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Table of Contents: Volume 11 Number 1, 16 January, 2016

ARTICLES

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Full Length Research Paper

Similarities between basic mechanisms of cosmic and biologic systems

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Similarities in the birth and development of cosmic and biologic systems provide unexpected proof for the major theories of formation of the universe - the Big Bang and the String theories. They include similarities in the theory of their formation, one unit origin, preexisting states, conception, fertilization, gestation, information, basic units, flatness, fluctuations, smoothness, lumpiness, reproductive and excretive organs, differentiation, composition, organization, function, expansion and homeostasis. Based on these similarities, alternative suggestions are proposed to explain various past and present cosmic events and phenomena, and to predict the future of the universe. The relevance of these predictions could be far reaching, and could revolutionize major concepts in cosmology.

Key words: Cosmology, universe, big bang, string theory, biology, hypothesis, similarities, birth, evolution, fate, predictions.

INTRODUCTION

The big bang theory for the birth and development of the universe seems to be a very close variant of the Darwinian theory of evolution of the biological systems. It suggests that due to physical/chemical environmental conditions, out of a quark soup, evolved elements, molecules, stars, galaxies, clusters, super- clusters, and finally a whole new universe. It resembles the Darwinian theory of evolution, that suggests that due to physical/chemical evolution in a liquid phase, there is evolution from inorganic to organic molecules,that aggregate into cells, organs, new individuals. Therefore it is not surprising that many of the major events and features are based on the same principles. Our knowledge of the universe has changed drastically during the last century. One hundred years ago it was thought that our galaxy is the universe; however, today it is suggested that there are at least 100 billion galaxies (Kauffman and van den Bosch, 2002; Krauss and Turner, 2004; Strauss, 2004; Turner, 2013). Lonely stars, are not so lonely after all, since with the improvement of the resolution techniques, most of them have been proven to be composed of pairs of stars (binary systems) (Piran, 1995).

These are only a few examples of the progress in our knowledge of the universe. However, in spite of this, cosmology still seems to be at its first steps. Main issues such as, which theory for its birth is correct, the Big Bang or the String theory, if it was born by an explosion

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or by bouncing , the meaning of time and constants, the number of universes, its shape, the number of its dimensions, its age, how to reconcile the general theory of relativity with the quantum theory, black holes or black stars, or weather it is only an illusion, are still widely debated. We do not know what is the composition of 95% of the universe, if it is going to collapse because of the gravitation, or fall apart due to its accelerated expansion, just to mention a few of the major mysteries (Barcelo et al., 2009; Barrow and Webb, 2005; Bekenstein, 2003; Bojowald, 2008; Bousso and Polchinski, 2004; Collins, 2004; Krauss and Turner, 2004; Krauss and Scherrer, 2008; Luminet et al., 1999; Starkman and Schwarz, 2005; Strauss, 2004; Tegmark, 2003; Turner, 2013; Veneziano, 2004).

Many of the yesterday's "facts" and theories have been proven to be wrong, and many of the today's "facts" and theories will be shown to be obsolete tomorrow (Turner, 2013). Therefore, there is a constant need for new and original ideas.

In spite of enormous size differences, some basic mechanisms seem to be similar. For instance, already about a hundred years ago, it was Rutherford that suggested similarities between the atomic and planetary systems- the planetary model of the atom. These similarities are between the extremes in the universe, from the smallest particles to the largest objects in the universe.

In the biological systems, the cell division and basic biochemical principles are also similar throughout a very wide range of sizes (Alberts et al., 2002; Cooper, 2000; Gilbert, 2000). For instance, the mechanism of cell division of a microscopic virus (about 20 nanometer) is essentially the same as that of a fly, ant, squirrel, dog, bird, fish, horse, elephant, or a 130 ton whale. This, inspite of an up to 10 to the 15^{th} times size difference! The basic principle is the same, the division of the genetic material, and production of two new cells, even that there could be some variations and certain details could be different (Alberts et al., 2002; Cooper, 2000; Gilbert, 2000). Therefore, it is possible that there are universal mechanisms of division and formation of new entities, and that could be true at even much higher size differences, such as in the case of star and cell formation (Kleinman, 2008). Recently, additional similarities of cosmic and biologic systems have been suggested; for example, the model of the "cellular universe"(Anjamrooz et al., 2011), and the model of "network cosmology" (Krioukov et al., 2012).

Comparison of major principles of cosmic and biologic systems suggested similarities that could explain some of the basic cosmic phenomena and events, and offered an unifying hypothesis for the universe (Kleinman, 2008). In this report, additional similarities are suggested, that provide unexpected support for the Big Bang and String theories, for the mechanisms of birth, development and fate of the universe. Based on them, predictions are made.

COMPARISON OF THE MAJOR EVENTS IN THE BIRTH AND EARLY DEVELOPMENT OF COSMIC AND BIOLOGIC SYSTEMS

Before the big bang

Cosmology

The Big Bang Theory (BBT) suggests that universe was born about 13.5 billion years ago ,when an infinitesimally small particle exploded (Rees, 1999, 2005; Krauss and Turner, 2004; Strauss, 2004). Before this event nothing existed, if nothing can exist… No time, matter, energy or space (Tegmark, 2003; Veneziano, 2004).

These assumptions are controversial, to start with. If nothing existed than how can it be explained that there was a particle that contained all the matter and energy of the whole future universe? In addition, if a particle existed before the Big Bang, then it was "hanging" in some place (space) for a certain period (time).

The question is how, when and why should the entire universe be condensed and packed into an infinitesimal particle. What caused the energy and matter to concentrate in the particle, and where they come from? Therefore, even by the logic of this theory the universe is the continuation of a pre-existing state, that contained all the components of the today's universe- time, matter, energy and space.

In addition, if one particle could exist in these conditions, than there could be many more particles, and potentially more than one Big Bang, and as a result many additional (parallel) universes. The proponents of this theory (String theory) suggest that the Big Bang was not the origin of the universe, but simply the outcome of a preexisting state. In their view, time is endless and contains many finite universes in an infinite space (multiverse) (Tegmark, 2003; Bousso and Polchinski, 2004; Veneziano, 2004; Rees, 1999, 2005), and our universe was born by the collapse of matter and energy into a black hole, and/or as a result of collision between two universes (‘’cosmic conception").

They describe the universes as pairs of membranes (branes), that undergo cyclic collisions and separations ("cosmic conception") (Tegmark, 2003; Veneziano, 2004; Barger, 2005; Carr and Giddings, 2005). As a result, following each cycle, there is production ("birth") of new universes. Lately, it was suggested that such colliding universes could share black holes (Carr and Giddings, 2005) ("reproductive-secretory organs"); therefore this could be the place where the exchange of matter and energy is taking place ("cosmic conception"), and the new stars of the embryonic universe are formed. This could be the explanation for the formation of new stars in the vicinity of the black hole of galaxies that are going through, or have recently undergone a close encounter or merger with a neighboring galaxy (Weaver, 2003; Barger, 2005).

Table 1. Similarities in birth and development.

