Influence of pressure and composition on electronic properties, phonon frequencies, and sound velocity for the zinc-blende GaAs$_{1-x}$N$_x$ alloy

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Abstract
We investigated the electronic, phonon frequencies, and sound velocity of GaAs$_{1-x}$N$_x$ ternary semiconductor alloys with the zinc-blende crystal structure over the entire nitrogen concentration range (with $x$ from 0 to 1) using the empirical pseudo-potential model within the virtual crystal approximation including the compositional disorder effect. The pressure-dependent electronic, phonon frequencies and sound velocity of GaAs$_{1-x}$N$_x$ ternary alloy have been studied. Our findings and the existing experimental data are found to be in good agreement. According to the dependence on pressure, a rising bandgap is predicted for GaAs$_{1-x}$N$_x$ alloys at high-pressure values. According to the findings of this study, the GaAs$_{1-x}$N$_x$ characteristics could have substantial optoelectronic applications in the infrared and mid-infrared spectral ranges.

Keywords Phonon frequencies · Sound velocity · Electronic properties · GaAs$_{1-x}$N$_x$ · Pressure

1 Introduction

The III–V semiconductors which contain nitrogen provide the foundation of the material for a variety of well-established commercial technologies [1]. The study of nitride-based III–V compound semiconductors has recently received a lot of attention. Because of their potential uses in solar cells, linear and nonlinear optics, and integrated optical systems, they have attracted a lot of attention [2]. GaAs$_{1-x}$N$_x$ ternary alloy appears to be a promising material for use in light detectors [3] and optical fibers [4]. Incorporating a little quantity of nitrogen into III–V compound semiconductors results in a strong bowing parameter modulation of the bandgap, allowing the alloys of interest to cover a wide range of wavelengths for essential industrial applications [5–8]. The electronic energy band structure parameters of semiconducting materials are crucial in determining the quality of samples of interest and also in guiding the design of optoelectronic devices, as well as their development and production [2]. The energy bandgap of semiconductor alloys is regarded as one of the most essential key characteristics for devices because it is closely related to the operating wavelength of optoelectronic devices. It is worthwhile to investigate and debate the physical properties of GaAs$_{1-x}$N$_x$ ternary alloys in terms of electronic structure, phonon frequencies, and sound velocity for this purpose. Furthermore, pressure is a critical component in determining the state of materials and due to the rapid development of the diamond anvil technique, study into materials under high pressure is becoming possible [9]. Due to the possibility of a sudden change in atom arrangement under applied pressure, the characteristics of high-pressure phases may differ significantly from those under normal conditions [9]. The effect of pressure on the electronic, optical, mechanical properties, phonon frequencies, and sound velocity of the semiconductor alloys has been studied by several authors [10–20].

Gueddim et al. [1] investigated the effect of nitrogen concentration on the electronic properties of zinc-blende GaAs$_{1-x}$N$_x$ alloys for small amounts of nitrogen. For GaAs$_{1-x}$N$_x$ ternary semiconductor alloys with the zinc-blende crystal structure, Bourarissa et al. [2] investigated the composition dependence of direct and indirect bandgap energies, refractive index, valence bandwidth, anti-symmetric gap, high frequency and static dielectric constants over the
entire nitrogen concentration range (x from 0 to 1). Jian et al. [9] studied the structural, mechanical, and electronic properties of GaAs$_{1-x}$N$_x$ ternary alloys with the zinc-blende crystal structure over the entire nitrogen concentration range using first-principles total-energy calculations within a density functional theory (DFT) framework. Although many studies have been used to analyze the properties of GaAs$_{1-x}$N$_x$, there has been relatively little works on the associated properties such as phonon frequencies and sound velocity of this alloy in the presence of pressure. Many methods are used to calculate the electronic properties among them the so-called empirical pseudo-potential method [21–26].

In this work, we investigated the effect of pressure and nitrogen content on the electronic behaviors such as the energy band structure and energy bandgaps, phonon frequencies, and sound velocity of GaAs$_{1-x}$N$_x$ alloys using the empirical pseudo-potential technique EPM under the virtual crystal approximation VCA.

