MATLAB Wavelet analysis of electron energy spectrum in one-dimensional quantum well with infinitely high walls for Al-Ga-As system (0 < x < 1)

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Abstract. This paper presents calculations of electronic states in AlₙGaₙ₋ₙ₃ As semiconductor nanostructures and simulates the envelope wave functions of quantum energy levels in a one-dimensional quantum well with infinitely high walls of a given width at various values of x. For the analysis of results the authors choose the function wtmm from the Matlab library that fixes the extremums and which is a characteristic of the fractality of the envelope wave functions of quantum energy levels.

1. Introduction

Nowadays, when new nanostructures are created, such as quantum dots or superlattices, the issue of studying AlₙGaₙ₋ₙ₃ As semiconductor nanostructures remains relevant, where x is the fraction of gallium atoms substituted by aluminum atoms, it usually varies from 0.15 to 0.35.

Figure 1 shows the band structure of AlₙGaₙ₋ₙ₃ As at different contents of x [1-2].

![Figure 1. Zone structure of AlₙGaₙ₋ₙ₃ As solid solution: a - x < 0.45, b - x > 0.45 [1]](image-url)
The electronic states in semiconductor nanostructures are determined by the effective mass method, based on the solution of the stationary Schrödinger equation, which is one-dimensional for the motion of electrons in the perpendicular plane of the layers (excluding cases where the potential relief is a function of time) [1-2]:

\[
\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(z,E)}{\partial z^2} + U(z) \cdot \psi(z,E) = E \cdot \psi(z,E),
\]

where \( m \) is the effective mass of the electron, \( E \) is its total energy, \( U(z) \) is the potential relief for the electron along the \( z \) axis directed perpendicular to the plane of the layers.

A solution of this Schrödinger equation is the \( z \)-component of the envelope of the wave function \( \psi(z,E) \) which characterizes the motion of electrons in the perpendicular plane of the layers and determines the probability of finding an electron with energy \( E \) of motion along the \( OZ \) axis at a point with coordinate \( z \) within the normalisation [1-2].

Consider simulation of the energy spectrum of an electron in a one-dimensional quantum well.

If a thin layer of narrow band material is placed between two quite thick layers of wide-band material, a potential well can be formed for an electron moving in a direction transverse to the planes of the layers (Fig. 2) (the energy is counted from the bottom of the conduction band of the well material). This kind of relief is called a rectangular potential well. For modeling we will consider a symmetric potential well (Fig. 2, b) [1-2].

Consider the idealized case of a potential well with infinitely high walls, in which case the envelope wave function \( \psi(z,E) \) outside the well is identically equal to zero and inside the well satisfies the Schrödinger equation (1) with boundary conditions [1-2]:

\[
\psi \left( \pm \frac{a}{2},E \right) = 0
\]

where \( a \) is the width of the potential well (thickness of the middle layer of the three-layer structure). Then \( \pm a/2 \) are coordinates of interfaces between the layers.

The solution at discrete energy \( E \) - eigenvalues of this equation (1) [3] has the form:

\[
E = \frac{\hbar^2}{2m} \left( \frac{\nu \pi}{a} \right)^2
\]

where \( \nu \) is the number of the energy level.

The system has symmetry along the \( OZ \) axis with respect to the origin, so the set of eigen solutions of the Schrödinger equation is divided into subgroups of even and odd solutions [1, 3-5]:
\[
\psi(z,E) = \begin{cases} 
\cos\left(\frac{v\pi}{a}z\right) & \text{at } v = 1, 3, 5, \ldots \\
\sin\left(\frac{v\pi}{a}z\right) & \text{at } v = 2, 4, 6, \ldots 
\end{cases} 
\]

where \(C\) is the normalisation factor, depending on \(v\).

2. Modelling the energy spectrum of an electron in a one-dimensional quantum well at different values of \(x\)

The following equations were proposed to describe the Al\(_x\)Ga\(_{1-x}\)As structure [1]:
- effective mass of the electrons in the \(\Gamma\)-minimum:
  \[m_e=(0.067+0.083x)m_e\]  
- lattice constant:
  \[a_0=(0.56533+0.00078x)\times10^{-9}\]  
- bandgap energy (eV):
  \[E_g = \begin{cases} 
(1.424+1.247x)q_e & \text{at } x < 0.45 \\
19+0.125x+0.143x^2q_e & \text{at } x \geq 0.45 
\end{cases} \]
- width of the quantum well, which depends on the number of atomic layers:
  \[a=NN \cdot a_0 \times 10^{-9}\]  

where \(m_e = 9.1093897\times10^{-31}\) - electron mass, \(q_e\) - electron charge, \(NN\) - number of monolayers.