Parameter theory	System	
	Cosmic	**Biologic**
Theory	BBT~ Darwinian evolution	Darwinian evolution
Born from one unit	Particle, singularity	Oocyte (Egg cell)
Conception	Collision (mating) of branes (galaxies, universes)	Male – female mating
Fertilization	Jet of energy & matter	Seminal fluid (sperm)
Explosion	Particles, anti particles	Ions : Ca, Na, K
	Temperature increase	Temperature increase
Gestation	One billion years	9 months – humans
Smoothness	Quark soup	Chorionic fluid
Fluctuations	Radiation (CMBR)	Calcium concentration
Lumpiness	Aggregation of :	Aggregation of :
	stars = galaxies = clusters = universe	Cells= organs= individual
Expansion(age)	Inflation (= young)	Growth (= young)
	Increasing no. stars	Increasing no. cells
Flatness	Flat, curved	Flat, curved
	Discoid	Embryonic disk
Basic units	Stars	Cells
Differentiation	Population: 3, 2 ,1 stars	Stem cell: RBC, WBC
Composition	Dark energy (70%)	H_2O (70%)
	Dark matter (25%)	Fat (25%)
	Common matter (5%)	N-organic compounds (5%)
Reproductive & excretive organs	Black hole:	Urino-genitals:
	(i) enhanced star formation	(i) enhanced cell formation
	(ii) disposal of cosmic debries	(ii) excretion of catabolites
Pre-existing state	Multiverses	Individuals
Cause of death	Death of its components (stars)	Death of its components (cells)
Homeostasis	Cosmic background radiation, temperature	Electrolytes , temperature
Organization	Filamentary network	Conjunctive tissue
	Stars, galaxies	Cells, organs
Information	Matter	DNA
	Law and order: physical – chemical- mathematical	physical – chemical- mathematical + biological
	Flatness, lumpiness	yes
	" God does not play dice"	yes
Functionality	Galaxies	Organs

Biology

The above cosmic phenomena have their biological parallel, in the formation in the uterus, of new embryonic cells, following a male- female close encounter (mating, biologic conception). The production of universes by the cyclical collision of branes (universes) (attraction, collision, separation, formation of new universes) resembles the male –female reproductive cycle (Knobil and Neill, 1988; Larsen, 2001). This is similar to the preexistence of individuals of different sexes, before the egg cell is fertilized, and the production of many more, new, parallel individuals.

The suggestion of finite universe in an infinite multiverse also has his equivalent in the biological model. The individual is finite, and he lives in infinite space. The cosmological finite would be a universe/galaxy, and its biologic correspondent an individual.

Predictions

Preexisting state: From the similarities to the biologic

systems, it could be predicted that the particle(s) that the universe(s) are born from are a continuation of a preexisting state, of parallel universes.

Black holes - reproductive / excretory organs: The cosmic black holes are thought to be the place where cosmic debris (stars that exploded) are disposed, and where there is an enhanced stars production. It also suggested that it contains the singularity, which could be the particle from which a new universe can emerge, following the collision of the branes ("cosmic conception"). This is similar to the reproductive / excretory organs of the biological systems (uro- genitals), that are the place of disposal of the catabolites and also of the reproductive organs containing the egg cells (Larsen, 2001).

One unit origin

Cosmology

The Big Bang theory (BBT) suggests that the universe originates from one infinitesimally small particle (singularity) (Joshi, 2009; Turner, 2013). Its sudden explosion led to the formation of all the different forms of mater, energy, space and time. It also suggests that all the infinite amounts of today's mater, space and energy existing in billions of galaxies, were encapsulated in the original infinitesimal small particle.

Biology

The biological systems also originate out of a single particle (oocyte, egg cell), that will evolve into an individual composed of trillions of new cells (Alberts et al., 2002; Cooper, 2000; Gilbert, 2000; Guyton and Hall, 1991). However, from the biological systems can be learned that there is no need for assuming that all those trillions of cells were packed in the cell of origin, but that it contained the information for their production ("cosmic DNA").

Predictions

Similar to the egg cell, the initial particle (singularity) contains only the information for the formation of all the components of the universe, and it does not contain all the existing and future mater and energy.

Big bang

Cosmology

The Big Bang theory (BBT) suggests that universe was born about 13.5 billion years ago, when an infinitesimally small, dense and hot particle exploded (Bousso and Polchinski, 2004; Collins, 2004; Krauss and Turner, 2004; Krauss and Scherrer, 2008; Strauss, 2004; Tegmark, 2003; Turner, 2013; Veneziano, 2004). In a few fractions of a second, space expanded violently, and formed a highly energetic soup of particles and antiparticles. Following the initial explosion, the BBT brings a very accurate description of the events, down to fractions of the first second. This seems questionable since there is still a controversy about the age of the universe, from 8 to 20 billion years.

The String theory suggests that this particle (singularity) was a continuation of an existing state, and its explosion was precipitated by collision with jets of mater and energy in a black hole ("cosmic fertilization"), perhaps during the collision of branes. During the collisions, there could be exchange of mater and energy through their black holes. This form of "cosmic intercourse" could be the mechanism of new galaxies and universes formation .These similarities would suggest the existence of "male " and " female" galaxies and/or universes.

Biology

In the biological systems there seems to be a similar process of fertilization, whereby the production of an embryo, is the result of the "collapse" of a "jet of matter " (seminal fluid of the male) containing about 300 million sperms, into the female Fallopian tube (black hole), hitting one egg cell (particle, singularity), and inducing an explosion in the concentration of calcium ions (Alberts et al, 2002 ; Cooper, 2000; Gilbert, 2000).

Predictions

The explosion of the initial particle (singularity) was precipitated by collision with jets of mater and energy in a black hole ("cosmic fertilization"), perhaps during the collision of branes. This suggests the existence of male and female universes (galaxies).

First 3-400,000 years

Cosmology

During this period, the BBT suggests that the universe was a flat and homogenous (smooth) soup of particles and antiparticles (quark soup) (Krauss and Turner, 2004; Krauss and Scherrer, 2008; Strauss, 2004; Tegmark, 2003; Turner, 2013). It was suggested that since energy and mass were interchangeable and in equilibrium, no radiation could escape during this period, and that this is

the reason why there is no information about this period.

The fact that initial measurements of the cosmic microwave background radiation (CMBR) showed that it was uniform from all directions, was taken as a proof for the Big Bang and for the homogeneity of the early universe (quark soup). Indeed, if the BB occurred in a vacuum, which by definition should be devoid of any resistance, then the radiation should be equal and uniform in all directions.

Biology

In the biological models we can see a similar situation. A single cell, the oocyte (the particle, singularity), upon fertilization by one sperm (the Big Bang), it is triggered into a process of rapid division and differentiation (inflation) in a homogeneous amniotic fluid (the quark soup, smoothness). In its first phases of its development, the embryo is flat (flatness- embryonic disc) (McLaghlan, 1994). During the whole period of pregnancy, the fetus (up to 3.5 kg) is floating in up to one liter of a homogeneous fluid (amniotic) (McLaghlan, 1994).

As soon as six seconds after fertilization there is an explosion in the concentration of Ca ions. This explosion is followed by prolonged oscillations in its concentration. There is evidence that these oscillations activate a cascade of reactions leading to cell division (Alberts et al., 2002; Gilbert, 2000). This chain reaction starts with explosion in concentration of calcium ions, followed by increase in the concentrations of ions of sodium and potassium, an increase in the pH and oxygen consumption, and activation of oxidative pathways, lipid metabolism, nicotinamide nucleotide reduction and enhanced protein, hormones (beta human chorionic gonadotrophin, progesterone, estrogens) and DNA synthesis (Alberts et al., 2002; Gilbert, 2000; Knobil and Neill, 1988; Srivastava and Talwar, 2004). As a result, the initial egg cell will divide and produce a new individual. Thus, one cell, provided that it has the proper environment and enough nutrients, can develop into an individual with trillions of different cells (Guyton and Hall, 1991; Larsen, 2001; McLaghlan, 1994; Rudolph and Rudolph, 2002). All this is possible due to the existence of the DNA molecule that has the information for this process. Perhaps that the initial particle, that supposedly was the origin of the universe, also contained the information for its further development.