### 2 Computational

The ternary alloy GaAs$_{1-x}$N$_x$ under study is bordered by the two binary materials GaAs and GaN. We began by computing the binary compounds’ direct and indirect energy bandgaps under the effects of pressure and composition. The second stage is to calculate the bowing parameters by studying the energy bandgaps of the ternary alloys in the virtual crystal approximation, which includes the effective disorder potential. The energy bandgaps and the electronic band structure were determined in the final stage using the computed results of the corresponding binary compounds of the ternary GaAs$_{1-x}$N$_x$ alloy under the effects of composition and pressure.

The energy eigenvalues are calculated by solving numerically the secular determinant equation [27–30]

$$\begin{align*}
\left| \frac{1}{2} [k + G']^2 - E_{\text{el}}(x, p) + \sum_{G \neq G'} V(\Delta G, x, p) \right| &= 0 \\
\text{where } V(\Delta G, x, p) \text{ is the } x \text{ and } p \text{-dependent pseudo-potential with } \Delta G = G - G', G \text{ and } G' \text{ are the reciprocal lattice vectors.}
\end{align*}$$

(1)

The potential of GaAs$_{1-x}$N$_x$ ternary alloy is calculated by the improved VCA. The symmetrical $W^S$ and anti-symmetrical $W^A$ form factors of GaAs$_{1-x}$N$_x$ are calculated using the associated binary compounds’ adjusted form factors GaAs and GaN as [31]:

$$W^{S,A}(x, p) = x W^{S,A}_{\text{GaAs}} + (1 - x) W^{S,A}_{\text{GaN}} - \delta \sqrt{x(1-x)} [W^{S,A}_{\text{GaAs}} - W^{S,A}_{\text{GaN}}]$$

(2)

where $\delta$ is a quantity that can be adjusted to simulate the disorder effect. In the case of our GaAs–GaN system, the potential described by relation (2) is employed by adjusting $\delta$ until a close agreement between the estimated and experimentally observed or calculated fundamental bandgap bowing parameters was achieved. A value of 0.6999 for $\delta$ yields a large fundamental bandgap bowing coefficient in the current calculations, which is compatible with the experiment. If $\delta$ is altered from 0.6999, we obtain bowing parameters that are incompatible with the experimental ones reported in Ref [32].

Three independent elastic constants $C_{11}$, $C_{12}$, and $C_{44}$ in a cubic lattice are acquired using appropriate lattice distortions [33–35]. The influence of strain on electronic properties necessitates a thorough understanding of the material’s mechanical properties, particularly the elastic constants that explain the response to macroscopic stress. For this reason, the elastic constants of the materials under investigation, namely $C_{11}$ and $C_{12}$, were computed using the same approach as Bouarissa [36], which was based mostly on Baranowski’s work [37], where $C_{11}$ and $C_{12}$ are represented as

$$c_{11} = \frac{\sqrt{3} \ h^2}{4d^5} \left[ 4.37(5 + \lambda) \left( 1 - a_p^2 \right)^{3/2} - 0.60751 \left( 1 - a_p^2 \right)^{1/2} \right]$$

(3)

$$c_{12} = \frac{\sqrt{3} \ h^2}{4d^5} \left[ 4.37(3 - \lambda) \left( 1 - a_p^2 \right)^{3/2} + 0.60751 \left( 1 - a_p^2 \right)^{1/2} \right]$$

(4)

where $d = \sqrt{\frac{a \pm 1}{3}}$, is the nearest-neighbor distance, $\lambda = 0.738$. The $c_{44}$ can be obtained using the valence force field model [38].

$$c_{44} = \frac{3 \left[ c_{11} + 2c_{12} \right]}{\left[ 7c_{11} + 2c_{12} \right]}$$

(5)

To calculate the sound velocity, we used the stiffness constants (cij) and the crystal density (g) [39] as

$$v = \sqrt{\frac{c_{ij}}{g}}$$

(6)

Lyddane–Sachs–Teller relations were used to compute the longitudinal and transverse phonon frequencies (LO and TO) [40, 41]

$$\frac{\omega_{TO}^2}{\omega_{LO}^2} = \frac{\varepsilon_{\infty}}{\varepsilon_0}$$

(7)

$$\omega_{TO}^2 - \omega_{LO}^2 = \frac{4\pi e^2}{M \Omega \varepsilon_{\infty}}$$

(8)
where $\Omega$, $M$, $e$, $e_T^*$, $\varepsilon_0$, and $\varepsilon_\infty$ are the volume occupied by one atom, twice the reduced mass, electron charge, transverse effective charge, static dielectric constant, and high-frequency dielectric constant, respectively. In our calculations, we used our own proprietary program based on MATLAB language.

