Diamond & Related Materials 31 (2013) 25–29

Contents lists available at SciVerse ScienceDirect

Diamond & Related Materials

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

First principle study of valence-band offsets at AlN/diamond heterojunctions☆☆

Leonardo Silvestri [a,]*, Jiri Cervenka [b], Steven Prawer [b], François Ladouceur [a]

[a] School of Electrical Engineering and Telecommunications, UNSW, Sydney, Australia
[b] School of Physics, The University of Melbourne, VIC, Australia

ARTICLE INFO

Article history:
Received 6 September 2012
Received in revised form 19 October 2012
Accepted 26 October 2012
Available online 2 November 2012

Keywords:
Diamond
Aluminium nitride
Heterojunction
Band alignment

ABSTRACT

We present a first principle study of the band alignment at AlN/diamond heterojunctions. We consider AlN (0001) and diamond with (100) and (111) orientations, assuming that the first AlN layer at the interface is made of N atoms. Our results show that the average valence-band offset is about 1.6 eV, corresponding to a staggered (type II) band alignment. We also find a weak dependence of the valence-band offset on strain and on the diamond orientation.

Crown Copyright © 2012 Published by Elsevier B.V. All rights reserved.

1. Introduction

Wurtzite aluminium nitride (*w*-AlN) has the widest direct bandgap among the group-III nitrides (about 6.2 eV [1]) and is currently being investigated for use in many electronic and optoelectronic devices, including UV detectors [2] and emitters [3]. It is also well established that *Si* doping of AlN produces *n*-type conductivity at room temperature, while it is very difficult to achieve *p*-type doping in this semiconductor. Diamond, in addition to its excellent thermal and optical properties, possesses a wide indirect bandgap of about 5.5 eV [4] and it can be efficiently *p*-doped with boron. For these reasons, heterojunctions between diamond and *w*-AlN show the potential to be used in UV emitting devices, high power/high frequency devices or as heat sinks in overheating electronic devices. Light emitting diodes [5,6] and field effect transistors [7] based on AlN/diamond heterojunctions have already been demonstrated. These devices have been fabricated by growing AlN layers on single crystal diamond substrates. More recently, polycrystalline diamond films have been grown by microwave-assisted chemical vapour deposition on single crystal AlN thin films. These thin film diamond/AlN heterojunctions have shown very efficient heat dissipation in the layers [8]. Despite the recent progress in fabrication of AlN/diamond heterojunctions, the understanding of their electronic structure is still lacking and has not been well explored. In particular, one of the most important parameters of heterojunctions, energy band offset, has not been established yet. To our knowledge a single measurement of the AlN/diamond band alignment has been reported [6] and most of the theoretical predictions rely on electron affinity-based arguments. These arguments give useful indications, however it is well known that the value of the electron affinity of a material strongly depends on the details of its surface, which is strongly affected by the presence of an interface. This is especially true for AlN (0001)/diamond interfaces, which are polar heterovalent heterojunctions that are in general expected to give rise to different band alignments depending on the relative orientation and strain.

In this work, we present the results of density functional theory (DFT) simulations of the electronic properties of *w*-AlN/diamond heterojunctions. In particular we have computed the valence band offset (VBO) for the (100) and (111) diamond and (0001) AlN heterojunctions, assuming that the first layer of AlN at the interface is made of nitrogen atoms. Although these structures resulted in various interface geometries and strains, our calculations showed that this has minor effect on the electronic valence offset. All our results predict a staggered (type II) band alignment at AlN/diamond interfaces.

2. Method

Valence-band offsets have been calculated by means of ab-initio DFT calculations using the macroscopic averaging technique as described in Ref. [9] for lattice-mismatched heterojunctions. The valence-band offset ΔE_{VBO} can be written as the sum of two terms as

$$E_v^{\text{diamond}} - E_v^{\text{AlN}} \equiv \Delta E_{VBO} = \Delta E_v + \Delta V, \quad (1)$$

where E_v indicates the energy of the valence-band maximum, ΔE_v is the band structure term and ΔV is the lineup term. ΔE_v is the difference

---

☆☆ Originally presented at the International Conference of Diamond and Carbon Materials.

