Empirical pseudopotential study of electronic, positron, and structural properties of Ga$_{1-x}$Al$_x$N

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Abstract

Electronic and positron band structures and charge densities of Ga$_{0.5}$Al$_{0.5}$N using the empirical pseudopotential method (EPM) are investigated. For the ternary alloy Ga$_{1-x}$Al$_x$N, the virtual crystal approximation (VCA) is coupled with the pseudopotential method. The energies along $\Gamma$, $X$ and $L$ of Ga$_{1-x}$Al$_x$N alloy as a function of the mole fraction are calculated. Angular correlation of positron annihilation radiation (ACPAR) along different crystallographic directions in Ga$_{0.5}$Al$_{0.5}$N is calculated. Other quantities such as ionicity character and bulk modulus by means of recent models with respect to the mole fraction are discussed.

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Keywords: GaAlN; Positron; EPM

1. Introduction

The nitrides semiconductors have received extensive attention during the last few years due to their superior properties which have not been seen in conventional semiconductors like Si and GaAs. Since their band gaps are not sufficiently large, Si and conventional III–V semiconductors are not suitable for designing and fabricating optoelectronic devices in the violet and blue region of the spectrum. Moreover, GaAs based electronic devices cannot be used at high temperatures. On the contrary, because of their wide band gaps and strong bond strengths, group-III nitrides can be used for violet, blue and green emitting devices and for high temperature transistors [1-3]. Regarding these important applications of nitride semiconductors in optoelectronic devices, detailed knowledge of their electronic properties is necessary.

Positron annihilation spectroscopy has a valuable tool to study the properties in solid [4,5]. Along side with the evolution of the experimental techniques and applications, it has been highly important to develop the theoretical machinery, which is needed to give a satisfactory interpretation and analysis to the experimental annihilation characteristics for getting about the electronic and atomic structure of condensed matter. The angular correlation of positron annihilation radiations (ACPAR) is a powerful method for studying the electronic structure of solids [6] because the positron mainly samples the valence electrons. This method has become an important tool both for the investigation of electronic structure of metals and for understanding the behaviour radiation in semiconductors. Since the momentum distribution of emitted photons is created by positron annihilation with an electron in a solid, the momentum distribution of the photons thus corresponds to that of the electrons. The method is considered to be an effective microscopic probe into the materials.

A number of ACPAR studies have been carried out in covalent elemental semiconductors; Si and Ge by different groups [7-13]. Since compound semiconductors are covalent materials with a degree of ionicity, they are expected to show different behaviour compared to group-IV semiconductors, since the probability of the positron annihilating with the negative ion is greater than that with the positive ion [14]. In the case of ionic solids it was also found [15] that the positrons annihilate mostly near the anion.
The investigation of electronic properties of solids using electronic and positron charge densities represents an increasing importance. So far, this work has been concerned with electronic charge densities which were found to be useful for understanding the chemical bonds and the modification of the band structures by interstitial impurities [16,17]. The growth of the recent development in this field is to look for a better physical understanding of the charge densities.

The aim of this article is to examine the electronic and positron properties of the GaAs(Nb)N and reports a theoretical framework for the electron-positron momentum densities along (001) and (110) directions. On the other hand, the positron wave function is obtained in an identical manner as use it here.

position and interpretation of the pseudopotential formalism established as a convenient work to study many problems the required pseudopotential coefficients are fitted to few se-

2. Computational details

A pseudopotential model is used in this calculation and the required pseudopotential coefficients are fitted to few selected experimental data. The pseudopotential approach is established as a convenient work to study many problems as the electronic structure of simple metals, semimetals and semiconductors. The following paragraphs contain a brief exposition and interpretation of the pseudopotential formalism as use it here.

The empirical pseudopotential parameters (EPP) of a semiconductor is defined as a superposition of pseudopotentials of the form \( V = V_L + V_{NL} \), where \( V_L \) and \( V_{NL} \) are local and non-local parts, respectively. In this calculation the non-local part is omitted.

In the EPP, a small number of parameters consistent with the electronic band structure EBS is used, these parameters are determined to be fully interdependent among them. Some authors [19] have attempted to understand the EBS of semiconductors in a wider energy range.