3 Results and discussion

The energy bandgaps for GaAs$_{1-x}$N$_x$ alloy as a function of composition at constant values of pressure $p=0$ and 120 kbar are displayed in Fig. 1a and b. It is noted that the direct ($E_\Gamma$) and indirect ($E_L$ and $E_X$) are nonlinearly increased with increase in the nitrogen composition from 0 to 1. This is due to the lattice constant diminishing with rising composition and the potential energy raises which leads to an increase in energy bandgaps. The GaAs$_{1-x}$N$_x$ alloy at ambient pressure is converted from direct to indirect semiconductor at the crossover energy 1.3 eV and at $x=0.12$ as shown in Fig. 1a, which matches the experimental value of 1.517 eV [42] and theoretical value of 1.5 eV [9] fairly well. Furthermore, the GaAs$_{1-x}$N$_x$ alloy at $p=120$ kbar is transformed from direct semiconductor to indirect one at 0.82 as in Fig. 1b. It is observed that the conversion point from direct to indirect semiconductor alloy for GaAs$_{1-x}$N$_x$ is raised by enhancing pressure. Naturally, the energy bandgaps of the ternary semiconductor alloys are correlated to the alloy composition by a quadratic relationship, with the bandgap bowing parameter described as the quadratic term of the relationship. The calculated results for the energy bandgaps for the GaAs$_{1-x}$N$_x$ alloy can be fitted by a polynomial as follows:

At $p=0$ kbar,

\[
E_L = 9.2668 x^2 - 4.9626 x + 1.7536 \tag{9}
\]

\[
E_\Gamma = 3.7805 x^2 - 2.1869 x + 1.4224 \tag{10}
\]

\[
E_X = 8.634 x^2 - 6.1561 x + 1.8222 \tag{11}
\]

At $p=120$ kbar,

\[
E_L = 8.7915 x^2 - 4.8549 x + 2.1012 \tag{12}
\]

\[
E_\Gamma = 3.0194 x^2 - 2.2471 x + 2.4475 \tag{13}
\]

\[
E_X = 8.0886 x^2 - 5.6847 x + 1.8079 \tag{14}
\]

Our data for the bowing parameters for conduction $L$, $\Gamma$ and $X$ valleys at 0 kbar are 9.2668 eV, 3.7805 eV, and 8.634 eV, respectively. The value of the bowing parameters for the GaAs$_{1-x}$N$_x$ acquired in the current work is reliable with those documented experimentally and theoretically [7, 43, 44]. It is seen that the bowing parameters are decreased with enhancing pressure from 0 to 120 kbar as shown in Eqs. (6–11). The energy bandgaps at $p=0$ kbar for GaAs$_{1-x}$N$_x$ alloy at $x=0$ (GaAs) and at $x=1$ (GaN) are $E_L=1.75$ eV, $E_\Gamma=1.42$ eV, $E_X=1.82$ eV, $E_L=6.25$ eV, $E_\Gamma=3.20$ eV, and $E_X=4.61$ eV, respectively. The experimental [45, 46] and theoretical [2, 47] data of the energy bandgaps for the GaAs$_{1-x}$N$_x$ at ambient pressure at $x=0$ (GaAs) and at

Fig. 1 Energy bandgaps for GaAs$_{1-x}$N$_x$ as function of composition at a $p=0$ kbar and b 120 kbar
\( x = 1 \) (GaN) are \( E_L = 1.72 \, \text{eV}, E_T = 1.42 \, \text{eV}, E_X = 1.81 \, \text{eV}, \)
\( E_L = 6.04 \, \text{eV}, E_T = 3.30 \, \text{eV}, \) and \( E_X = 4.57 \, \text{eV}, \) respectively. This comparison shows that our results are in excellent agreement with experimental and theoretical data at the normal pressure. The energy bandgap values produced in this study at \( p = 120 \, \text{kbar} \) are predictions and may be used as a guide for future studies.

