THREE DIMENSIONAL MODELLING OF QUANTUM CASCADE LASERS' CHARACTERISTIC PARAMETERS

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KUANTUM KASKAT LAZERLERİN KARAKTERİSTİK PARAMETRELERİNİN ÜÇ BOYUTLU MODELLENMESİ

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ABSTRACT

Quantum Cascade (QC) lasers are semiconductor lasers that contain quantum wells. Quantum wells provide distinct quality for QC lasers. Changing width of quantum wells cause to obtain different wavelengths for QC lasers. QC lasers have critical characteristic quantities such as optical gain, linewidth enhancement factor and refractive index change. These parameters differ according to conditions. In this study; relating to injection current and wavelength the changes of optical gain, linewidth enhancement factor (Alpha parameter) and refractive index change which are characteristic parameters of QC lasers are modelled three dimensionally considering experimental values. Surface fitting techniques: regression analysis (lowest, polynomial) and method of least squares are applied to provide the optimal surface. Both the training and test results are used to obtain surface curves of characteristic quantities with minimum error. Except method of least squares, MATLAB program is used to find the surfaces and the errors of techniques. In this study, we present the best fitting technique to find the ideal parameters for each different QCLs' variables.

Keywords: Quantum Cascade Laser, Regression Analysis, Surface Fitting, Least Square Method

ÖZET

Kuantum kaskat (QC) lazerler, kuantum kuyuları içeren yarı iletken lazerlerdir. Kuantum kuyuları, QC lazerlere farklı bir nitelik sağlar. Kuantum kuyularının derinliğinin değiştirilmesi, QC lazerlerin farklı dalga boylarına ulaşmasına neden olur. QC lazerlerin optik kazanç, çizgi genişleme faktörü ve kırınım indis değişimi gibi ayırt edici özellikleri vardır. Bu parametreler, içinde bulunulan koşullara göre farklılık gösterir. Bu çalışmada, akım ve dalga boylarına göre değişiklik gösteren optik kazanç, çizgi genişleme faktörü (alfa parametre) ve kırınım indis değişimi QC lazerler için deney verileri kullanılarak üç boyutlu modellenmiştir. En uygun yüzeyi bulabilmek için regresyon analiziyle birlikte yüzey uydurma yöntemi uygulanmıştır. Test ve deney sonuçları, minimum hataya sahip özellikler içeren yüzey eğrisi elde etmek için kullanılmıştır. En küçük kareler yöntemi dışındaki metotlar için MATLAB programı kullanılmıştır. Çalışma sonunda, kullanılan metotlar içinde QC lazerlerin özelliklerine uygun ideal verileri bulan en iyi yüzey uydurma tekniği saptanmıştır.

Anahtar Kelimeler: Kuantum Kaskat Lazer, Regresyon Analizi, Yüzey Uydurma, En Küçük Kareler Yöntemi

1. INTRODUCTION

Laser is an optical resource which depends on behaviors of electrons surrounded in active region [1]. Laser as a name is presented by using the first letters of the words in "Light Amplification by Stimulated Emission of Radiation". Forming of laser is related in difference between energy levels. Electrons that are found in atoms or molecules in the active region determine their movements according to energy levels. During transition of electrons; absorption or emission can occur related to energy levels. The transitions of electrons between energy levels occur naturally or stimulated, as absorption and emission. Emission is the process of the transition of an electron from high energy level to low energy level by releasing a photon. Emission occurs in two ways; naturally or stimulated. If an electron in high energy level release a photon to move low energy level not naturally by the effects of photons in the same region, this transition is called stimulated transition. For stimulated emission, the energy of photon which performs stimulation released must consist as much as the difference of energy between the current energy and the energy level of the atom will move. Absorption occurs when an electron in the lower level absorps a photon to move high energy level [2]. To form a laser, three compoents are needed: gain or laser medium (solid, liquid, gas or semi conductor medium), optical resonator that produces optical gain and manage transitions of photons and an energy source (pump source that provides atoms to be stimulated) [3].

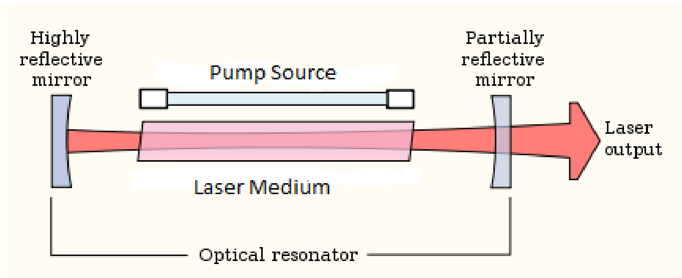


Figure 1 Diagram of a laser

Lasers are grouped according to active laser medium used. There are various types of lasers as solid, liquid, gas, semi conductor. The semiconductor laser is the most widely used of all lasers. As the name of semi conductor suggests, semi conductor medium is used to provide optical gain. Semi conductor lasers have practical importance in usage so it is manufactured in the largest quantities [4].