* Corresponding author.
E-mail address: l.silvestri@unsw.edu.au (L. Silvestri).

0925-9635/$ – see front matter. Crown Copyright © 2012 Published by Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.diamond.2012.10.010

between the two band edges when the single-particle eigenvalues are referred to the corresponding average electrostatic potential in the bulk. In order to calculate this term we performed a self consistent field calculation for each bulk material taking into account the strain present in the particular heterojunction considered. ΔV is the lineup of the electrostatic potential generated by the electronic pseudocharge distribution and by the charge of the bare ion cores. In order to evaluate this term we performed supercell calculations using a slab geometry, as described below. After convergence of the supercell self consistent field calculations is achieved, we calculate the planar average, $\bar{V}(z)$, of the electrostatic potential $V(x,y,z)$ over planes parallel to the interface as a function of the distance perpendicular to the interface z. Finally, we define the double macroscopic average

$$\bar{\bar{V}}(z) = \int dz' \int dz'' w_{l_1}(z-z') w_{l_2}(z-z'') \bar{V}(z''), \tag{2}$$

where

$$w_l = \frac{1}{l}\Theta(l/2-|z|) \tag{3}$$

and $\Theta(z)$ is the unit-step function. The values of l_1 and l_2 correspond to the (strained) lattice constants of diamond and AlN along z, respectively.

Ab-initio simulations have been performed with the open source QUANTUM ESPRESSO package [10] using the Perdew–Burke–Ernzerhof (PBE) functional [11], ultrasoft pseudopotentials and a plane wave energy cutoff of 408 eV. All the supercells contained a single heterojunction consisting of two adjacent slabs of AlN and diamond, respectively, separated by 1.4 Å of vacuum. The supercell size in the direction orthogonal to the interface has been chosen such that the width of the vacuum between periodically repeated structures was about 15 Å. All the diamond slabs we used contained at least 12 carbon layers, while the AlN slabs had least 4 bilayers. These slabs are thick enough to recover the bulk behaviour far from the interface. The relaxed AlN lattice parameters have been set to the PBE optimised values, $a=3.118$ Å, $c=5.008$ Å, and $u=0.3812$, which in turn give a band gap of 4.09 eV. [12] The PBE optimised lattice constant used for the relaxed diamond substrate is $a=3.574$ Å and the corresponding band gap is 4.11 eV. Up to a 4×2×1 Monkhorst–Pack [13] mesh has been used for Brillouin zone sampling depending on the supercell size. Dangling bonds of Al and N surface atoms have been saturated with fractional charge hydrogen atoms. Carbon atoms at the (111) surface have been saturated with hydrogen, while the (100) surface has been left clean, because no realistic surface reconstruction was practical enough to be used in our supercell simulations.

In constructing the supercell we assume that the substrate is unaffected by the presence of the overlayer, and we match a multiple of the in-plane lattice constant of the overlayer to a multiple of the in-plane lattice constant of the unstrained substrate. This kind of arrangement is a consequence of the large lattice mismatch between AlN and diamond, and it introduces misfit dislocations at the interface, which are necessarily formed in order to release part of the in-plane elastic stress. The same interface geometry has been observed experimentally when AlN layers have been grown on single crystal diamond substrates [14]. The residual in-plane strain in the overlayer gives rise to some residual stress that in our simulations has been released by including a strain with opposite sign in the direction perpendicular to the interface. In our simulations we calculated the overlayer lattice constant along z by means of the linear elasticity theory using literature values for the diamond [15] and AlN [16] elastic constants.