Predictions

Origin: The division of the initial particle is the origin of the universe, and not the quark soup. This would be similar to the production of an individual composed of trillions of cells, out of the division of a single egg cell, and not from its surrounding amniotic fluid (Larsen, 2001; McLaghlan, 1994; Guyton and Hall, 1991).

The quark soup: Is only providing the optimal conditions for the division of the initial particle/singularity, similarly to the feeding, protecting role of the of the amniotic fluid for the division of the egg cell (Alberts et al., 2002; Gilbert, 2000; Knobil and Neill, 1988; Srivastava and Talwar, 2004).

Oscillations/variations: In radiation (cosmos) or Ca ions (biology) induce and facilitate star or cell formation, from the initial particle/singularity or egg cell (Alberts et al., 2002; Gilbert, 2000; Knobil and Neill, 1988; Srivastava and Talwar, 2004). They do not induce new star or cell formation out of the homogeneous soup (quark or chorionic), but they only enhance the division of the egg cell or the cosmic particle.

Where do the quark soup come from?: The BBT and ST assume that the BB was the continuation of an existing state (a particle that existed before the explosion). The division of this particle will produce the embryonic universe, which in turn will produce the quark soup. This is similar to the biological models, in which first there is the appearance of the embryonic cells and only thereafter; partly due to their own secretions, they are engulfed in fluids (amniotic, yolk, chorionic) in surrounding cavities produced by its differentiating cells (McLaghlan, 1994).

Homeostatic mechanisms: The relative uniformity of the radiation is only one feature of the present universe, which does not necessarily has to do, or prove the way, or cause of its creation. It is like deducing from the fact that our body has physiological constants, with only slight variations in their values (e.g. temperature, Na, K, Cl, cholesterol, iron, albumin, globulin, protein), that we were born by an explosion, out of a homogeneous soup, and that the small variations in their values were responsible for the production of the cells (stars) and organs (galaxies) of our body. The uniformity of certain cosmic and biologic features only prove the existence of homeostatic mechanisms that maintain their unity and integrity (Guyton and Hall, 1991; Gilbert, 2000; Longo et al., 2011; Rudolph and Rudolph, 2002).

Information: The initial particle/singularity, that was the origin of the universe, contained the information for its further development and for the formation of the various forms of matter and energy. The infinite quantity of matter and energy of the universe were not packed in an infinitesimal small particle. This would be similar to the information contained in the egg cell (DNA) coding for the formation of trillions of cells (Alberts et al, 2002; Gilbert, 2000; Knobil and Neill, 1988; Srivastava and Talwar, 2004; Larsen, 2001; McLaghlan, 1994).

300,000 to one hundred million years

Cosmology

BBT suggests that at the beginning of this period, matter

separated from energy, and the free photons produced the so called "cosmic microwave background radiation" (CMBR). Why should they separate, and why only after about 400,000 years is an interesting question by itself. Following the first 300-400,000 years, the BBT suggests that there is a period of about 100 million of years, during which under the effect of random, minute variation in the environmental conditions (radiation, temperature, gravitation), the dark matter and hydrogen (H) kept aggregating to larger and larger bodies, eventually producing the first stars (Balick and Frank, 2004; Boss, 1995; Larson and Bromm, 2004; Caldwell and Kamionkovski, 2001; Carr and Giddings, 2005; Gibbs, 2002; Turner, 2013).

However, there are some problems with this theory. First, some of these variations have never been directly detected, and their fluctuations are so faint, that detecting them is so difficult as detecting the addition of a single grain of sand to all of the beaches of Long Island NY, or noticing a change in the distance between Saturn to the Sun by the width of a hydrogen atom. These are the gravitational waves that supposedly produced the first compressions of quark soup, and started the aggregation of matter (Gibbs, 2002). Second, recent analysis of the temperature of the radiation revealed mysterious discrepancies in their variation ("out of tune"), that lead some scientists to question the validity of the BBT (Starkman and Schwarz, 2005).Third, even if such variations exist, they are not a direct, nor indirect proof for the process of star formation, but rather the indication for existence of homeostatic mechanisms.

The BBT suggests that the first stars were huge and contained mostly H and helium (population III stars).The today's new stars are metal rich (population I stars), and the old ones are metal poor (population II stars) (Larson and Bromm, 2004).Therefore it seems that there is a process of star evolution and differentiation.

Biology

The body has also constants that have only very small variations (temperature, concentration of various blood components, etc) (Guyton and Hall, 1991; Knobil and Neill, 1988; Longo et al., 2011; Rudolph and Rudolph, 2002; Srivastava and Talwar, 2004). Their function is to provide optimal conditions for cell division, and maintenance of the functions and integrity of the body. They are the homeostatic mechanism of the biologic systems.

In the biologic systems there is also cell evolution and differentiation (McLaghlan, 1994; Rudolph and Rudolph, 2002). The initial embryonic cells are toti-potent (morula, can differentiate into all types of cells) and can transform into more differentiated multi-potent (ectoderm, endoderm, can differentiate only to a limited group of cells) and finally into mono-potent specialized cells (red blood cells, cannot differentiate into other cells). Similarly to the first stars, also the first embryonic cells were much larger than the later, more differentiated cells (McClatchey, 1994).

Predictions

Constants with minute variations: (CMBR, magnetic waves, temperature) are the homeostatic mechanisms of the universe and not the factors that induce the star formation out of the quark soup.

Star division, differentiation and fragmentation: Following the BB, the initial particle/singularity differentiated into several stars classes (1, 2, 3). This is similar to the differentiation of the egg cell into a variety of different cells (McLaghlan, 1994). In addition, this process occurs today in the stellar nurseries, similarly to the differentiation of the stem cells in the bone marrow (McClatchey, 1994; Longo et al., 2011).

In the solar system, the Sun (population III) could be the equivalent of a multi-potent cell, that differentiated into several specialized planets, some metal rich (Earth), and other metal poor (Jupiter). Alternatively, they could be produced by a star fragmentation. This is also a known phenomenon of cell production in biological models. For instance, the platelets (type of blood cells) are produced by the fragmentation of giant megakaryocytes (McClatchey, 1994). However, this is a minor pathway for cell production, and the vast majority come from cell division.

Similarities in formation and life cycles of stars and cells were previously suggested (Kleinman, 2008). Therefore, the evolution of the universe could be explained by star divisions and fragmentations, starting from its "embryonic phase", and continuing to the present days.

The tiny fluctuations: It is in the radiation, temperature, gravitation: are the result of a homeostatic mechanism, and not the cause for matter aggregation and star formation.

The 100- 1000 million years

Cosmology

The BBT assumes that after an additional 100-250 million years, the stars started organizing into young galaxies (proto-galaxies), at the intersections (nodules) of a vast filamentary network. Altogether, about one billion years after the BB, the proto-galaxies transformed into adult galaxies, which further organized into clusters and super-clusters, filamentary structures, stretching billions of years through the universe ,and in between gigantic voids of empty space (Rees 1999, 2005; Turner, 2013).

Frequently used ways to represent the universes are the bubbles, that are continuously born and expending in valleys of a vast landscape (Bousso and Polchinski,

2004; Rees, 1999, 2005; Tegmark, 2003). Alternatively, the multiverse is suggested to be as a huge balloon, containing zillions of smaller bubbles, each representing a different universe (Magueijo, 2001).