The pseudopotential Hamiltonian is

\[
H = \frac{\hbar^2}{2m} \nabla^2 + V_L(r),
\]

contains an effective potential, which is expanded as Fourier series in a reciprocal lattice space. For a binary compound the expansion is written in two parts, symmetric and antisymmetric, with respect to an interchange of two atoms about their mid-point,

\[
V_L(r) = \sum_{G} \left[ S^L(\vec{G}) V^L(\vec{G}) + i S^R(\vec{G}) V^R(\vec{G}) \right] \exp(i \vec{G} r),
\]

where \( S^L(\vec{G}), V^L(\vec{G}), S^R(\vec{G}) \) and \( V^R(\vec{G}) \) are the symmetric and antisymmetric structure and form factors, respectively.

The EPP is determined by a non-linear least-square method, in which all the parameters are simultaneously op-timized under a criterion of minimising the root-mean square (r.m.s) deviation. The experimental electronic structure is used.

This non-linear least-square method requires that the r.m.s. deviation of the calculated level spacing (LS) from the exper-

imental ones is defined by

\[
\delta = \left[ \sum_{i,j} \frac{\Delta E_{i,j}^2}{m} - N \right]^{1/2},
\]

should be minimum.

\[
\Delta E_{i,j}^2 = E_{i,j}^{exp} - E_{i,j}^{cal},
\]

where \( E_{i,j}^{exp} \) and \( E_{i,j}^{cal} \) are the observed and the calculated LS’s between the \( n \)th state at the wave vector \( K = K_i \) and the \( j \)th at \( K = K_j \), respectively, in the \( m \) chosen pairs \((i,j)\). \( N \) is the number of the EPP. The calculated energies are given by solving the EPP secular equation. The starting values of the parameters are improved step by step by iterations until \( \delta \) is minimized. The parameters are denoted by \( P_n (n + 1) = P_n (n) + \Delta P_n \), where \( P_n (n) \) is the value at the \( n \)th iteration. The correction \( \Delta P_n \) is determined simultaneously by solving the system of the linear equations:

\[
\sum_{i=1}^{m} \left[ \sum_{j=1}^{m} \left[ (Q_i^u(K_i) - Q_i^u(K_j))(Q_j^v(K_j) - Q_j^v(K_i)) \right] \Delta P_{u} \right] = \sum_{i=1}^{m} \left[ \sum_{j=1}^{m} \left[ E_{i,j}^{exp} - E_{i,j}^{cal}(n) \right] Q_i^u(K_i) - Q_j^v(K_j) \right];
\]

where \( u = (1, 2, \ldots, N) \) and \( E_{i,j}^{cal}(n) \) is the value at the \( n \)th iteration and \( Q_n \) is given by

\[
Q_n^u(K_i) = \sum_{q \neq \delta} C_q(K_i) \left[ \frac{\partial H_p(K_i)}{\partial P_n} \right] C_q^*(K_i),
\]

where \( H_p(K_i) \) is the pseudo-hamiltonian matrix at \( K = K_i \) in the plane wave representation and the \( \delta \) pseudowave function at \( K = K_i \) is expanded as

\[
\Psi_{\delta}(K_i) = \sum_{q} C_q(K_i) \exp(i(K_i + \delta_q) r),
\]

where \( \delta_q \) is the reciprocal lattice vector. Eq. (7) shows that all the parameters are determined automatically in an independent way.

Here the approach of Aourag et al. [11,14] is followed for evaluating the positron wave function. With the assump-
tion that there is only one positron for many electrons, there is no exchange part because there is no positron–positron interaction. The positron potential is purely Coulombic in nature. There is a repulsive ion core potential and an attractive Hartree potential. In addition to these two parts, there
is a third part which comes from the electron–positron correlation. The total positron potential can thus be expressed as:

\[ V = V_i + V_e + V_{\text{ep}}, \]

where \( V_i \) is the potential due to the ion cores, \( V_e \) is the potential due to the valence electrons, and \( V_{\text{ep}} \) is the electron–positron correlation potential. The electron–positron correlation is a slow function of the electron density. It is generally flat in the interstitial region and swamped by \( V_i(r) \) and \( V_e(r) \) in the ion core region. It is not considered here since the crystal ion core potential must be periodic; it can always be written in terms of the atomic equivalent,

\[ V_i = \sum \sum v_i(r - R_n - T_i), \]

where \( R_n \) is a set of all Bravais lattice vectors and \( T_i \) is a non-primitive vector of a two-atom basis.