Quantum cascade lasers (unipolar lasers) are the semi conductor lasers that contain quantum wells and demonstrated in 1994 by Federico Capasso and Jerome Faist. Quantum wells are so narrow that cause electrons in it to reveal different behaviors. The electrons in quantum wells move between different energy levels. Thus photons spread out. The wideness of well affect the energy of photons. When the wideness of well decreases, the energy of photon increases [5]. Electron transition in semi conductor lasers occurs between conductional and valence band. Differently, in quantum cascade lasers, these bands comprise subbands. The medium between quantum wells that electron transits is called active region. Electrons traverse through active regions using subbands. The transition from valence band to a lower band, a photon is emitted. In transition through structure, a photon is emitted each passing next active region. QCLs contain many quantum wells which means multiple photons can be generated by a single electron [6].

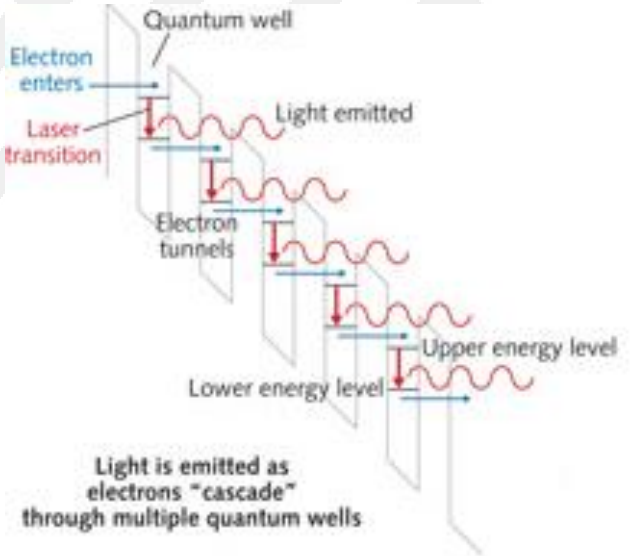


Figure 2 Transition of an electron in Quantum Cascade Laser

One of the distinct properties of QCLs is that short pump pulses of energy sources can be used to gain watt-level peak powers even at room temperature. Narrow linewidth, wavelength tunability and running in the room temperature of QCLs make them preferable in applications in several different fields [8].

QCL is used in a huge variety in real world applications. QCL based systems are used in medical, industrial, security, space and environmental fields. It is used as sensitive medical diagnosis detector. Various types of cancers can be early detected. QCL is a very important laser type for military applications, too. Since explosive materials were used in terror attacks first, explosive detection technology has standed out by countries that face terrorism. QCL is used in standoff explosives detection equipment. In homes QCL based systems are also used for personal security. It is also used in aviation, cruise is controlled automotically and radar is improved for avoiding collisions in the air. Another field in which QCL is used is mid-infrared imaging. Gas sensors that analyze content of gas and detect the amount of chemical compunds (CH4, CO, N2O, NH3, SO2, HCL etc.) in the atmosphere. For example these sensors detect nitric oxide in air, which causes acid rain [9, 10, 11]. QCL is also used as spectrometer to find applications in exploration of space.

Quantum wells which are the constituents of quantum cascade lasers, are composed of different materials joining in layers. Because of this, they are called as heterostructures. Heterostructures contain different semiconductors that have divers energy levels. This diversity causes an ambiguity as how the different bands in the two materials will line up in energy with one another. The term “band offset ratio is “ steps in at that time. The band offset ratio is the ratio of difference in conduction band energies to the difference in valence band energies. Conduction band is the structure which contains high energy electrons and valence band is the band which is separated by a band gap from conduction band and contains low energy electrons. If both electrons and holes see higher energies after calculating band offset ratio, this type is called type 1 system. In type 2 system, electrons and holes in heterostructures have their lowest energies [12].

The types of transition between bands in a quantum well can vary. It can be between states of a single subband (without passing through a band gap), subbands of same band or subbands of different bands.

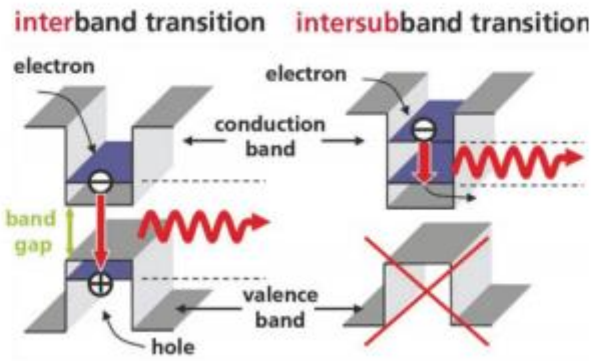


Figure 3 Transitions of an electron in type I and type II QCls

Type 1 Quantum Wells: In type 1 quantum wells, energy transition occurs between the bands of single subband [14].

In conduction band of quantum wells, photons can be created by intersubband transitions between subbands. So wavelength of laser is not restricted by the material used in band gap. The wavelength of type I QCls can vary in a big range. Layers thicknesses play an important role in this variation of wavelength [15].

Type II Quantum Wells: In type II lasers, electrons and holes aren't confined in the same layer . There is a photon transition between different subbands [16].

In type 2 QCLs, it is seen that conduction band of one semiconductor ovelapping on the valence band of another closest semiconductor. A photon is emitted by tunneling of electron between these bands. After this emission, transition goes on the other connected region. Type 2 QCLs have higher efficiency, the number of photon created is very high. It is also a big advantage that being formed at nearly room temperature. They are used in a various applications such as hot electron transistors, resonant tunneling diodes and detectors [17].