Biology

The above process, of stars grouping into galaxies, clusters and super-clusters, resembles the grouping of cells into organs and various systems (digestive, vascular, nervous, etc).The filamentary network organization of the universe is similar to the conjunctive tissues of the biological systems (Guyton and Hall, 1991; Gilbert, 2000; McLaghlan, 1994; Longo et al, 2011). The bubbles model of the universe is similar to the biological models. For example, a cell, inside an embryo, floating in the chorionic cavity, surrounded by the chorionic plate, inside the cytotrophoblast, in the syncytiotrophoblast, in the uterus, in the body of a female (McLaghlan, 1994). The zillions of bubbles (universes) inside a multiverse, could be the equivalent to the trillions of cells inside an animal (Guyton and Hall, 1991).

Predictions

Birth of the universe: The BBT suggests that the universe in its present form, evolved only after one billion years of development, after the Big Bang, and thereafter it only continuously inflated. Therefore, similarly to the biological systems, this period could be taken as the "pregnancy phase", during which the universe was in his embryonic phase, and its real birth was only one billion years after its conception – the Big Bang.

According to this classification, the history of a new universe can be divided into several phases. The collision of the branes is the "conception", followed by the "fertilization" that occurs when a jet of matter and energy hits the singularity/particle. Then, there is one billion years of "pregnancy", during which it is in the "embryonic" phase. Only at the end of this period comes the "birth" of the universe.

Functionality: The organization of the stars into galaxies resembles the organization of cells into a variety of functional organs (endocrine, digestive, nervous, etc.). This similarity suggests several possibilities. First, that inside the galaxies there are functional organs such as, the nebula that produces new stars (bone marrow), and the black holes (reproductive/excretory). Second, that similar to the animal kingdom, different types of galaxies, have different function ("cannibalism").

The 1-14 billion years

Cosmology

The universe is continuously expanding. The BBT suggest that this is a result of the initial explosion. Alternatively, it is suggested that this expansion is caused by the mysterious black energy. Lately it was suggested that this expansion would eventually lead to its destruction (Krauss and Scherrer, 2008; Turner, 2013).

Biology

Similarly, in the biological systems, there is a continuous expansion, from the initial one cell, to an individual with trillions of cells (Guyton and Hall, 1991; Gilbert, 2000; McLaghlan, 1994; Longo et al., 2011; Rudolph and Rudolph, 2002). This expansion continues until the individual reaches maturity, than it reaches a relative steady state. Finally, with the onset of the process of aging, the individual will undergo a certain reduction in his size, and will eventually die. His death is not because of an unlimited expansion, nor because of his collapse, but because of the death of his cellular components.

Similarly it can be assumed, that the fact that the universe expands, is not because of the initial explosion, but because of the multiplication of its stars. Therefore, its expansion is not a sign of its disintegration, but of its growth and its young age. The expansion will stop when it will reach maturity, than will follow a long period of steady state, and then it will die due to the death of its stars, and not because of unlimited expansion nor due to its collapse. Therefore, the similarities between the cosmic and biologic systems, could provide an explanation to the expansion, and predict the fate of the universe.

Predictions

Composition: Cosmic and biologic systems have a similar distribution of their main components. It is suggested that the universe has about, 72% dark energy, 24% dark matter, and 4% ordinary matter (Turner, 2013). A typical neonate has a similar distribution, about 75% water, 15% fat and 10% N containing organic substances (Rudolph and Rudolph, 2002). The properties of these components suggest similarities. For instance, it was suggested that the dark matter interacts weekly with ordinary matter, therefore it could be equivalent to the water in the biologic systems. On the other hand, the dark energy could be equivalent to fat, which is a known source of energy.

Inflation/ expansion: This process is an expression of normal growth and development of the newly born universe. The fact that the universe is expanding indicates that is young. Its expansion is due to the multiplication of its components (stars), and not because of the dark energy. The dark energy is a result of its growth, and not its cause. The fact that the amount of energy is several times larger than expected, indicates it

has its origin from outside, from other universes (multiverses). The expansion will stop when the universe will reach maturity, and then it will remain at a steady state, until it will start deteriorating due to the death of its components- the stars. Therefore, the expansion is only an expression of its development, is not caused by the Big Bang explosion and it will not lead to its extinction.

Age of the universe: The fact that the universe has a higher percentage of energy than a newborn (72% dark energy versus 15% fat), suggests that it is in later phases of development (adult, old?). From the biological systems it can be seen that the percentage of fat increases with age (Rudolph and Rudolph, 2002). It has been suggested that the domination of the dark energy started only after about one billion years, after the production of the galaxies, cluster and super clusters (Turner, 2013). Therefore, also by these criteria there is similarity between the cosmic and biologic systems.

From the biologic systems (humans) it can be seen that the period of pregnancy (9 months) is about 10% of the life span (about 80 years). If the universe in its present form, was formed only after one billion years of evolution (birth date?), than its life span should be 10 billion years. Therefore, either that the suggestion that its age is about 13.5 billion years is incorrect, or that its "gestation" period was longer than one billion years. Alternatively, the ratio of pregnancy: life span is different in the two systems.

Information: The explosion of the initial particle (Big Bang), in a vacuum should produce a spherical universe. Therefore, the fact that the universe is flat (flatness), indicates that its birth and development were determined not only by physical laws, but also by additional factors such as information.

DISCUSSION

The major theories of birth and development of the universe resemble the Darwinian theory of evolution of the biological systems. The later suggests that, (in brackets their suggested cosmic counterparts), first there was a physical – chemical event (Big Bang), leading the evolution of molecules in a liquid media (quark soup – particles), and to the formation of inorganic and then organic molecules (elements) (Miller and Urey, 1959; Turner, 2013). These molecules evolved into complex biochemical molecules, that eventually assembled into primitive cells (stars). The cells aggregated into multi - cellular organisms (galaxies), that evolved into higher and higher levels of organization- the plant and animal kingdom (clusters, universes).

Regardless of their size, there are some basic phenomena, components that are common to all forms of matter in the universe. For instance, they all share the same elements at various ratios. The orbiting motion is common from the smallest particles, the electrons around the protons (the planetary model of the atom, Rutherford), and to the huge moons around the planets, the planets around the stars, the stars around the center of the galaxy. The same is true for biological systems, from the submicron sized viruses, and up to millions of times larger animals (whales, hundreds of tons), they all share similar genetic, biochemical, components, processes and information (DNA, RNA, proteins, enzymes, etc).Therefore, the differences in the size, do not exclude possible basic similarities between small (the biological systems) and the big (the universe).

Therefore is not surprising that the similarities listed in this article (Table 1), about the principles of birth and development of cosmic and biologic systems provide evidence for the validity of major, basic principles of BBT, and the String theory. However, they also raise questions, and suggestions for different, new ways of interpretation of the known cosmic events, and proposes predictions for the birth, development and fate of the universe.

In both the cosmic and biologic systems, their birth originates from one entity (particle, singularity - egg cell), which is initiated to develop into a flat creature (flatness-embryonic disk), floating in a homogeneous (smoothness) media (quark soup - chorionic fluid). However, based on the example of the biologic systems, it is suggested that the first stars derived from the original particle/singularity, and the quark soup is not the origin of the embryonic universe, but is a product of it.

The suggestion of the BBT, that the whole energy and matter of the universe were packed in the initial particle (or singularity by the String theory), indicate that it was the continuation of a preexisting state. The sudden development from the initial particle either by a spontaneous explosion (BBT), or by collision with a jet of matter and energy (ST), into a new universe, has its parallel in the biologic systems. A new individual can develop out of a single egg cell, when it is hit by a jet of biological matter (seminal fluid, containing millions of sperm cells). This is the case of the highly organized biological systems, of the animal kingdom. However, in the lower biological systems, like unicellular bacteria, a single cell can also develop into trillions of new cells, provided it has the optimal environment (nutrients, temperature, etc).