For modelling purposes, the following parameters are assumed constant: number of monolayers \(NN = 20\) and the first four allowed energy levels \(v = 4\). The results of the simulations at different values of \(x\) are shown in Table 1 and Figure 3.

| Structure description parameters | Fraction of gallium atoms substituted by aluminum atoms, \(x\) |
|---------------------------------|-----------------------------------------------------|
| \(m_e\) | 0       | 0.2   | 0.4   | 0.6   | 0.8   | 1.0   |
|       | 6.1033e-32 | 7.6154e-32 | 9.1276e-32 | 1.0640e-31 | 1.2152e-31 | 1.3664e-31 |
| \(a_0\) | 1.4240  | 1.6734 | 1.9228 | 2.0265 | 2.0915 | 2.1680 |
| \(E_g\) | 5.6533e-10 | 5.6549e-10 | 5.6564e-10 | 5.6580e-10 | 5.6595e-10 | 5.6611e-10 |
| \(a\)  | 11.3066 | 11.3097 | 11.3128 | 11.3160 | 11.3191 | 11.3222 |

Figure 3. Graphs of dependence on structure description parameters \(a\) and \(x\):
a) effective mass of the electrons in the $\Gamma$-minimum $m_n$, b) lattice constant $a_0$, c) bandgap energy $E_g$, d) width of the quantum well, which depends on the number of atomic layers $a$.

Analysis of the graphs shows that all dependences are linear, which simplifies the finding of the structure parameters of Al$_x$Ga$_{1-x}$As by formulas (5 - 8). Only one of these parameters depends on the parameter - number of monolayers $NN$.

Figure 4 shows the dependence of the quantum well width depending on the number of atomic layers $a$ at the parameter number of monolayers $NN = 10, 20, 30$. The graphs coincide at $NN = 10 = 30$.

![Figure 4. Dependence of quantum well width depending on the number of atomic layers $a$ at the parameter number of monolayers $NN = 10, 20, 30$](image)

3. Holder exponent (Lipschitz exponent and scaling exponent) as a tool for fractal analysis

The Holder exponent (Lipschitz exponent and scaling exponent) is used for signal analysis tasks in purpose of revealing their regular changes or features on the processing interval and is a tool for fractal signal analysis [4-6].

The signal $f(t)$, satisfies the Holder condition $\text{Hol}$, so there is a constant $C_H$:

$$\left| f(t) - f(\tau) \right| \leq C_H |t - \tau|^\text{Hol}, \quad 0 < \text{Hol} < 1$$

(9)

it can be represented as the exponent value raised to the power, so the difference in the time argument will be proportional to the difference in the values of the signal $f(t)$ at a given time interval [6].

If we perform a wavelet transform of this signal and write it in terms of scaling (the scale parameter tends to zero), the transform is [4-6]:

$$E \left[ W_{\phi}(t, A, \phi) \right]^2 \approx |A|^{2\text{Hol}+1}, \quad A \rightarrow 0$$

(10)

where $A$ is the scale parameter of the wavelet transform, $E<*>$- averaging sign.

The analysis of expression (10) shows that various kinds of signal regularities are clearly visible in the area of small values of the scaling factor [6].

In Matlab, this function is implemented by the $\text{wtmm}$ function, which finds the maximum value of the wavelet transform modulus. By default, the wavelet transform of the original signal is performed by a second-order Gaussian wavelet, which differs from the "Mexican Hat" wavelet by the correction normalizing coefficient.
The authors chose the following syntax for this function [7], which draws lines of wavelet maxima and displays them as a table on the right side of the Holder local exponent estimation graph by which we can judge the fractality of the signal:

\texttt{wtmm(signal, 'ScalingExponent', 'local')}

4. Analysis of results

For modeling, we take the values of $x$ from 0 to 1 in steps of 0.1.