In the point core approximation,

\[ v_i = \frac{Z^2}{r}, \]

where \( Z \) is the number of valence electrons, on the other hand, the Coulombic potential due to the valence electrons is expressed as

\[ v_e(r) = -\frac{e^2}{r} \int \frac{Q_e(r')}{|r - r'|} d^3r', \]

where \( Q_e(r) \) is the charge density of the valence electrons for the binary compounds. \( Q_e(r) \) has been calculated using EPM scheme according to

\[ Q_e(r) = \sum_{n=1}^{\infty} \sum_{k=1}^{Z} |\psi_{ak}(r)|^2, \]

where \( \psi_{ak}(r) \) is the electron wave function. The positron density is evaluated by using \( \psi_{ak}(r) \) as in Eq. (12). In this calculation, the wave function has taken the fully thermalised positron (\( n = 1 \) and \( k = 0 \)).

\[ Q_p(r) = |\psi_{a(k=1,k=0)}(r)|^2. \]

The EPM scheme employs an extended plane wave’s basis, where the pseudowave function is expressed as an expansion over an arbitrary large number of plane waves as cleared in Eq. (7).

The positron after entering the solid gets thermalised and attracts the surrounding electrons (mostly valence electrons). The pair subsequently gets annihilated to emit two \( \gamma \)-rays. The probability of annihilation of the electron–positron pair with momentum \( p \) is proportional to the pair momentum density,

\[ M^{2\gamma}(\vec{p}) = \sum \sum |\sigma_{\nu}(k)|^2 \int |\psi_{ak}(\vec{r})\psi_{ak}(\vec{r})^\ast| d^3r. \]

(in the calculation there are about 600 \( k \)-points used to sample the Brillouin zone in each direction). \( \sigma_{\nu}(k) \) is the occupation number. In the long-slit angular correlation experiment one measures a component of the pair momentum density as given by

\[ N(p_z) = \int \int M^{2\gamma}(p_x p_y) dp_x dp_y. \]

The lattice constant of the alloy \( A_{1-x}B_xC \) (AC: GaN, BC: AlN) is determined by using Vegard’s rule as:

\[ a(x) = (1 - x)a_{AC} + x a_{BC}. \]

where \( x \) is the mole fraction and \( a_{AC} \) and \( a_{BC} \) are the lattice constants of the pure semiconductors AC and BC, respectively. Note that the lattice constant is a function of the alloy concentration \( x \), also the reciprocal lattice vector in the expansions is dependent upon \( x \). Therefore symmetric \( V^s \) and antisymmetric \( V^a \) forms of lattice constants different from the natural lattice constants of AlN and GaN were obtained by a polynomial fit to \( V \) as a function of \( |G' - G| \).

The alloy potential is calculated within the virtual crystal approximation, which treats an alloy as a perfectly periodic crystal with an average potential at each sublattice site and does not include the effects of periodic fluctuations in the crystal potentials. This model expects a linear variation of the principal parameters of the alloy. Particularly, the potential of the crystal is defined by a linear interpolation between the crystal constituents.

\[ V(x) = (1 - x)V_{AC} + x V_{BC}. \]

The electronic wave function has been calculated within the EPM scheme [20]. The form factors have been adjusted in order to have a good agreement between calculated and experimental band gaps. The adjusted symmetric and antisymmetric form factors are listed in Table 1. The calculated principal band gaps along with those obtained by experiment are listed in Table 2. A good agreement is observed. The fitting of the calculated principal energy bands to the experimental ones (EPM is capable for this mission), which encourages to make an application study comparable to results of experiments and others, in addition to wide band gaps and strong bond strengths, as indicated in introduction, these calculations and properties mean the ternary alloy is suitable for optoelectronics.