The continuation of a preexisting state, also suggests that similarly to the biological systems, where all the information for the production of the new individual exists in the DNA of the egg cell, the particle, the singularity , also posses the information for the production of the new universe. In addition, the fact that universe is flat and not spherical (as it should be by the physical laws of a particle exploding in a vacuum), that there is diversity and evolution of its components, and that there is an organized association of stars into galaxies, clusters, super clusters, also indicates that it is following a pattern contained in its initial information ("DNA"). This is similar to the information driven cell differentiation and

aggregation into organs and a variety of physiological systems leading to the formation of a new individual. From the fact that the organs of an individual have different functions, it can be predicted that their cosmic counterparts, the galaxies could also have specific functions that are needed for the integrity and proper function of the universe. Indeed, there are a variety of shapes of galaxies, and perhaps each type is associated with certain specific functions. In addition, inside the galaxies there could be functional organs, such as nebula (star nurseries- bone marrow), or the black holes (reproductive/excretive- uro/genitals).

The reproductive / excretory organs of the biological systems (uro- genitals), that are the place of disposal of the catabolites, and of the reproductive organs containing the egg cells, have their parallel in the cosmic black hole. It is also supposed to be the place where cosmic debries (stars that exploded) are disposed, and where there is an enhanced star production. It also contains the singularity, which could be the particle from which a new universe can emerge, following the Big Bang.

The basic units of the biological systems are the cells, similarly to the basic units of the universe – the stars (Kleinman, 2008). Their proliferation lead to the growth (inflation, expansion) of both systems. Thus, the inflation of the universe is not a sign of its destruction, but to the contrary, a sign of a vital, young and growing universe. Similar to the biologic systems, its growth will stop when it will reach maturity, and its death will be caused by the death of its components (stars), and not because its expansion or collapse.

An additional feature that indicates the similarity between the cosmic and biologic systems is their composition. They are composed of similar percentages of their major components (Table 1). It is suggested that the black matter is amorphous, thus resembling the water in the biologic systems, at the time that the dark energy resembles the energy contained in the fat. The similarities between the constant values of certain parameters of the cosmos (radiation, temperature, etc) and of the biological systems (temperature, blood components, etc), seems to indicate the existence of homeostatic mechanisms, designed to preserve and maintain their integrity.

The BBT assumes that the stars and today's universe were produced by random variations in the environment, a kind of casino. However, we know that there is lāw and order in the universe, therefore the "casino" approach does not seem feasible ("God does not play dice" Einstein). Instead, a logical explanation can be derived from the biological systems.

Could one explain the birth of a new individual by quantum mechanics, extended relativity, physical, chemical or mathematical laws? The answer is no. Each one of the various levels of organization, mathematical, physical, chemical, biological, has his own laws. In order to understand biological phenomena one needs to use a synthesis of all the above in a more complex form (biochemistry, biophysics), together with a new science – biology, that was created to understand specific processes related to this higher level of organization (genetics, endocrinology, immunology, neurology, reproduction, etc).

The universe, with its suggested eleven dimensions, seems to be a much more complex, and much higher level of organization than our known three dimensional world. Therefore, if the physical, chemical, mathematical laws cannot explain the birth of an individual, one cannot expect that they would be able to explain the birth and development of an even higher level of organization - the universe. To do so, there is need to use a synthesis of the laws of all known levels of organization (including biological), upgrading, adapting, and integrating them into a new science- the supra-biological cosmology. Until such a science is developed, in order to understand the universe, we need to learn from the closest level of its organization, the biological model.

In conclusion, the similarities in the birth and development of biologic and cosmic systems provide an unexpected proof for the basic assumptions of the major theories of the birth and development of the universe – the Big Bang and the string theories. In addition, they provide alternative, different interpretations, explanations and predictions for many of their observations and assumption. The significance of these predictions could have far reaching consequences, and could revolutionize major concepts in cosmology.

Conflict of Interests

The authors have not declared any conflict of interests.

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Full Length Research Paper

Theoretical calculation of half-metallic ferromagnetism in $Al_{1-x}V_xN$ compound

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Using the first-principles in the framework of density functional theory, the structural properties, electronic structure, and magnetism of V-doped aluminum nitride (AlN) were investigated. The calculations were carried out using the method based on pseudopotential, employed exactly as implemented in Quantum ESPRESSO code. For (x = 6.25%) $Al_{0.9375}V_{0.0625}N$ and (x = 12.5%) $Al_{0.875}V_{0.125}N$ concentrations, a half-metallic behavior with 100% carrier spin polarization of the conduction carriers in the ground state was found. The calculations showed that the substitution of a V atom at the Al site ($Al_{0.9375}V_{0.0625}N$ compound) introduces a magnetic moment of 2.0 μ_B, while two V atom substitutions ($Al_{0.875}V_{0.125}N$ compound) introduce a magnetic moment of 4.0 μ_B. These magnetic properties came from hybridization and polarization of states V-3d and their first neighboring Al-2p and first neighboring N-2p atoms. The calculated magnetic properties indicate that V-doped AlN compound can potentially be used in diluted magnetic semiconductors or as spin injectors.

Key words: Aluminum nitride (AlN), first-principles calculations, magnetic ordering.

INTRODUCTION

Aluminum nitride (AlN) normally crystallizes in the wurtzite structure (Beloufa et al., 2009). This material has recently attracted the attention of researchers due to their excellent properties, has been widely used in: design Light-Emitting Diodes (LEDs) and Laser Diodes (LDs) (Taniyasu and Kasu, 2008), in electronic packaging material and applied to optical disk as well as lithographic photo masks (Jonnard et al., 2004; Carcia et al., 1996; Carcia et al., 1997). Due to its stability, high temperature, considerable thermal conductivity, low thermal expansion and high resistance to gases and chemicals (Beheshtian et al., 2012) has been used in many electronic devices which must work in high temperature, high power, and corrosive ambients. In last years, AlN has received extensive attention, because of its possible use as a diluted magnetic semiconductor (DMS) with potential applications in the field of spintronics. For these applications, ferromagnetism at room temperature is a requirement. Recently, high-temperature ferromagnetism has been reported by many researchers in several types of transition-metal (TM)-doped semiconducting oxides and nitrides (Gonzalez et al., 2011; Vargas-Hernadez et al., 2015; Frazier et al., 2003). In particular, many theoretical and experimental works performed on the

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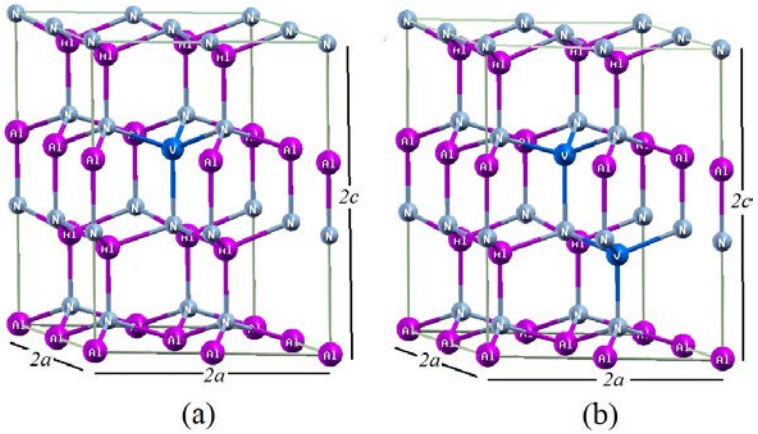

Figure 1. Unit cell of the ternary compound: (a) $Al_{0.9375}V_{0.0625}N$, (b) $Al_{0.875}V_{0.125}N$ after structural relaxation.

