

Electron Band Structure of Gadolinium Gallium Nitride

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Theoretical determination of the electron band structure of $Gd_xGa_{1-x}N$ semiconductor compound alloy is made in this paper. The authors model the GdGaN alloy on Gd content. Segregated Gd species in wurtzite GaN containing Gd are not considered, only alloyed species with Gd substituting on Ga site. For this arrangement a new ternary semiconductor $Gd_xGa_{1-x}N$ with $0 < x < 1$ is identified and it has two binary constituents – GaN and GdN. This condition allows the authors to introduce a primitive cell of binary constituent GdN satisfying the following conditions: a) Gd atom substitutes for a Ga atom saving the tetrahedral shape of the crystal cell; b) Gd atom has valence equal to 2 and the N atom has valence equal to 5; c) the Gd-N bond is ion-covalent. Using the conditions a), b) and c) it is found that the hybrid $2sp^3$ orbital of N atom attracts an electron from the $5d$ orbital of Gd atom, due to existence of polar energy 1.32 eV, and this electron replaces on the $6p$ orbital of Gd atom. In this way the Gd-N bond becomes of sp^3 type.

The variational principle is used for determination of the energy relations in this replacement. The following parameters of the GdN binary constituent are found: 1) Charge transfer between $5d$ -orbital of Gd atom and $6p$ -orbital of the same atom is 0.9976 electrons and as result the valence electron cloud of Gd atom is replaced in direction to N atom, i.e. donor behavior can be expected from the alloyed Gd atoms. 3) Using the Hartree-Fock method the authors have found that the electron energy term of the $6p$ -orbital of Gd atom, which forms GdN tetrahedral cell, is -2.00 eV. LCAO electron band structures of wurtzite $Gd_xGa_{1-x}N$ for temperature 300K are calculated by the previously developed method [1, 2]. A multinary crystal is considered to be a periodical crystal having a large primitive super-cell, containing a finite number of quasi-elementary cells. It is found [1] that the electron energy in a primitive super-cell of the multinary crystal can be presented in the following way.

$$E(\mathbf{r}) = \sum_{\mathbf{q}} \delta(\mathbf{r} - \mathbf{R}_{\mathbf{q}}) E(\mathbf{q}) \quad (1)$$

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Where \mathbf{r} is the radius-vector of the electron, $E(\mathbf{q})$ is electron energy in the quasi-elementary cell \mathbf{q} having radius-vector $\mathbf{R}_{\mathbf{q}} = q_1\mathbf{a}_1 + q_2\mathbf{a}_2 + q_3\mathbf{a}_3$ (\mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 are the three basis vectors of the primitive super-cell), and $\delta(\mathbf{r} - \mathbf{R}_{\mathbf{q}})$ is a delta-function. The electron band structure of the multinary crystal can be determined on the basis of the interactions within the primitive super-cell, which determine the corresponding sub-bands. As a matter of fact the electron band structure of the multinary crystal determined in this way contains the same sub-bands as those determined for the primitive super-cell of the same multinary crystal without consideration of the localizations of the interactions. However here the sub-bands are localized in the corresponding quasi-elementary cells. This structure is given in Fig.1 as only the sub-band of the bottom of the conduction band (CB) and the sub-band of the top of the valence band (VB) are provided in consideration that the energy of the vacuum level is zero. The results show: a) Semi-metallic behavior must be expected due to overlapping between VB and CB in sectors 4 (Gd dominating) and 5 (pure GdN) of Fig.1 where VB rises in direction Σ and goes above CB minima. b) The magnetic properties are determined mainly by $4f$ electrons of Gd atom. It can be considered possible interaction $4f \leftrightarrow VB$ of sector 1 (pure GaN), which means that if a $4f$ electron moves to VB the total magnetic momentum per atom changes.

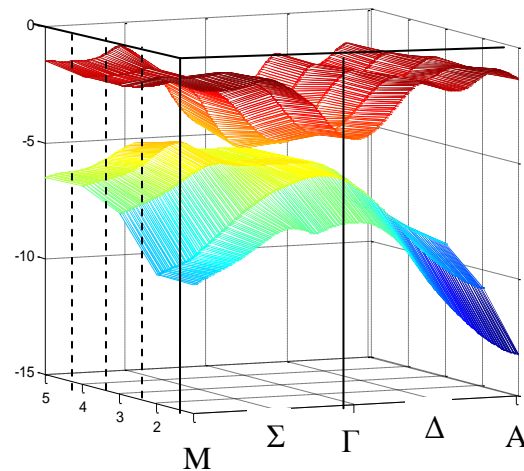


Fig. 1. Electron band structure of $Gd_xGa_{1-x}N$

[1] D. Alexandrov, Journal of Crystal Growth, 246, p.325, 2002

[2] D. Alexandrov et al., Physica Status Solidi, 203, p.25, 2006