Table 1

<table>
<thead>
<tr>
<th>Compound</th>
<th>( a_{\text{opt}} )</th>
<th>V(4S)</th>
<th>V(4P)</th>
<th>V(4D)</th>
<th>V(4F)</th>
<th>V(4L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>4.50</td>
<td>0.380</td>
<td>0.000</td>
<td>0.070</td>
<td>0.280</td>
<td>0.200</td>
</tr>
<tr>
<td>GaN, Al, N</td>
<td>4.63</td>
<td>0.310</td>
<td>0.070</td>
<td>0.280</td>
<td>0.265</td>
<td>0.027</td>
</tr>
<tr>
<td>AlN</td>
<td>4.32</td>
<td>0.300</td>
<td>0.110</td>
<td>0.280</td>
<td>0.333</td>
<td>0.015</td>
</tr>
</tbody>
</table>
Table 2
The principal energy bands are in eV of zinc-blende GaN and AlN

<table>
<thead>
<tr>
<th>GaN</th>
<th>AlN</th>
</tr>
</thead>
<tbody>
<tr>
<td>E\textsubscript{\textGamma\textGamma}</td>
<td>3.38, 3.1, 3.2, 3.48, 2.08, 2.65, 2.00</td>
</tr>
<tr>
<td>E\textsubscript{\textGamma\textX}</td>
<td>4.57, 4.7, 5.10, 4.9</td>
</tr>
<tr>
<td>E\textsubscript{\textGamma\textL}</td>
<td>5.64, 6.2, 9.42, 9.3</td>
</tr>
</tbody>
</table>

\* Ref. [21].
\* Ref. [22].
\* Ref. [23].
\* Ref. [24].
\* Ref. [25].

3. Results and discussion

The electronic and positron band structures for Ga\textsubscript{0.5}Al\textsubscript{0.5}N are displayed in Figs. 1 and 2, respectively. The first obvious observation is the similarity between the electron and positron energy spectra, with the exception that the positron energy spectrum does not exhibit a band gap. The lowest positron energy state is the \textGamma\textGamma state at \textk\textGamma = 0; the corresponding eigenvalue \textE lies several eV above the interstitial potential.

The dispersion for an electron in the empty lattice model has the form:

\[ E = \frac{\hbar^2}{2m} |k + k_0|^2, \]  

(18)

where \textk\textGamma is the translational reciprocal lattice vector. To simplify the discussion, firstly choose a system of units which reduces (18) to

\[ E = (x + n_1)^2 + (y + n_2)^2 + (z + n_3)^2, \]  

(19)

where \textx, \texty, and \textz are the components of \textk and are continuous variables ranging throughout the first Brillouin zone, and \textn is integer representing discrete values of \textk\textGamma.

The evolution of the energy values along \textGamma\textGamma, \textGamma\textX, and \textGamma\textL directions for different mole fractions are examined as shown in Fig. 3. The different energy values decrease with increasing mole fraction. One may conclude that when the mole fraction or alloy concentration \textx increases, the transformation from first one binary semiconductor, GaN, to other one, AlN, through the ternary alloy Ga\textsubscript{1-x}Al\textsubscript{x}N is shown. A notice is observed at \textx = 0.58 where it regards a separation between the indirect band gap of Ga\textsubscript{1-x}Al\textsubscript{x}N alloy system and the direct band gap of the same system due to concentration change of the alloy.

The total valance charge density \textQ(\textr) in Eq. (12) is computed using the wave function \textΨ(\textr) and obtained from solving the secular equation of the EPM scheme [20]. The total valence charge density is obtained by summing over the four occupied valence bands. Fig. 4 presents the results of calculated electronic distribution (all the results are displayed along the \{1 1 1\} direction (bond axis)). In Fig. 4, the pseudocharge density for the sum of the valence bands for Ga\textsubscript{0.5}Al\textsubscript{0.5}N is shown. To illustrate the results of the bonding
characteristics in detail, the charge density is evaluated at more than 1600 points in the plane which intersects both the Ga, Al and N sites in the primitive cell.

The investigation of the chemical trends in solid-state properties appears as an extremely useful part of a new material research. From the charge density, one can notice that the profiles are not symmetric, most of the charge is localized at the anion site, and thus the nature of the bond is covalent with an ionic character. Similar results were obtained by Chadi and Cohen [26].