magnetic properties of AlN via TM doping (Fan and He, 2010; Wu et al., 2003; Li et al., 2008; Yang 2002) showed that it may be a promising candidate for spintronics. However, it was found out that the magnetic TM dopants in TM-doped DMS segregate to form ferromagnetic clusters, precipitate, or secondary phases (Park et al., 2004; Kaspar et al., 2008; Zhou et al., 2008). This represents a big obstacle for practical applications of diluted magnetic semiconductors. It is at this point that the theoretical calculations play a key role, because theoretical methods are able to reliably predict the relative stability, the atomic and electronic properties of increasingly complex structures, for example, theoretically it can calculate the energy formation parameter which is important for obtaining sufficient magnetization at room temperature. On the other hand, it has been reported that MT = Sc-, Cr-, Co-, Mn-, Er-, Mg-, Ca- and Cu MT-doped AlN are ferromagnetic (FM) (Lei et al., 2009; Wu et al., 2006, 2007; Yang et al., 2007; Dridi et al., 2011; Zhang et al., 2008). But the investigation of AlN:V system is rare, either theoretically or experimentally. For these reasons, this paper presents a systematic theoretical study of the electronic and magnetic properties of V-doped AlN.

COMPUTATIONAL METHODS

The theoretical calculations were performed using the Quantum ESPRESSO package (Giannozzi et al., 2009). Within the density functional theory (DFT) framework, the DFT is an extremely successful approach for the description of the ground-state properties of metals, semiconductors, and insulators. The correlation and exchange effects of the electrons were treated using the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) (Perdew et al., 1997). Electron–ion interactions were treated with the pseudopotential method (Vanderbilt, 1990; Laasonen et al., 1993). Electron wave functions were expanded into plane waves with a kinetic-energy cutoff of 40 Ry. For the charge density, a kinetic energy cutoff of 400 Ry was used. A 6×6×4 Monkhorst-Pack mesh (Monkhorst et al., 1976) was used to generate the k-points in the unit cell. The calculations were performed taking into account the spin polarization. All the crystal structures were fully relaxed via geometrical optimization by displacement of the atoms in the z axis. Structural optimizations are finished when the total energy converged to less than 10^{-7} eV/atom and the magnitude of the force acting on each ion is less than 10 meV/Å. To calculate the structural, electronic, and magnetic properties of pure AlN, a 32-atom *2a* × *2b* × *2c* wurtzite supercell was considered. The concentrations $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ were obtained by substituting one and two Al-atoms in the supercell. Pure AlN and $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds were modeled according to the special quasirandom structures approach and the disorder aspects were ignored (Zunger et al., 1990). Figure 1 shows the supercell of the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds obtained after of the structural relaxation.

RESULTS AND DISCUSSION

Structural parameters

To determine the structural properties in the ground state, such as the lattice constant (a_0), the bulk modulus (B_0), the c/a ratio, the total energy (E_0) and the magnetic moment (μ) per supercell of pure AlN, $Al_{0.9375}V_{0.0625}N$, and $Al_{0.875}V_{0.125}N$ concentrations in the wurtzite structure, the total energy was calculated as a function of the volume and the results were fit to the Murnaghan equation of state (Murnaghan, 1944). Additionally, for the $Al_{0.9375}V_{0.0625}N$ compound, the total energy variation was calculated as a function of the volume for the FM and non-magnetic phases, while $Al_{0.875}V_{0.125}N$ compound allows the calculation of the relative energies of FM and antiferromagnetic (AFM) phases, in order to find the most favorable magnetic ordering. Figure 2 shows the energy-volume curves.

Table 1 shows the lattice constant (a_0), the c/a value, the bulk modulus (B_0), the total energy (E_0), and the magnetic moment (μ_β) per supercell. The solid line is

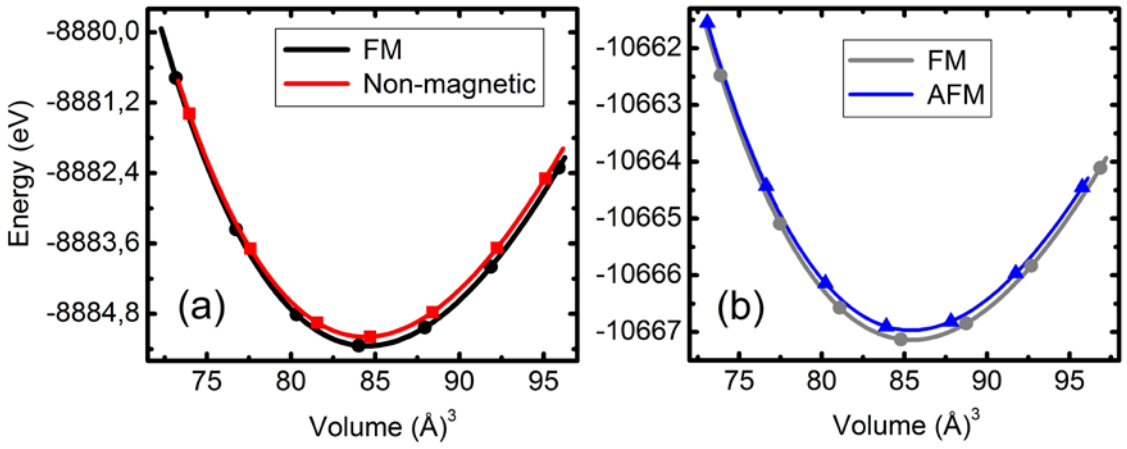

Figure 2. Total energy as a function of volume for (a) $Al_{0.9375}V_{0.0625}N$, (b) $Al_{0.875}V_{0.125}N$.

Table 1. Lattice constant, c/a ratio, bulk modulus, total energy, and magnetic moment per supercell of pure AlN, $Al_{0.9375}V_{0.0625}N$, and $Al_{0.875}V_{0.125}N$.

Compound	a_0(Å)	c/a	B_0 (GPa)	E_0 (eV)	μ (μ_β/cell)
AlN	3.121	1.603	192.93	- 7101.912	0.0
	3.110[a]	1.601[a]	192[b]	-	-
$Al_{0.9375}V_{0.0625}N$	3.117	1.604	191.86	- 8885.344	2.0
	3.125[c]	1.602[c]	-	-	2.0[c]
	3.112[d]	1.600[d]	-	-	2.0[d]
$Al_{0.875}V_{0.125}N$	3.114	1.608	191.11	- 10667.056	4.0

[a]Experimental reference (Schulz and Thieman, 1977), [b]Theoretical reference (Peng et al., 2008), [c]Theoretical reference (Yao et al., 2013), [d]Theoretical reference (Dihn et al., 2005).

the fit to the Murnaghan equation of state.

The lattice constant *a* and c/a ratio value calculated for the pure AlN agree well with values reported experimentally, since it differs by less than 1%. The values of the bulk modules of the pure AlN, $Al_{0.9375}V_{0.0625}N$, and $Al_{0.875}V_{0.125}N$ concentrations are higher, which confirms that they are quite rigid, making them good candidates for possible application in devices operated at high temperature and high power, as well as in hard coatings.

For $Al_{0.9375}V_{0.0625}N$ compound, the values calculated for lattice constant *a*, c/a ratio and magnetic moment are in good agreements with that reported theoretically by Yao et al. (2013) and Dihn and Katayma-Yoshida (2005). However, for $Al_{0.875}V_{0.125}N$ compound, Yao et al., (2013) and Dihn and Katayma-Yoshida (2005) did not give the structural parameter value and the magnetic moment value; these values are given for the first time as shown in Table 1.