Differences between type I and type II lasers: In type 1 systems, absorption of an electron is stronger than the absorption of electron in system of type II because of transition in same band [14]. In type II systems, transition occurs between different subbands. For the same side, type II systems release lower energy for electrons and holes[17]. In type II laser system, combination of electrons and holes provides photon generation. So the band gap of semiconductor material affects laser wavelength directly. In type 1 laser system, transition occurs intersubband not in the holes so the wavelength of laser is not affected by the material of band gap [13].

Why these calculations are done in the experiments of these laser types : (For type 1 calculations) It is defined that there are important parameters that affect QCLs directly. One of them is linewidth enhancement factor. The LEF is a parameter which affects determination of spectral linewidth of semiconductor lasers considerably so the measurements of LEF under different conditions take an important role for lasers efficiency [18]. A large LEF is not desirable in the high power operations because of causing large chirp in filamentation of operations. There has been many reports about verification of LEF in type 1 QCLs but there has been no report about LEF near zero at the gain peak. There are many factors that affect LEF. Some of them are device self heating and refractive index change. Device self heating provide type 1 QCL more effective because the threshold current of a QCL is higher than others. There are also transitions other than lasing. These transitions affect refractive index change. In these transition states, there can be various electron populations that are not close to lasing wavelength. These populations can also affect refractive index change at the lasing wavelength. The experiments are also done to determine effects of transitions other than lasing one against refractive index change [18]. In the study of type II laser; on the amplified spontaneous emission spectra, LEFs of type II laser on different refractive index change and gain are determined.

In which conditions are the calculations done: For type I lasers, a liquid nitrogen cryostat is used for the QCL sample to be set under a given current source. QCL emits light and the light is collimated and directed to the spectrometer. This light which is emitted from QCL is anaylsed. Current is lined as 2 mA increment from the begining measure. Device self heating is also used in the experiment. Similarly, a liquid nitrogen cryostat is used for QCL sample to be operated. In the end the radiation of laser is collimated and referred to the Fourier transform infrared spectrometer as declared in the type I QCL measurements. The gain is calculated by Hakki-Paoli method.

Why do we need three dimensional surfaces: Modelling is applied to this experiment data because measurement of linewidth enhancement factor is not very easy according to different environments. For optimal environment, many different conditions are needed according to types of laser. By modelling these surfaces, linewidth enhancement factor can be attained without preparing required currents other than given and applied current points. For this purpose, different surface fitting algorithms were used on the given data points.

1.1. Characteristic Quantities Of Quantum Cascade Lasers

Quantum cascade lasers possess many advantages compared as standard semiconductor laser. Consisting quantum wells and barrier materials provide convenience in wavelength, bias voltage, output power. Direct electronic transition for light generation is another advantage of QCLs [11]. Wavelength can be modified by changing the width of QCL well and QCLs can run in the room temperature. As a result, QCLs provide high brightness, they are tunable and contain narrow band [19]. Quantum cascade lasers have threee important characteristic parameters as linewidth enhancement factor, optical gain and refractive index.

1.1.1. Linewidth Enhancement factor (LEF)

Linewidth enhancement factor (α- factor) is an effective parameter which determines spectral linewidth of semi conductor lasers [20]. α- factor has an important role in the changes of filamentation in devices, linewidth, laser dynamics etc… [21].

1.1.2. Optical Gain

Optical gain is the increase in the ratio of number of photons to the extent of unit radiation. It can also be defined as the degree that provides to increase optical power of semi conductor lasers [23]. Optical gain changes according to quantities of photons proportionally. Changes in optical gain obtains to attain information about capabilities of tools as shown by the formula below:

$$\text{Efficiency} = \text{Optical power} / \text{Electrical power}$$

Optical gain can be defined as:

$$g=g0\left[1-exp\frac{(E-\Delta E_F}{kT}\right]$$

E= Energy Level

go= Naturally Radiaton Ratio

ΔEF= Quasi-Fermi Level

K= Boltzmann Constant

T= Temperature (Kelvin) [21]

1.1.3. Refractive Index:

Refraction is the act of wave when it enters through a different medium. The wave bends according to its speed in the new medium. Bending of wave depends on the refractive indices of two media [23]. Refractive index is the ratio of speed of light in vacuuum to speed of light to which it passes.

Refractive index is calculated as

$$n_i=\frac{c}{v_i}$$

C = The speed of light in the vacuum (299792458 m/s) (constant)

V_I = The speed of light in the medium passed

n_i=Refractive index [24].

Refractive index is affected by the variables like temperature, pressure and wavelength. It changes by temperature because temperature impacts density of medium. When the density of medium changes, its velocity changes. The refractive index changes certainly depending on velocity. Velocity of light depends on frequency so refractive index changes by the increase and decrease of medium frequency. When the wavelength of conductive medium increases, refractive index of light decreases. The variety in the refractive index by the effects of frequency and wavelenght is called dispersion. Dispersion can be observed normally or abnormally. In case of close absorbtion bands, rapid changings occur in the refractive index which is called abnormal dispersion. The others which do not cause rapid changing of refractive index are called normal dispersion [25].