1) Consider the dependence of quantised energy levels of an electron in a rectangular quantum well on different values of $x$ (Figure 5). Analysis of the graphs showed that an increase in the value of $x$ leads to a decrease in the energy levels.

\begin{figure}
\centering
\subfloat[$x=0$]{
\includegraphics[width=0.3\textwidth]{fig5_a.png}}
\hfill
\subfloat[$x=0.1$]{
\includegraphics[width=0.3\textwidth]{fig5_b.png}}
\hfill
\subfloat[$x=0.2$]{
\includegraphics[width=0.3\textwidth]{fig5_c.png}}
\subfloat[$x=0.3$]{
\includegraphics[width=0.3\textwidth]{fig5_d.png}}
\hfill
\subfloat[$x=0.4$]{
\includegraphics[width=0.3\textwidth]{fig5_e.png}}
\hfill
\subfloat[$x=0.5$]{
\includegraphics[width=0.3\textwidth]{fig5_f.png}}
\subfloat[$x=0.6$]{
\includegraphics[width=0.3\textwidth]{fig5_g.png}}
\hfill
\subfloat[$x=0.7$]{
\includegraphics[width=0.3\textwidth]{fig5_h.png}}
\hfill
\subfloat[$x=0.8$]{
\includegraphics[width=0.3\textwidth]{fig5_i.png}}
\subfloat[$x=0.9$]{
\includegraphics[width=0.3\textwidth]{fig5_j.png}}
\hfill
\subfloat[$x=1$]{
\includegraphics[width=0.3\textwidth]{fig5_k.png}}
\caption{Dependence of quantised energy levels on $x$.}
\end{figure}
**Figure 5.** The dependence of quantised energy levels of an electron in a rectangular quantum well with values of $x$

2) The wavelet analysis with the *wtmm* function will be performed in the range of 0.1 to 0.4, assuming that the fraction of gallium atoms substituted by aluminum atoms $x$ usually varies between 0.15 and 0.35 [1 - 2]. The visual representation of the plots of the local Holder exponent estimation is shown only in Figure 5b, since in the other cases they are very similar because of the small deviations of the lines of maximums for each envelope function.

![Figure 5](image1.png)

**Figure 6.** Wave function envelopes of an electron in the rectangular quantum well at different values of $x$

![Figure 6](image2.png)

**Figure 7.** Results of wavelet analysis in the form of local Holder exponent estimation plots at four wave function envelopes ($x=0.1$)

![Figure 7](image3.png)

**Figure 8.** Results of wavelet analysis in the form of local Holder exponent estimation plots at four wave function envelopes ($x=0.2$)

![Figure 8](image4.png)
Figure 9. Results of wavelet analysis in the form of local Holder exponent estimation plots at four wave function envelopes (x=0.3).

Figure 10. Results of wavelet analysis in the form of local Holder exponent estimation plots at four wave function envelopes (x=0.4).

Analysis of the results of Figures 7-10 shows that the values of local Holder exponents for the four wave function envelopes coincide, which indicates the equality of extremum values for each envelope function for different values of x. Depending on the value of x, the coordinates of points of extremum change by insignificant value, for example, for the first envelope function the second coordinate of extremum (in units of counts) is 5655 (x=0.1) – 5656 (x=0.2) – 5656 (x=0.3) – 5657 (x=0.4).

A formula for conversion from sample to \( z \) can be derived from this:

\[
\hat{z}_i = -\frac{a}{2} + s\text{hag} \cdot (nN_i - 1)
\]

(11)

where \( s\text{hag} \) is the step, \( nN_i \) is the number of counts of a given point (sample).

3) Wavelet analysis with the wtmm function at x=0 for different numbers of monolayers: 10 monolayers, 20 monolayers, and 30 monolayers (Table 3). Table 2 shows quantised energy levels for the considered numbers of monolayers.

| Number of monolayers, \( NN \) | Quantised energy levels |
|--------------------------------|-------------------------|
|                               | 1           | 2           | 3           | 4           |
| 10                             | 0.0281e-36 | 0.1125e-36 | 0.2532e-36 | 0.4502e-36 |
| 20                             | 0.0070e-36 | 0.0281e-36 | 0.0633e-36 | 0.1125e-36 |
| 30                             | 0.0313e-37 | 0.1250e-37 | 0.2814e-37 | 0.5002e-37 |

Table 3

Wave function envelopes and quantised energy levels (x=0) (wtmm function) with step \( s\text{hag} = 1.0000e-03 \)
10 monolayers

\[ a = 5.6533, \]
\[ nN = 5654 \]

20 monolayers

\[ a = 11.3066, \]
\[ nN = 11307 \]

30 monolayers

\[ a = 16.9599, \]
\[ nN = 16960 \]

5. Conclusion
This paper presents the results of a wavelet analysis of the electron energy spectrum in a one-dimensional quantum well with infinitely high walls Al\(_x\)Ga\(_{1-x}\)As at different values of \(x\) (\(x\) values from
0 to 1) and at different numbers of monolayers ($NN = 10, 20, 30$), using the $wtmm$ function calculating the Holder exponent to determine the coordinates of extrema and analyze the fractality of envelope functions. The obtained values can be used to determine the coordinates of extremums of envelope functions.

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