For 6.25% concentration of V doping, the lattice constant in the $Al_{0.9375}V_{0.0625}N$ compound changes only slightly with respect to pure AlN. There is a reduction of 0.128% for *a*, which resulted from the minor difference in atomic radius between V (1.34 Å) and Al (1.43 Å). For 12.5%, the reduction on the lattice constant is 0.224%.

Figure 2a shows that for the $Al_{0.9375}V_{0.0625}N$ compound, the calculated total energy of spin polarized state (FM phase) is lower than that of the non-spin polarized state (non-magnetic phase) by about 55.4 meV, while that for the $Al_{0.875}V_{0.125}N$ compound (Figure 2b), in the ground state (FM state) is lower than the AFM state by about ΔE = 21.2 meV. This indicates that the ground state of V-doped AlN is ferromagnetic.

The spin polarization calculations for $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds result in a magnetic moment of 2.0 and 4.0 μ_β per supercell, respectively. The magnetization for $Al_{0.9375}V_{0.0625}N$ is the same magnitude than that of $Ga_{0.9375}V_{0.0625}N$ compound (Guangrui et al., 2012). This demonstrates that it is very likely for V to order ferromagnetically in AlN.

In order to verify the relative stability of the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds, the

Table 2. Formation energy.

Compound	E_f (eV)
$Al_{0.9375}V_{0.0625}N$	2.66
$Al_{0.875}V_{0.125}N$	3.04

corresponding formation energy is calculated, which is expressed as:

$$E_f = E_{V:AlN} - E_{AlN} - nE_V + nE_{Al}$$

where $E_{V:AlN}$, E_{AlN}, E_V and E_{Al} are the energies in the ground state of V-doped AlN, pure wurtzite AlN, bcc V, and fcc Al, respectively (Murillo et al., 2015). The integer n is the number of V atoms that substitute for Al. The total energy E_V and E_{Al} in their ground states was calculated. The energy values are -1955.656 eV and -169.564 eV, respectively. Additionally, to ensure the results are accurate, a formation enthalpy of -3.31 eV for AlN wurtzite was obtained, which is in good agreement with the experimental value of -3.28 eV and the theoretical value of -3.33 eV (Shi et al., 2008; Thapa et al., 2010). Table 2 shows the calculated values of formation energy E_f.

The value of the formation energy of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds are positive. Therefore, the compounds are metastable and the moderate formation energy values indicate that the compounds can easily be grown experimentally. Additionally, it was found out that the value of formation energy for $Al_{0.9375}V_{0.0625}N$ is significantly lesser than the Cr-doped AlN (E_f = 4.41 eV) (Cui et al., 2004), Mg-doped AlN (E_f = 3.80 eV) (Sandhya et al., 2014). This indicates that V-doped AlN is energetically preferred and therefore this proves that is most likely to obtain sufficient magnetization, a room temperature in V-doped AlN. Additionally, the heat energy K_BT (where K_B is constant Boltzmann and T is the temperature) was calculated. In this case K_BT = 26.55 eV. It was found out that the heat energy K_BT (26.55 meV) is greater than the energy difference ΔE (21.2 meV). This result confirms that it is possible to obtain sufficient magnetization, a room temperature in V-doped AlN

Electronic and magnetic properties

The theoretical lattice constants and c/a ratio of the AlN and the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds shown in Table 1 were used to calculate the band structure and the spin-polarized density of states (DOS) along the high-symmetry direction in the first Brillouin zone.

The band structure for pure AlN and $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds are shown in Figure 3. Figure 3a shows the band structure of pure AlN. This confirms the direct semiconductor behavior, with the top of the valence band and the bottom of the conduction band located at the point of the Brillouin zone. A direct band gap of about 4.3 eV was found. The magnitude of this gap is smaller than the value reported experimentally (6.2 eV) for AlN in the wurtzite structure (Vurgaftman et al, 2001). This occurs because the GGA approximation underestimates the forbidden energy gap in semiconductors. The valence band is mainly determined by Al-2p states and N-2p makes a minor contribution.

Figure 3b and c shows the band structure of the ternary $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds, respectively. It can be observed that the minority spin (down) states preserve a band gap (with an energy gap larger than 4.4 eV), but in the majority spin (up) states being metallic, because there is a penetration towards the prohibited energy zone of the states 3d-V in greater proportion and states N-2p and Al-2p in lesser proportion. Therefore, due to the introduction of one and two V atoms into the structure of AlN, it loses its semiconductor nature. The allowed ternary $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds exhibit half-metallic behavior. It can be seen that the spin up orientation of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds is partially filled, because they exhibit dispersed bands above the Fermi level. High polarization of the conduction carriers is confirmed by the fact that the V atom dopants couple ferromagnetically and that there is a high presence of conduction carriers in the majority spin channel. These compounds exhibit a spin polarization of 100% of the conduction carriers in the ground state, and they are responsible for the conduction in V-doped AlN. This is a requirement for spin injectors (Díaz et al., 2015). This finding suggests that these ternary compounds can be efficiently used in spintronics.

In order to fully understand the mechanism by which the FM state in $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds is stabilized and at the same time identify the contribution of each atom to the ferromagnetism, the total density of states (TDOS) and partial density of states (PDOS) for the $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds were calculated. Figure 4a and b shows the TDOS and PDOS: 3d states of V atom, 2p states of the first neighboring Al atom, and the first neighboring N atom of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds, respectively. The total density of states confirms that due to the V substitution at the Al site, the compound has a half-metallic character. This behavior occurs because in the valence band near the Fermi level, majority of the spins are metallic and the minority spins are semiconductors. According to the energy scale, Figure 4a shows that in the valence band near the Fermi level, the spin-up density is mainly dominated by the V-3d states and to a lesser extent by the Al-2p and N-2p states, which cross the Fermi level. This indicates the magnetic moment comes from 3d-V orbitals mainly and the Al-2p and N-2p states in minor