The phonon frequencies play an essential role in a wide range of crystalline material properties and dynamical behaviors, including thermal properties, mechanical properties, phase transitions, and superconductivity \([48]\). The longitudinal \( \omega_{\text{Lo}} \) and transversal \( \omega_{\text{To}} \) phonon frequencies in \( 10^{13} \, \text{s}^{-1} \) for GaAs\(_{1-x}\)N\(_x\) alloy at the center (\( \Gamma \)) of the Brillouin zone (BZ), as a function of composition \( x \) at ambient pressure, are shown in Fig. 2. It is noted that the longitudinal \( \omega_{\text{Lo}} \) and transversal \( \omega_{\text{To}} \) phonon frequencies are nonlinearly increased with the increase in nitrogen concentration. From Fig. 2, it is seen that the longitudinal \( \omega_{\text{Lo}} \) phonon frequency has high values than the transversal \( \omega_{\text{To}} \) phonon frequency. In the case of GaAs\(_{1-x}\)N\(_x\) at \( x = 0 \) (GaAs), our calculated results of \( \omega_{\text{Lo}} \) and \( \omega_{\text{To}} \) are in good accord with the experimental data quoted in Refs. \([41]\). Also, the calculated values of \( \omega_{\text{Lo}} \) and \( \omega_{\text{To}} \) for GaAs\(_{1-x}\)N\(_x\) at \( x = 1 \) (GaN) are in good agreement with those cited in Refs. \([49, 50]\). The analytical expressions for both \( \omega_{\text{Lo}} \) and \( \omega_{\text{To}} \) in \( 10^{13} \, \text{s}^{-1} \) for GaAs\(_{1-x}\)N\(_x\) give the following relations:

\[
\omega_{\text{Lo}} = 13.062x^2 - 2.6424x + 6.7883
\]

\[
\omega_{\text{To}} = 9.8075x^2 - 1.391x + 6.4897
\]

Equations (12, 13) can be used to calculate the \( \omega_{\text{Lo}} \) and \( \omega_{\text{To}} \) for any value of composition in the range (0–1) for the GaAs\(_{1-x}\)N\(_x\) alloy. The phonon dispersion schematic can be determined by the same method by calculating the longitudinal \( \omega_{\text{Lo}} \) and transversal \( \omega_{\text{To}} \) phonon frequencies at \( \Gamma \) and \( X \) high symmetry points and plotting them with the wave vector.

Acoustic velocity is important in determining crystal density and mechanical properties such as elastic constants, bulk modulus, shear modulus, and Young’s modulus. The composition-dependent sound velocity in \( 10^5 \, \text{cm} \, \text{sec}^{-1} \) for the GaAs\(_{1-x}\)N\(_x\) alloy at ambient pressure is displayed in Fig. 3. It is seen that the sound velocity in the directions [100], [110], and [111] is increased with increase in the composition \( x \) from 0 to 1. This is due to the elastic constants \((C_{11}, C_{12}, \text{and } C_{44})\) are increased by increasing composition. Our calculated results for the sound velocity for the considered alloy at \( x = 0 \) (GaAs) in the directions [100], [110], and [111] are \( v_{LA} = 5.00 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( v_{TA1,T2} = 3.18 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( v_{LA} = 5.29 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( v_{TA1} = 2.66 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( v_{TA2} = 3.18 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( v_{LA} = 5.39 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( v_{TA1,T2} = 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), respectively. The experimental values which are given by Adachi \([39]\) are \( 4.73, 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( 3.34, 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( 5.24, 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( 2.47, 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( 3.34, 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( 5.39, 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), \( 2.79, 2.85 \times 10^5 \, \text{cm} \, \text{sec}^{-1} \), respectively. This comparison shows that there is a good agreement.
agreement between our values and the experimental data. The calculated results for GaAs$_{1-x}$N$_x$ alloy at $x = 1$ (GaN) are $7.24 \times 10^5$ cm sec$^{-1}$, $4.58 \times 10^5$ cm sec$^{-1}$, $7.66 \times 10^5$ cm sec$^{-1}$, $3.83 \times 10^5$ cm sec$^{-1}$, $4.58 \times 10^5$ cm sec$^{-1}$, $7.80 \times 10^5$ cm sec$^{-1}$, $4.10 \times 10^5$ cm sec$^{-1}$. Also, the rest calculated data for the compositions (0.1 to 0.9) are predictions that could be used as a guide for future investigation.