1.2. Regression Analysis

Regression analysis is a method which determines relationship between two or more variables and provides to predict new values by the help of defining a mean of dependence of random values [26]. Relationships between annual rainfall and drought, fertilizer amount used on land and yield taken of products, malnutrition and being ill frequently are the examples of regression analysis. In the example above, it is given that there is a relationship between malnutrition and being ill frequently. In this example malnutrition is reason and being ill frequently is result. According to regression analysis, being ill frequently is dependent and malnutrition is independent variable. Regression analysis analyzes not only relationship between two variables, number of independent variables can be increased. Regression analysis can be grouped according to function type used or number of independent variables of equation. In a regression analysis one dependent and one or multiple independent variables can take place. One independent variable means simple regression and multiple independent variables mean multiple regression. Linear and nonlinear regression analysis are types of regression as to function used in the equation.

For finding result ranges linear and non linear regression, in linear regression there is no need any conversion but in non linear regression different conversion methods are used to conclude. At the beginning, required functions (logarithma, square root…) are used to turn the equation into linear form and then the equation in linear form is resolved by using linear methods. Finally converted equation is returned to the non linear phase at the beginning. Non linear prediction methods are used when the coefficient can not be converted to linear phase. These non linear prediction methods are Gauss Newton, gradient and etc.

1.2.1. Simple Linear Regression Analysis

Simple linear regression is a type of regression which reveals the relation between one dependent and one independent variables. For a relation as (x,y), it can be said that x and y are related to each other partially. Variable x informs about variable y.

Therefore y is called as result, dependent; x is called as independent, explanatory, exogenous variable [27].

$$y = \beta_0 + \beta_1 x + \varepsilon$$

Simple Linear Regression Equation

In the equation above, β0 is called as constant or intercept, β1 is called as coefficient or slope, informs about steepness of the regression line, ε is the error term.

1.2.2. Multivariate Linear Regression Analysis:

It is a type of regression model composed of multiple independent variables and one variable that depends on these independent variables. By using this type of regression, effects of independent variables on the dependent variable and the magnitude of these effects can be examined [28].

For n observations, the equation for multiple linear regression is

$$yi = \beta_{0} + \beta_{1xi1} + \beta_{2xi2} + ... \beta_{pxip} + \varepsilon_{i}$$

p is the number of explanatory variables.

1.3. Surface Fitting Techniques

Surface fitting is an analysis that is used to find out the best fitting model for a relationship between dependent and more than one independent variables of computer graphics or desings [29].

The closeness between the real surface and the surface created by fitting technique is the base of surface fitting. The aim of surface fitting is to obtain the nearest surfaces by minimizing distance between them. For this purpose different surface fitting techniques are used and comapred to reach the ideal result [30].

Surface fitting has a widely used areas as in medicine, mathematics, engineering, earth sciences etc. [31].

In this study we used polynomial interpolation, custom equation, Locally Weighted Smoothing (Lowess) methods.

Least Square Method: Least square method is a type of regression which provides the best line or surface for given data points [33]. The aim is to minimize the sum of squares of errors for results of each single equation.

For surface fitting the steps and logic are same with 2D linear fitting. A set of samples are given. Dependent and independent variables are shown by letters as x, y and z. “z" is declared as the dependent variable, x and y are as independent variables. The equation “z = Ax + By + C” is the surface which the samples best fit. The main part is that error function between the given points and effectual surface equation is minimized. The error function is equalized to zero. So the equation can easily be solved. The result shows the best surface by applying least squares [32].

$$E(A,B,C) = \sum_{i=1}^{m} \left| \left(A_{x_i} + \mathrm{B}y_{\mathrm{i}} + \mathrm{C} \right) - \mathrm{z}_{\mathrm{i}} \right|^{2}$$

is defined. The hyperparaboloid graph derived when the gradient occurs

∇E = (0, 0, 0).

$$(0,0,0) = \nabla E = 2\sum_{i=1}^{m} [(Ax_i + By_i + C) - z_i](x_i, y_i, 1)$$

Lowess (Locally Weighted Scatterplot Smoothing): It is a type of regression method which is used to present a surface by using a function of the independent variables locally among multiple smoothing methods. It is also called as LOESS (locally weighted smoothing). By using lowess method much wider regression surfaces can be obtained as per polynomial methods [34]. Lowess method is not interested in the global relationship determined using the whole dataset , instead it is interested in the local relationship between a response variable and a predictor variable over their ranges [36].

Lowess method implements a non parametric method and generally used when the user does not have a suitable parametric form of surface. Lowess procedure is a good choice for fitting if data includes outliers.

There are two types of lowess applied method: linear and quadratic.

In lowess, a regression surface is fitted to data points by choosing a neighborhood and a local approximation is obtained by this way. At the center of neighborhoods, linear or quadratic functions are fitted to apply weighted least square. After fitting process, the percentage of data points is acquired by choosing the radius of each neighborhood. Smoothing parameter is another variable that defines the fraction of data. This parameter controls the smoothness in the surfaces of each neighborhood. A smooth decreasing function of data points' distances from the center of the neighborhood is used to weight data points in the local neighborhood [37].

Polynomial Regression: It is a linear regression method which obtains to predict a single y variable by separating x variable into a nth order polynomial. A polynomial function which approximates a set of data points, is created by polynomial regression. It is also included in multiple linear regression.

$$Y=a + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \ldots + \beta_n x^n$$

The degrees in polynomial regression can be increased according to difference between R squares in related power equations [38].

