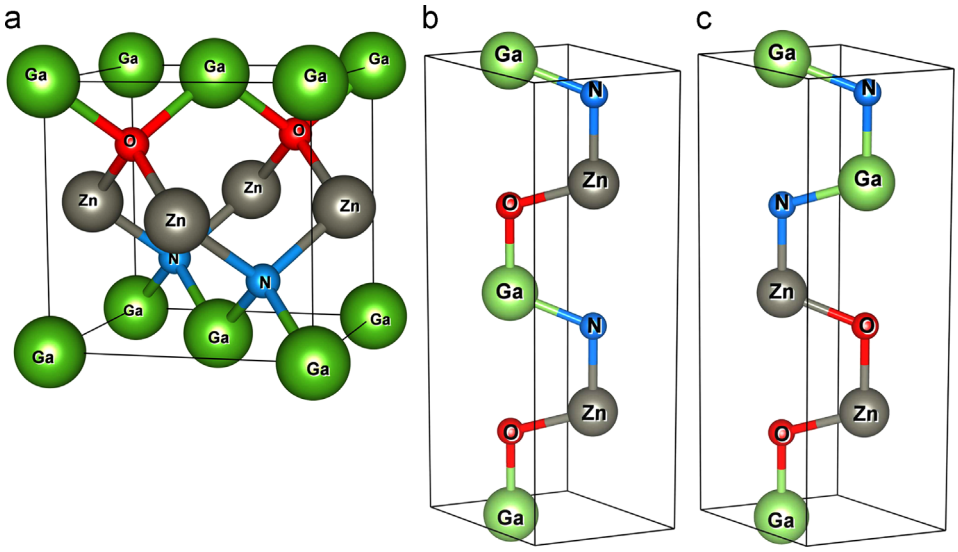

Fig. 1. Unit supercells of (a) $1 \times 1 \times 1$ zincblende $(GaN)_1/(ZnO)_1$, (b) $1 \times 1 \times 2$ wurtzite $(GaN)_1/(ZnO)_1$ and (c) $1 \times 1 \times 2$ wurtzite $(GaN)_2/(ZnO)_2$.