Also, the positron charge density $Q_p(r)$ is computed according to Eq. (13), where the origin of this calculation is at the bond site. The calculated positron charge density along the ⟨111⟩ direction for Ga$_{0.5}$Al$_{0.5}$N is shown in Fig. 5. The positron charge density is maximum in the interstitial region while the electron charge density is maximum at the bond center; this is the difference between the electronic and positron charge densities. The exclusion of the positron from the ion cores and the regions of the valence bands are clear. The positron is pushed out of the cell containing the larger valence and the larger ion core so it is pushed, out of the Ga cell in GaN and out of the Al cell in AlN. However, the used approximation does not require a large number of plane waves because it has no wiggles in the ion core region [27]. The wave functions are represented by plane waves as cleared in Eq. (7).

Fig. 6a and b shows the sections of the 2D electron–positron momentum densities for Ga$_{0.5}$Al$_{0.5}$N obtained by integration of the appropriate plane along ⟨001⟩ and ⟨110⟩ directions, respectively. In the low-momentum region the lineshapes for ⟨001⟩ and ⟨110⟩ directions are seen to be flatter. The nature of data in the low-momentum region is
Fig. 5. Distribution of the thermalised positron for Ga$_{0.5}$Al$_{0.5}$N along $\langle 111 \rangle$ direction.

Fig. 6. Integrated electron–positron momentum density of Ga$_{0.5}$Al$_{0.5}$N along (a) $\langle 001 \rangle$ and (b) $\langle 110 \rangle$ directions.
governed by \( \sigma \) and \( \pi \) bonds of the sp\(^3\) hybridised bonding orbitals.

For GaN \((x = 0)\), one could see an admixture of \((4p, 2p)\) \(\sigma\) and \((4p, 2p)\) \(\pi^*\) bonds which reduce a dip in the low-momentum region for both \(\langle 001\rangle\) and \(\langle 110\rangle\) directions. The same feature is observed for AlN \((x = 1)\) along \(\langle 110\rangle\) due to an admixture of \((4p, 1p)\) \(\sigma\) and \((4p, 2p)\) \(\pi^*\) bonds as observed by Panda et al. [28] in GaSb, and Berko et al. [29] in GaAs. However, because AlN is more metallic compared to GaN (the ionicity value \(f_{i\text{GaN}} = 0.773, f_{i\text{GaP}} = 0.758\) [30]), the wave functions in AlN are more diffused due to its smaller band gap compared to GaN. Under alloying effect, the overall values of \(M(p)\) are enhanced and the sharp peaking observed in \(\text{Ga}_{1-x}\text{Al}_x\text{N}\) in the direction \(\langle 110\rangle\) becomes a very low dip in the direction \(\langle 001\rangle\). This may be due to the weakness of the \(\sigma\) bond.

The refinement of the calculations is taking into account the core contributions would not change the results significantly because of the resulting smaller core contribution is almost compensated by the parabolic part due to the annihilation with the valence electrons. However, the pseudopotential method used in calculation reflects only the low-momentum components (LMC). Annihilation with electrons in the ion core involves high-momentum components (HMC), which cannot describe by the pseudopotential function due to their localisation.

In order to test the validity of our recent model [30] on the ternary alloy, the calculation of \(\text{Ga}_{1-x}\text{Al}_x\text{N}\) using hetropolar gap is carried out, hence the ionicity character \(f_i\) in the \(\text{Ga}_{1-x}\text{Al}_x\text{N}\) alloy system is calculated. The computation of \(f_i\) is trivial and the accuracy of the results reaches that of ab initio calculation. Also, ab inito calculations are complex and required significant efforts, more empirical approaches have been developed [31] where yield analytic results that can be used for exploring trends and to compute properties of materials. The EPM offers advantage of applicability to broad class of materials and illustrated trends not only for GaAlN but also for ZnMgSe and ZnSSe alloys [32–34]. In many applications, these empirical approaches do not give highly accurate results for each specific material but still very useful. The used formula [30] is

\[
 f_i = \left( \frac{E_g}{E_g - 1} \right)^{-1} - 0.75 - \frac{1}{E_g} - 0.66 \tag{20}
\]

where \(E_g\) is the energy gap between the first and the second valence bands at point \(X\) and 1 is equal to 1 eV. The calculated ionicity values are compared with Phillips [31] and Garcia and Cohen [35]. The comparison is given in Table 3. This result shows that the calculated ionicity values exhibit the same chemical trends as those found in the values derived by Phillips and in accordance with results of Garcia and Cohen [35]. Fig. 7 shows the variations of \(f_i\) with the mole fraction \(x\). It is clearly seen that the ionicity decreases continuously with