The electronic band structure is one of the most significant basic properties of a material and is in particular essential in electronic, photo-electronic, and photocatalytic applications [51]. The electronic band structure of semiconductors has a significant impact on the material’s final electronic and optical properties, as well as the functionality of the devices that incorporate them [52]. The energy band structure for GaAs$_{0.5}$N$_{0.5}$ alloy for two different values of pressure $p = 0$ kbar (solid lines) and $p = 120$ kbar (dashed lines) at L, Γ and X high symmetry points is displayed in Fig. 4. It is seen that the valence bands are slightly affected by pressure, while the conduction bands are greatly affected by the applied pressure. It is perceived from Fig. 4 that the differences between the two curves for the two pressures are more obvious at the Γ-point which is 727 meV, and both the two symmetry X-( 206 meV) and L-( 248 meV) points.

The energy bandgap is a significant factor in determining a material’s electrical conductivity and plays a very vital role in the electronic properties of a solid. The variation in energy bandgaps $E_L$, $E_\Gamma$, and $E_X$ for GaAs$_{0.5}$N$_{0.5}$ alloy concerning pressure is displayed in Fig. 5. It is seen that the direct $E_\Gamma$ and indirect $E_L$ and $E_X$ are increased with enhancing pressure. This is because rising pressure reduces the crystal’s dimension, as seen by variations in the lattice constant, increasing the electron’s potential energy. It is observed that the GaAs$_{0.5}$N$_{0.5}$ alloy is an indirect semiconductor over the whole region of pressure. This is because the $E_X$ has lower values of energy than $E_L$ and $E_\Gamma$. A quadratic fit to our data for $E_L$, $E_\Gamma$ and $E_X$ energy bandgaps as a function of the pressure of the alloy of interest gives

$$E_L(p) = 1.8388 + 0.0036p - 1 \times 10^{-05}p^2$$  \hspace{1cm} (17) \\
$$E_\Gamma(p) = 1.4315 + 0.0085p - 2 \times 10^{-05}p^2$$  \hspace{1cm} (18) \\
$$E_X(p) = 1.1109 + 0.0004p + 1 \times 10^{-05}p^2$$  \hspace{1cm} (19)

Figure 6 shows the calculated LO(Γ) and TO(Γ) phonon frequencies and their dependence on the pressure for the zinc-blende GaAs$_{1-x}$N$_x$ alloys at various values of nitrogen concentration (0, 0.5, and 1). As obvious in our results, the frequencies of these two modes diminish with the pressure.
for N composition 0 and 0.5. We have also noted that for \( x = 1 \), the LO(Γ) and TO(Γ) phonon are enhanced with increasing pressure. The calculated results for \( \omega_{\text{LO}} \) and \( \omega_{\text{TO}} \) for the alloy of interest for  \( x = 0 \) (GaAs) and for  \( x = 1 \) (GaN) at  \( p = 0 \) kbar are 6.78 × 10^{13} \text{ s}^{-1}, 6.48 × 10^{13} \text{ s}^{-1}, 19.31 × 10^{13} \text{ s}^{-1}, \) and 16.67 × 10^{13} \text{ s}^{-1}. The experimental [41] and published values [49, 50, 53] for \( \omega_{\text{LO}} \) and \( \omega_{\text{TO}} \) are in reasonable agreement for the considered alloy for  \( x = 0 \) (GaAs) and  \( x = 1 \) (GaN) at  \( p = 0 \) kbar. The following analytical formulas can be used to describe the fluctuation of the LO and TO of the alloy of interest with pressure.

For GaAs\(_{1-x}\)N\(_x\) alloy, these formulas (17–22) can be used to predict the LO and TO phonon frequencies for any pressure value in the range (0–120) kbar. This is owing to an absence of experimental and theoretical data regarding the ZB structure of GaAs\(_{1-x}\)N\(_x\) alloy at high pressures in the literature.

