



Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlatticesExploring global phase stability of $(\text{VN})_1/(\text{InN})_1$ and $(\text{CrN})_1/(\text{GaN})_1$ superlattices from density-functional theoryN. Belmiloud^a, A. Zaoui^{b,*}, D. Madouri^c, M. Ferhat^a^a Département de Génie Physique, (LPMF), Faculté des Sciences, Université des Sciences et de la Technologie d'Oran, Mohamed Boudiaf (USTO), Oran, Algeria^b LCGE, Polytech'Lille, Université Lille 1 Sciences et Technologies, Cité Scientifique, Avenue Paul Langevin, 59655 Villeneuve D'Ascq Cedex, France^c Département de Physique, Université d'Oran Es-Senia, Oran, Algeria

ARTICLE INFO

Article history:

Received 8 October 2016

Accepted 12 October 2016

Available online xxx

Keywords:

DFT

 $(\text{VN})_1/(\text{InN})_1$ $(\text{CrN})_1/(\text{GaN})_1$

Magnetism

ABSTRACT

The quest for design half-metallic ferromagnets superlattice (HMFS) materials has captivated marked attention due to their potential applications in spin-based electronics. Unfortunately, the HMFS proposal still questionable if the stability of such compound is not satisfied. Herein, the importance of the global phase stability of half-metallic ferromagnets $(\text{VN})_1/(\text{InN})_1$ and $(\text{CrN})_1/(\text{GaN})_1$ superlattices is explored via *ab-initio* pseudopotential density-functional theory. We find that (i) the computed negative values of the formation enthalpy indicate that these superlattices are at least metastable. (ii) The calculated elastic constants and phonon dispersion curves evince the respective mechanical and dynamical stability of $(\text{VN})_1/(\text{InN})_1$ and $(\text{CrN})_1/(\text{GaN})_1$ superlattices. (iii) For moderate temperature ($T > 400\text{--}450\text{ K}$), the positive vibrational entropy and negative free energy of vibration enhances thermodynamic stability of $(\text{VN})_1/(\text{InN})_1$ and $(\text{CrN})_1/(\text{GaN})_1$ superlattices. Our general global phase stability for the specific superlattices investigated evidence credible experimental feasibilities.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

Recently the world witnessed a revolution called spintronics which manipulate the charge and the spin freedom of electrons as information carriers [1,2]. The spin-based electronics has given unexpected opportunities to design potential materials for electronic-spin devices applications, beyond conventional semiconductors compounds. The synthesis of heterostructures and multilayers systems with atomic-scale precision has unveiled new perspectives for inquiring uncommon phenomena such as the giant magnetic resistance (GMR) effects. In the original historical experiments leading to the discovery of the GMR, one group, led by P. Grünberg used a trilayer system Fe/Cr/Fe, while the other group, led by A. Fert used multilayers of the form $(\text{Fe/Cr})(001)$.

Other example of marked relevance are the half-metallic ferromagnets (HMF), i.e., materials evidencing metallic character for one spin channel, while the other spin direction has a gap at Fermi level. Since the first predicted HMF by de Groot et al. [3] in 1983 based on first-principles calculations for Heusler alloys, many further systems such magnetic multi layers and

* Corresponding author.

E-mail address: azaoui@polytech-lille.fr (A. Zaoui).