1.4. Performance Metrics

R Square: R squared is a measure that defines closeness between data and fitted regression line. It is also called as square of the multiple correlation coefficient or coefficient of determination.

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

SSR = the sum of squared regression, (It is defined as the sum of the squared differences between the prediction for each observation and the population mean.)

SSR =Sum of $(y_{predicted}-y_{mean})^2$

SSE = the sum of squared error, (calculates the sum of the squared errors of the prediction function. For the beter approximation function, SSE should be smaller.)

SSE=Sum of $(y_{observed}-y_{predicted})^2$ [38, 39]

SST = the sum of squared total

SST= SSR+SSE= Sum of$(y_{observed}-y_{predicted})$2

The value of R squared range between 0 and 1.

Adjusted R square: Adjusted R square is a value that measures the proportion of variation. The difference fronm R square is that it is interested in variation explained by only independent variables that really affect the dependent variable.

$$\text{Adjusted } r^2 = 1 - (1 - r^2) * \frac{(n-1)}{(n-2)}$$

Root Mean Square Error: Root mean square error is the square root of the average of squared differences between the real and predicted values of a given model. By using RMSE, closeness between observed data and predicted data can be indicated. Higher values of RMSE indicate worse fit so lower values of RMSE express that the accuration of predicted response has a higher value [40].

$$\sqrt{\frac{\sum_i^n (yi - \bar{yi})^2}{n}}$$

Standard Error: The standard error is a parametric that show how much the predicted points can be smaller or larger than the actual values. Standard deviation is a value that shows how far away each given number from their mean. Standard error is calculated as dividing standard deviation by the square root of the sample size. Calculation of Standard deviation has some basic steps. Firstly, the squares of the differences between data points and mean are taken. Each squared value is added and the sum is divided by the amount of numbers minus one. Then the square root of result of division is taken and standard error is calculated [41, 42,43].

$$SD = \sqrt{\frac{\sum (x - \bar{x})^2}{n-1}}$$

SD= Standard deviation

X= each value

$\bar{x}$=mean value of the sample

n=number of values [45]

$$SE = \frac{SD}{\sqrt{n}}$$

SE=Standard error

If the sample size increases, standard error decreases.

Multiple R: It is the correlation coefficient used in multiple regression analysis. It determines the proportion of the variance of the dependent variable that is related with independent variables. The value of multiple R varies between 0 and 1. The value 0 for multiple R means no relationship and the value 1 means considerable relationship for the equation [44].

Significance F: It is a variable that determines the probability of output in the regression could have been obtained by chance.

P Values: P value is a value that determines statistical significance in a hypothesis. When the p value is smaller than 0.005, null hypothesis(It is a hypothesis that proposes there is no meaningful statistical significance in the given observations) is rejected and a relationship between the variables comes out. A smaller p value means stronger relationship between variables.

2. METHODS

According to measurements of linewidth enhancement factor spectra calculated from the measured differential refractive index change and the differential gain with a current increment of 2 mA in type I QCL (Figure 4) [19] ;Gain and Linewidth Enhancement Factor of Type-I Quantum-Cascade Lasers and calculated linewidth enhancement factor values via measured differential index change and the differential gain with a current interval of 0.2 mA at various currents in type II QCLs (Figure -5)18 Linewidth enhancement factor of a type-I1 quantum-cascade laser) are modelled by using surface fitting techniques.

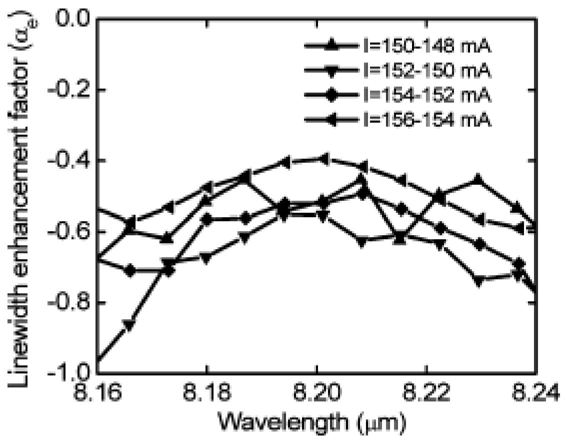


Figure 4 Linewidth enhancement factor spectra calculated from the measured differential refractive index change and the differential gain with a current increment of 2 mA.

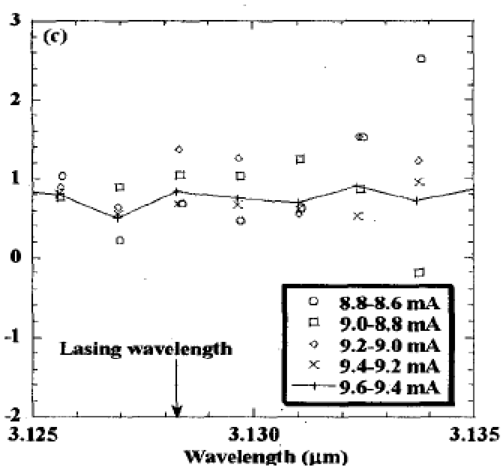


Figure 5 The linewidth enhancement factor is calculated from the measured differential index change and the differential gam with a current interval of 0.2 mA at various currents

The necessary points which will be used in surface fitting are extracted from the given graphics for type I and type II QCLs. The program which is used for this purpose is Ungraph version 5.