<table>
<thead>
<tr>
<th>Compound</th>
<th>(f_i) (calculated)</th>
<th>(f_i) (Phillips [31])</th>
<th>(f_i) (Garcia and Cohen [35])</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>0.773</td>
<td>0.500</td>
<td>0.780</td>
</tr>
<tr>
<td>(\text{Ga}<em>{0.5}\text{Al}</em>{0.5}\text{N})</td>
<td>0.766</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AlN</td>
<td>0.758</td>
<td>0.449</td>
<td>0.794</td>
</tr>
</tbody>
</table>

Table 4 shows the calculated Bulk moduli are in GPa for GaN, AlN and \(\text{Ga}_{1-x}\text{Al}_x\text{N}\) are compared with experimental and Al-Douri et al. [37] values

<table>
<thead>
<tr>
<th>Compound</th>
<th>(B_0) (GPa) (calculated)</th>
<th>(B_0) (GPa) (experimental)</th>
<th>(B_0) (GPa) (Al-Douri et al. [37])</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>197.88</td>
<td>237, 245, 195</td>
<td>164</td>
</tr>
<tr>
<td>(\text{Ga}<em>{0.5}\text{Al}</em>{0.5}\text{N})</td>
<td>196.41</td>
<td>192.89</td>
<td>207.9, 135</td>
</tr>
<tr>
<td>AlN</td>
<td>192.89</td>
<td>207.9</td>
<td>135</td>
</tr>
</tbody>
</table>

* Ref. [38].
increasing of the mole fraction between 0.773 (ionicity value of GaN) and 0.758 (ionicity value of AlN). These results show that the ionicities calculated here exhibit the same chemical trends as those found in the values derived from the Phillips theory or others.

Also, using electronic charge densities, the bulk modulus \( B_0 \) of the Ga\(_{1-x}\)Al\(_x\)N alloy is computed. The computation of \( B_0 \) is to test our new model [36], where used the well-known formula

\[
B_0 = (2400 - \lambda 1000)(S_c + 1)^{1.2}
\]

(21)

where \( S_c \) is the area of the cation side of the total valence charge density, and \( \lambda \) is a parameter appropriate for the group-IV (\( \lambda = 0 \)), III-V (\( \lambda = 1 \)) and II-VI (\( \lambda = 1.5 \)) semiconductors.

The calculated \( B_0 \) values are compared with experimental and Al-Douri et al. [37] (the energy gap along \( \Gamma-X \) and the transition pressure are used to calculate the bulk modulus in an empirical formula by our group) values. The comparison is given in Table 4. The results show that the calculated \( B_0 \) values exhibit the same trends and in reasonable agreement as other values derived experimentally and Al-Douri et al. [37]. It is shown from Fig. 8 that the variations of \( B_0 \) are in exponential decreasing with increasing of mole fraction between 197.88 GPa (\( B_0 \) value of GaN) and 192.89 GPa (\( B_0 \) value of AlN). The calculated bulk modulus exhibit the same trends as those found in the values derived by others [37,38].

4. Conclusions

It was shown that the electronic and positron energy spectra are similar with an absence of band gap in the positron energy spectrum. The positron tends to be pushed out of the cell containing the larger valence and the larger ion core. Therefore, the effect of the positron wave function is small compared to that of the electrons. The difference is that the positron density is maximum in the interstitial region, while the electron density is maximum at the bond centre. Ga\(_{1-x}\)Al\(_x\)N alloy system exhibits a direct gap at \( x = 0.58 \) and play an impetus for using through violet, blue and green emitting devices and for high temperature transistors.

Using the heteropolar gap, the obtained ionicity values for Ga\(_{1-x}\)Al\(_x\)N alloy are in agreement with the values obtained by Phillips. Also, based on the charge density, the calculated \( B_0 \) values for Ga\(_{1-x}\)Al\(_x\)N alloy are in reasonable agreement with experimental values.

References