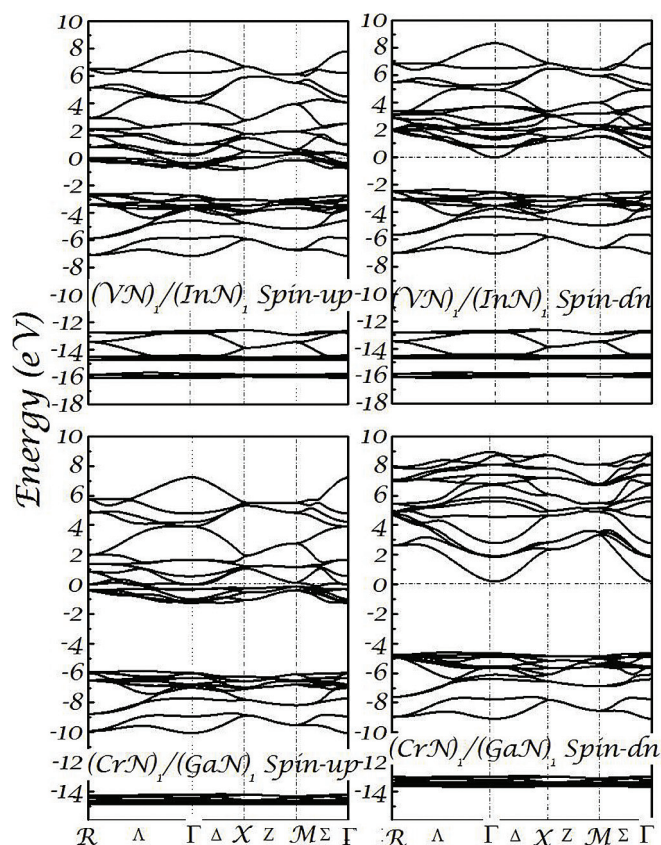


Fig. 1. Band structure of majority-spin, minority-spin of $(\text{VN})_1/(\text{InN})_1$ and majority-spin, minority-spin of $(\text{CrN})_1/(\text{GaN})_1$ superlattices. Fermi-level is set to zero.

superlattice have been found to be half-metallic ferromagnets, such as $(\text{CrP})_1/(\text{GaP})_1$ [4], $(\text{ZnO})_1/(\text{CuO})_1$ [5], CaN/InN , and SrN/GaP [6], $\text{SnO}_2/\text{CrO}_2$ [7], $(\text{MnSb})/(\text{GaSb})$ [8], $(\text{CrN})_1/(\text{GaN})_1$ and $(\text{VN})_1/(\text{InN})_1$ [9], $(\text{MnN})_1/(\text{XN})_1$ ($\text{X} = \text{Al}, \text{Ga}, \text{In}$) [10], $(\text{LaMnO}_3)_2/(\text{SrTiO}_3)_8$ [11], and $(\text{MX})_1/(\text{YX})_1$ ($\text{M} = \text{Sr}$ or Ba , $\text{X} = \text{N}, \text{P}$, or As , and $\text{Y} = \text{Al}, \text{Ga}$, or In) [12].

Unfortunately, for practical applications, these predicted HFM superlattices haven't been synthesized. Moreover, the prediction of technological useful properties of these HFM superlattices is widely irrelevant if the proposed hypothetical half-metallic ferromagnets materials are unstable. To our knowledge, the global phase stability (via thermodynamic, elastic, and dynamic calculations) of such of compounds has not been addressed. In this work using first-principles DFT calculations, we address this issue by examining the global stability of prototypical HFM superlattices $(\text{VN})_1/(\text{InN})_1$ (001) and $(\text{CrN})_1/(\text{GaN})_1$ (001), where we systematically probe their elastic, dynamic and thermodynamic stabilities.

2. Method and results

The total-energy calculations were carried out with the Quantum ESPRESSO Package [13] in the framework of density functional theory (DFT) within the Perdew-Burke-Ernzerhof version of the generalized gradient approximation (GGA) [14], using a plane-wave ultrasoft Vanderbilt pseudopotentials [15]. A plane-wave kinetic energy cutoff of 70 Ry was employed, and an energy cut-off of 400 Ry was included for the charge density. A Gaussian smearing of 0.02 Ry has been applied. Monkhorst-Pack [MP] k -points mesh [16] with resolution better than $2\pi \times 0.035 \text{ \AA}^{-1}$ were used. The phonon properties are calculated using the density functional perturbation theory (DFPT). A $4 \times 4 \times 4$ q -points MP mesh resulting in 18 dynamical matrices has been used to perform inverse Fourier transformation. To simulate the $(\text{VN})_1/(\text{InN})_1$ and $(\text{CrN})_1/(\text{GaN})_1$ in the (001) direction, cubic supercells containing 8 atoms are employed. The internal atomic positions were fully relaxed until the maximum force on a single atom becomes less than $1 \text{ meV/\AA}$. The total energy was converged to within 1 meV/cell . Finally we consider only the ferromagnetism case.

The spin-polarized band structures of $(\text{VN})_1/(\text{InN})_1$ and of $(\text{CrN})_1/(\text{GaN})_1$ superlattices are presented in Fig. 1. As found previously for both materials [9], the majority-spin channel show metallic character, whereas, the minority-spin bands are semiconducting. Further the calculated total magnetic moments are $4\mu_B$ for $(\text{VN})_1/(\text{InN})_1$ and $6\mu_B$ for $(\text{CrN})_1/(\text{GaN})_1$ superlattices. Accordingly, these two systems are HM ferromagnets.

Download English Version:

<https://daneshyari.com/en/article/7941699>

Download Persian Version:

<https://daneshyari.com/article/7941699>

[Daneshyari.com](https://daneshyari.com)