It is possible to proceed with the bulk sound velocity utilizing the relation (3) once the elastic constants (\( C_{11}, C_{12}, \) and \( C_{44} \)) have been determined. The variation in the acoustic wave speeds propagating in the [100], [110], and [111] directions with respect to pressure at different composition (0, 0.5, and 1) for GaAs\(_{1-x}\)N\(_x\) alloy is depicted in Fig. 7. Through this figure, one can note that both \( V_L \) and \( V_T \) increase monotonically with increasing pressure on going from 0 to 120 kbar for the composition  \( x = 1 \). This is due to the elastic constants are increased with rising in pressure at  \( x = 1 \). Furthermore, the acoustic wave speeds propagating in the [100], [110], and [111] directions decrease with enhancing pressure from 0 to 120 kbar for the compositions 0 and 0.5. This is because when pressure rises, the elastic constants decrease at  \( x = 0, 0.5 \). The velocities are almost constant against the pressure in GaN because the crystal density is nearly constant against the pressure. However, they are changing significantly in GaAs and GaAs\(_{0.5}\)N\(_{0.5}\). This is due to the density of crystal changes against the pressure in GaAs and GaAs\(_{0.5}\)N\(_{0.5}\). The calculated results of the longitudinal wave mode speed (\( v_L \)) and transverse wave mode speed (\( v_T \)) at  \( p = 0 \) kbar for GaAs\(_{1-x}\)N\(_x\) alloy for  \( x = 0 \) (GaAs) are \( v_{LA} = 5.00 \times 10^5 \text{ cm sec}^{-1} \), \( v_{TA1+TA2} = 3.18 \times 10^5 \text{ cm sec}^{-1} \), \( v_{LA-110} = 5.39 \times 10^5 \text{ cm sec}^{-1} \), \( v_{TA1+TA2-110} = 2.85 \times 10^5 \text{ cm sec}^{-1} \), \( v_{LA-110} = 5.29 \times 10^5 \text{ cm sec}^{-1} \), \( v_{TA1+TA2-110} = 2.66 \times 10^5 \text{ cm sec}^{-1} \), \( v_{TA2-110} = 3.18 \times 10^5 \text{ cm sec}^{-1} \), respectively. The calculated values for GaAs\(_{1-x}\)N\(_x\) alloy at  \( p = 0 \) kbar for  \( x = 1 \) (GaN) are \( v_{LA} = 7.24 \times 10^5 \text{ cm sec}^{-1} \), respectively.
$v_{TA1_{-}TA2_{-}100} = 4.58 \times 10^5 \text{ cm sec}^{-1}$, $v_{LA_{-}111} = 7.80 \times 10^5 \text{ cm sec}^{-1}$, $v_{TA1_{-}TA2_{-}111} = 4.10 \times 10^5 \text{ cm sec}^{-1}$, $v_{LA_{-}110} = 7.66 \times 10^5 \text{ cm sec}^{-1}$, $v_{TA1_{-}110} = 3.83 \times 10^5 \text{ cm sec}^{-1}$, $v_{TA2_{-}110} = 4.58 \times 10^5 \text{ cm sec}^{-1}$, respectively. A satisfactory agreement is obtained between our calculated data and the available experimental results [39].

4 Conclusion

The empirical pseudo-potential model under the virtual crystal approximation combined with the compositional disorder effect has been performed to study the electronic properties, phonon frequencies, and the acoustic wave velocity of zinc-blende ternary alloy GaAs$_{1-x}$N$_x$. The present theoretical study investigates the energy bandgaps, energy band structure, sound velocity, and the phonon frequency...
of zinc-blende GaAs$_{1-x}$N$_x$ alloys in the nitrogen concentration range 0–1 and in the pressure range 0–120 kbar. The bandgap of GaAs$_{1-x}$N$_x$ alloys is observed to rise in response to applied pressure, suggesting that applying pressure could be another effective method for controlling the bandgap of GaAs$_{1-x}$N$_x$ alloys. Our results are found to be in reasonable agreement with the available known data in the literature. Due to the absence of the experimental and theoretical values for the considered parameters of GaAs$_{1-x}$N$_x$ alloy in the pressure range 30–120 kbar, our results are predictions. The GaAs$_{1-x}$N$_x$ features may have significant optoelectronic applications in the infrared and mid-infrared spectral ranges.

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**Declarations**

**Conflict of interests** The authors have not disclosed any Conflict of interests.

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