Ungraph is a digitizing program that is used to extract data from graph, picture or maps. Processing an image by ungraph involves necessary steps. Initially image is loaded on the program and the coordinate system is defined by selecting basic points. This process is done to scale the image. After that process, a favorable digitizing method is selected and applied to the image. Digitizing methods of ungraph program are divided into 3 groups: functional, non- functional and scatter digitization. In functional digitization, line on the image is followed from left to right without turning back to x direction. In non-functional digitization image is followed left to right also and turning back to x direction is possible. In scatter digitization , data on the line is determined by user mouse clicks on the line. The number of user selected points means the number of data determined. Finally the points are saved as a list.

2.1. Determining coordinates of points for type I

According to Ungraph 5 program, before extracting data from graphics, a real world coordinate system is defined. 1st, 2nd and skew points are determined (Figure 6).

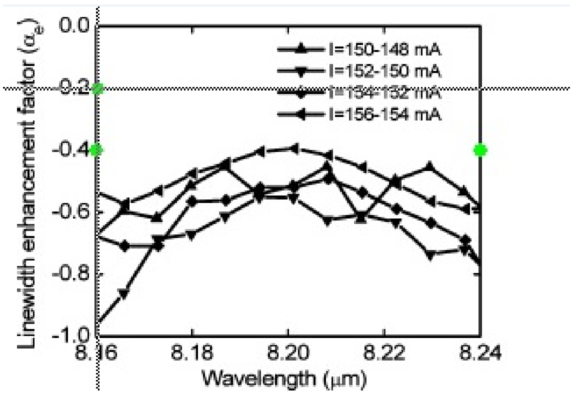


Figure 6 Points of coordinate system for type I QCLs properties

The 1st point (8.24,-0.4), the skew point (0,-0.4) and the 2nd point (0,-0.4) are figured out. After determining coordinate system, scatter digitizing method used to list dataset of selected points for each given current intervals. 51 (x,y) coordinates are set for each intervals. Data between given currents are shown as the figures below.