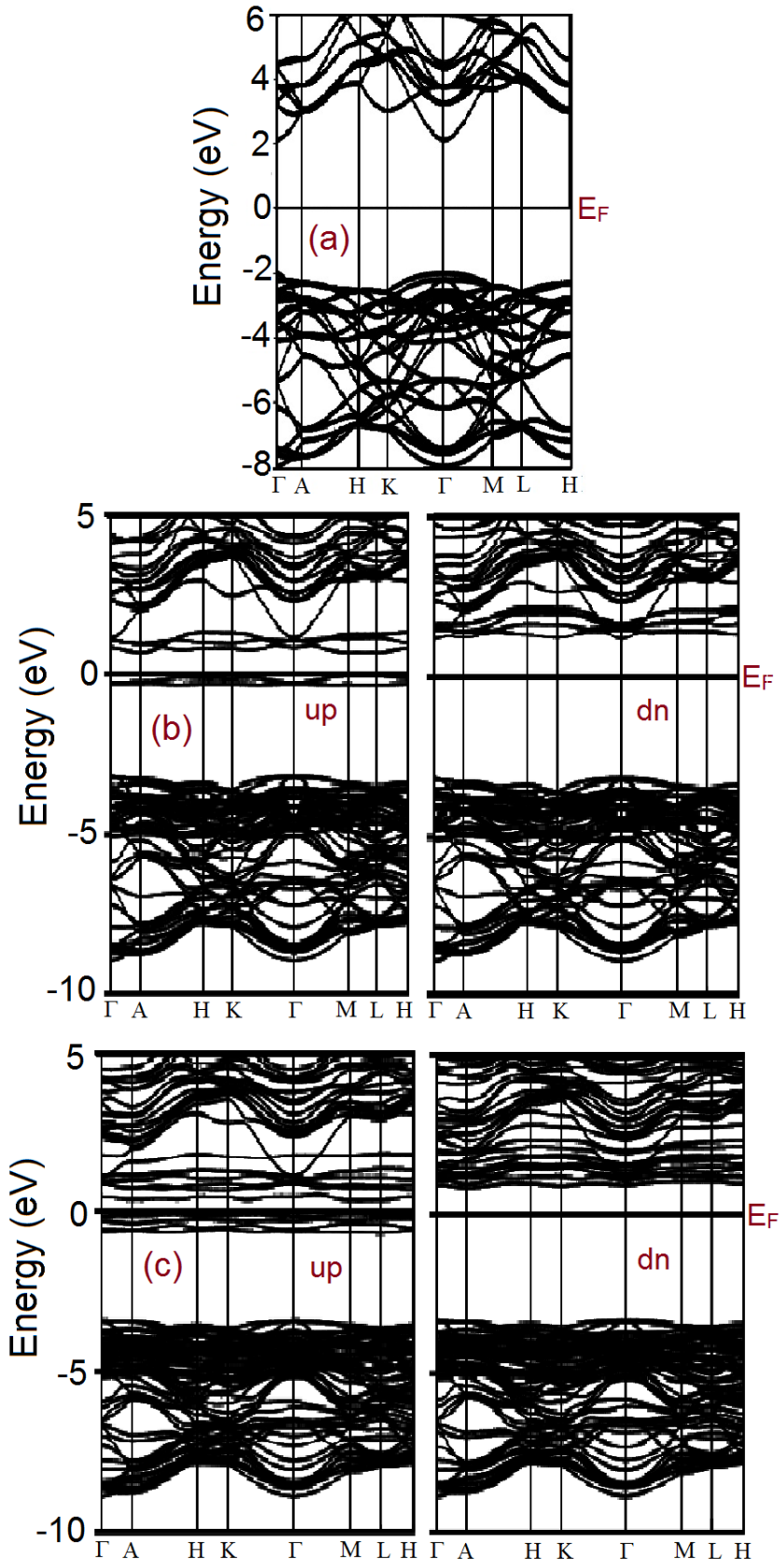

Figure 3. Electronic energy bands for: (a) pure AlN, (b) $Al_{0.9375}V_{0.0625}N$, (c) $Al_{0.875}V_{0.125}N$.

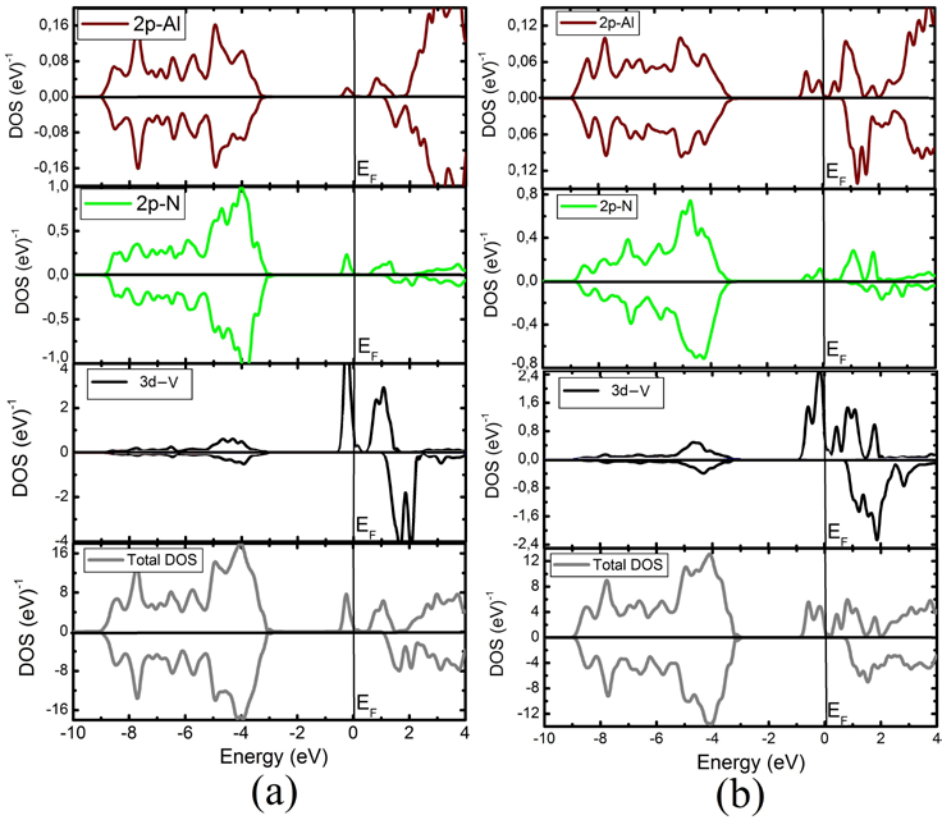

Figure 4. Partial and total density of states for the allowed ternary (a) $Al_{0.9375}V_{0.0625}N$ and (b) $Al_{0.875}V_{0.125}N$ compounds.

contributions.

Figure 4b shows that in the $Al_{0.875}V_{0.125}N$ compound, the magnetic moment induced by two V dopant and the corresponding moment distribution are nearly consistent with those in the cases of a single V atom substitution in a supercell.

Figure 4a and b shows that in the majority spin, the partial density of states belonging to the V-3d orbital exhibits a high peak near the Fermi level, about -0.5 eV for $Al_{0.9375}V_{0.0625}N$ and -0.65 eV for $Al_{0.875}V_{0.125}N$, thus indicating localized states in that region. In the valence band around the Fermi level, the V-3d states overlap with another two peaks of smaller amplitude belonging to N-2p and Al-2p. Therefore, there is hybridization between the V-3d, N-2p, and Al-2p orbitals. Additionally, the TDOS confirms the presence of some unoccupied bands above the Fermi level, because there is no contribution of spin down and the majority spin exhibits a hybridization and polarization between the V-3d, N-2p, and Al-2p states, resulting in a magnetic moment of 2.0 μ_β/Cell for $Al_{0.9375}V_{0.0625}N$ and 4.0 μ_β/Cell for $Al_{0.875}V_{0.125}N$. The magnetic moment is due to the V^{3+} configuration (with electronic configuration $[Ar]3d^2$). This implies that when the V atom occupies at the Al site in the AlN, it gives up three electrons and two valence electrons remain (d^2 configuration). These valence electrons couple ferromagnetically and as a result the two electrons produce a total magnetic moment of 2 μ_β/atom-V. Touati et al., (2008)[41] reported a valence of V^{3+} for infrared luminescence in V-doped GaN samples grown with MOVPE on a sapphire substrate. Finally, the magnetic moment of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds are integers, therefore, this confirms that each compound is ferromagnetic and half-metallic.

Conclusions

First-principles total energy calculations to determine the structural, electronic, and magnetic properties of $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds were carried out. The calculated values of the bulk modules were quite high; therefore, the ternary compounds are quite rigid, which makes them attractive for potential applications at high temperatures and for hard coatings. Also, the compounds were found to exhibit ferromagnetic and half-metallic behavior; due to polarization and hybridization, the orbitals V-3d, 2p-N, and 2p-Al cross the Fermi level. Finally, it was found that $Al_{0.9375}V_{0.0625}N$ and $Al_{0.875}V_{0.125}N$ compounds exhibit magnetic properties with magnetic

moments 2 μ_β and 4 μ_β per supercell, respectively. These properties show that these compounds are good candidates for possible application in diluted magnetic semiconductors, spin injectors, and other spintronics applications.

Conflict of Interests

The authors have not declared any conflict of interests.

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