We conclude this section with some remarks about the general validity of the approach we followed. Band lineups are a ground state property, since they only depend on the charge density at the heterojunction, therefore the use of the PBE functional gives reliable results [17]. The PBE functional, on the other hand, is known to underestimate semiconductor band gaps and produce inaccurate alignment of the bands with the macroscopic average potential in the bulk. Our calculations predict a band gap of about 4.1 eV for both diamond and AlN, to be compared with the experimental values of 5.5 and 6.2 eV, respectively. We note, however, that in the present work we are only considering valence-band offsets and the bandgap value is never used. As for the alignment of the valence-band edge with the macroscopic average potential in the individual materials, we can estimate the absolute error on the VBOs due to the use of PBE functional to be of the order of 0.1 eV. As an example, Wadhera et al. found HSE and PBE valence-band offsets for AlGaAs/GaAs heterojunctions to be within 0.05 eV [18] and Moses et al. found VBOs between AlN and GaN to differ by 0.15 eV [19].

3. Results and discussion

In this section we consider in detail four AlN/diamond heterojunctions (C indicates diamond):

H1. 4 bilayers of AlN (0001) grown on 12 layers of C (100), with in-plane orientation relationship $[10\bar{1}0]_{\mathrm{AlN}} \| [011]_{\mathrm{C}}$ and lattice matching as in Fig. 1(a).

H2. 12 layers of C (100) grown on 4 bilayers of AlN $(000\bar{1})$ with $[10\bar{1}0]_{\mathrm{AlN}} \| [011]_{\mathrm{C}}$ and lattice matching as in Fig. 1(a).

H3. 4 bilayers of AlN (0001) grown on 12 layers of C (111) with $[10\bar{1}0]_{\mathrm{AlN}} \| [1\bar{1}0]_{\mathrm{C}}$ and lattice matching as in Fig. 1(b).

H4. 8 bilayers of AlN (0001) grown on 12 layers of C (111) with $[10\bar{1}0]_{\mathrm{AlN}} \| [1\bar{1}0]_{\mathrm{C}}$ and lattice matching as in Fig. 1(c).

As already mentioned, in our calculations we keep the substrate lattice fixed in its relaxed geometry, while atoms in the overlayer are matched to the substrate. The strain imposed on the overlayer for each heterojunction is reported in Table 1. The in-plane strain is due to the lattice matching conditions shown in Fig. 1, while the strain perpendicular to the interface has been calculated with the linear elasticity theory, as discussed in the previous section. We note that in all

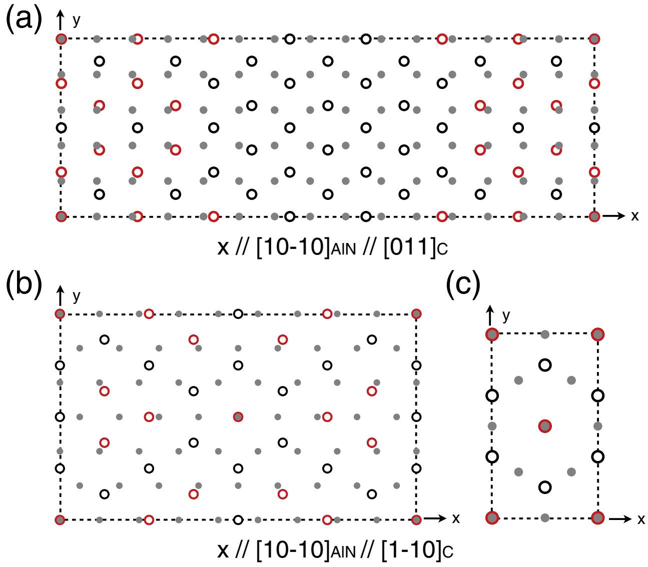

Fig. 1. Top view of the supercells used in the simulations of heterojunctions H1 and H2 (a), H3 (b) and H4 (c), as described in the text. Grey discs and empty circles represent the carbon and nitrogen atomic layers closest to the interface, respectively. Red and black empty circles are used to indicate N atoms bonded to C and N atoms with dangling bonds, respectively. Dashed lines show the in-plane unit cell.

Download English Version:

https://daneshyari.com/en/article/701839

Download Persian Version:

https://daneshyari.com/article/701839

Daneshyari.com