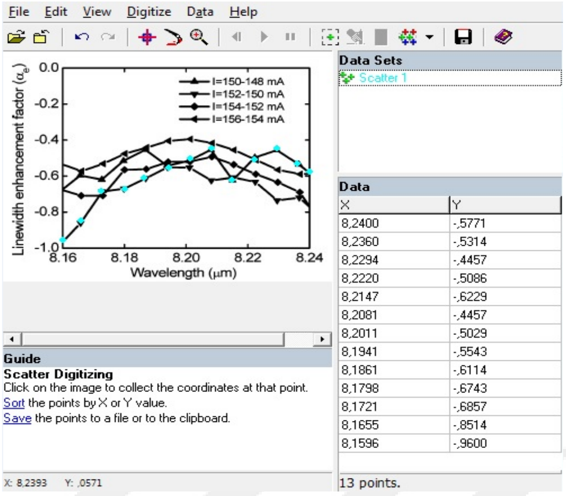


Figure 7 Points at current between 150-148 mA

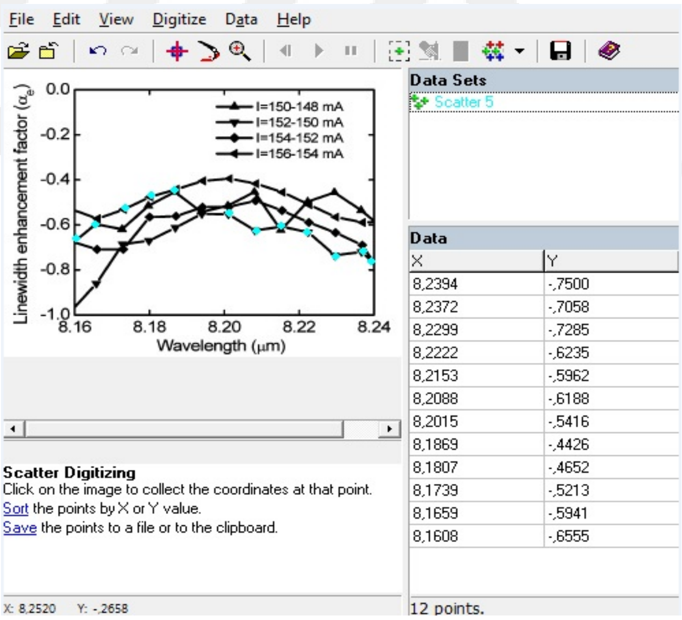


Figure 8 Points at current between 152 150 mA

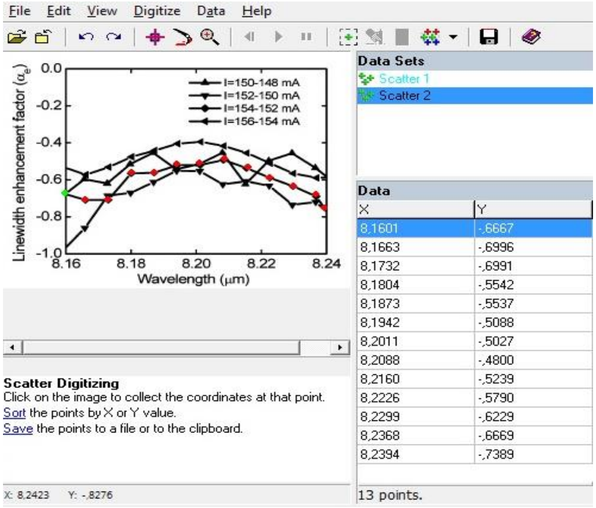


Figure 9 Points at current between 154-152mA

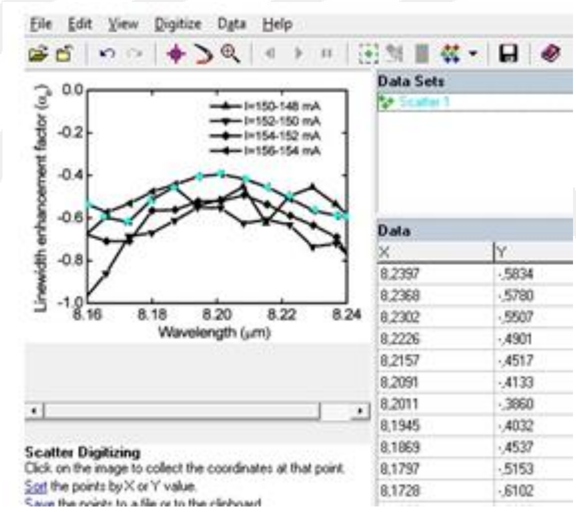


Figure 10 Points at current between 156-154 mA

All the points are distributed and saved to x-values2.txt, y-values2.txt and z-values2.txt files as to their names. The files are loaded to the program.

2.2. Modelling parameters of type I QCLs by using surface fitting techniques:

Several surface fitting techniques can be applied to given parameters to obtain best fit. In this study, different fitting techniques are applied to the characteristic parameters of QCLs. Matlab R2013a version is used for modelling. Curve fitting tool is the main application to fit surfaces. Least squared method of planar fitting is one of the methods carried out. The other methods are custom equation, lowess linear, lowess quadratic, polynomial degrees2 and polynomial degrees 3. By applying the methods; R squared, sum of squared errors, adjusted R squared and root mean squared error of equations are compared to obtain best fit. For least squared method of planar fitting, in excel data regression analysis is used in additon to matlab.

2.3. Planar Fitting of 3D Points of Form by Least Squared Method to Type I QCLs:

It is known that z value is dependent to independent values as x and y in a multivariate equation. When we assume that the plane z = Ax + By + C, by using given x , y and z values A, B and C are determined .

$$E(A,B,C) = \sum_{i=1}^{m} \left| \left(A_{x_i} + \mathrm{B}y_i + \mathrm{C} \right) - z_i \right|^2$$

is defined. The hyperparaboloid graph derived when the gradient occurs

$\nabla E = (0, 0, 0)$.

$$(0,0,0) = \nabla E = 2\sum_{i=1}^{m} [(Ax_i + By_i + C) - z_i](x_i, y_i, 1)$$

According to the formula the equation below is obtained.

$$\begin{bmatrix} \sum_{i=1}^{m} x_i^2 & \sum_{i=1}^{m} x_i y_i & \sum_{i=1}^{m} x_i \\ \sum_{i=1}^{m} x_i y_i & \sum_{i=1}^{m} y_i^2 & \sum_{i=1}^{m} y_i \\ \sum_{i=1}^{m} x_i & \sum_{i=1}^{m} y_i & \sum_{i=1}^{m} 1 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{m} x_i z_i \\ \sum_{i=1}^{m} y_i z_i \\ \sum_{i=1}^{m} z_i \end{bmatrix}$$

$$z = Ax + By + C.$$

The values of A, B and C are found thereby the equation is resolved. All data are loaded to values x, y, z. x=importdata('x-values2.txt'); y=importdata('y-values2.txt'); z=importdata('z-values2.txt'); As per formula adapted to matlab,

```
x=importdata('x-values2.txt');
y=importdata('y-values2.txt');
z=importdata('z-values2.txt');
N=size(x);
sum_x=0; sum_y=0; sum_z=0; sum1=0; sum_xkare=0; sum_ykare=0;
multiply_xy=0; multiply_xz=0; multiply_yz=0;
for i=1:N
    sum_x=sum_x+x(i);
    sum_y=sum_y+y(i);
    sum_z=sum_z+z(i);
    sum1=sum1+1;
    sum_xkare=sum_xkare+x(i)^2;
    sum_ykare=sum_ykare+y(i)^2;

    multiply_xy=multiply_xy+x(i)*y(i);
    multiply_xz=multiply_xz+x(i)*z(i);
    multiply_yz=multiply_yz+y(i)*z(i);
end


D=[sum_xkare, multiply_xy, sum_x;
    multiply_xy, sum_ykare, sum_y;
    sum_x, sum_y, sum1];

F=[multiply_xz;multiply_yz;sum_z];
Dinv=pinv(D);
E=Dinv*F;

fprintf('The equation is:\n');
fprintf('z=%.16f*x+%.16f*y+%.16f\n',E(1,1),E(2,1),E(3,1));
fprintf('Please enter a x and y value to find z\n');
x1=input('x=');
y1=input('y=');
z1=(E(1)*x1)+(E(2)*y1)+E(3);
fprintf('z=%.8f\n',z1);
```

Figure 11 Matlab code for least square method

When the written formula is executed in matlab, the equation is found as z=0.5952750876776918*x+0.0164522379263978*y+-7.9628150236458168

A=0.5952750876776918 B=0.0164522379263978 C=-7.9628150236458168

In addition to matlab solution data are examined also in excel file.In the excel file data-data analysis is clicked.

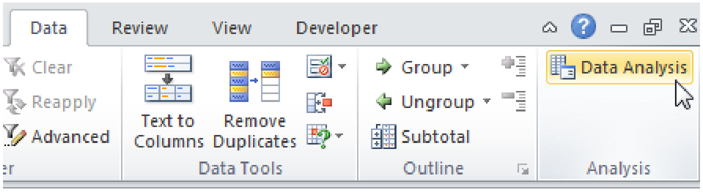


Figure 12 View of data analysis in excel

In the opened window, regression is selected

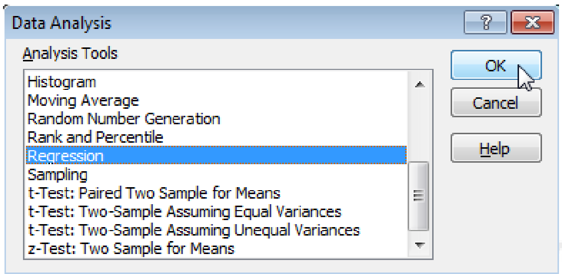


Figure 13 Data analysis tools in excel

The input ranges of x, y z are determined. After regression applied, the results are found as:

Table 2.1 Regression statistics of type I

Regression Statistics	
Multiple R	0,357654933
R Square	0,127917051
Adjusted R Square	0,091580262
Standard error	0,108340708
Observations	51

Table 2.2 Regression results of type I

	Df	*SS*	*MS*	*F*	*Significance F*
Regression	2	0,082640934	0,041328	3,52031	0,037444418
Residual	48	0,563410029	0,011738		
Total	50	0,646050963			

SS= Sum of Squares

MS= Mean Squared Error

F= Overall F test for the null hypothesis

Table 2.3 Regression results of type I -part 2

	Coefficients	Std Error	t Stat	P-values	Düşük %95	Lower %95	Upper95,0 %
Intercept	-7,962815	4,875565061	-1,63321	0,108969	-17,7657954	1,840165	-17,7658
x	0,59527509	0,581781231	1,023194	0,311345	-0,5744746	1,765025	-0,57447
y	0,01645224	0,006732281	2,443784	0,01826	0,00291608	0,029988	0,002916

Lower %95 = The lower boundary for the confidence interval

Upper %95 = The upper boundary for the confidence interval

2.3.1. Applying Custom Equation (Type I)

In custom equation method, there is a given equation to use, the user can prefer this equation or can create a different one. In our study, given equation is used to find the surface. Custom equation is selected on the curve fitting tool. The graphic and results are:

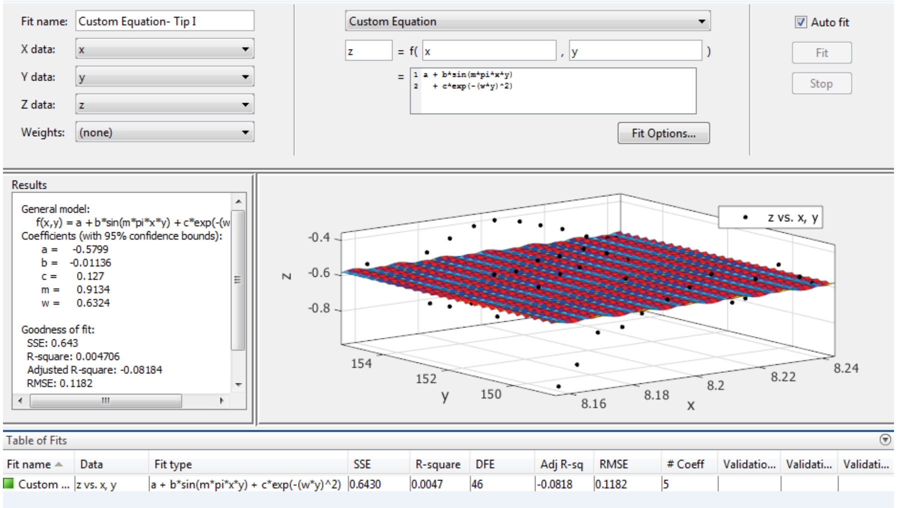


Figure 14 Surface of type I QCLs characteristics after custom equation

General model of the equation:

f(x,y) = a + b*sin(m*pi*x*y) + c*exp(-(w*y)^2)

Coefficients (with 95% confidence bounds):

a = -0.5799 b = -0.01136 c = 0.127

m = 0.9134 w = 0.6324

Goodness of fit:

SSE: 0.643 R-square: 0.004706 Adjusted R-square: -0,08184

RMSE: 0.1182

2.3.2. Applying Locally Weighted Smoothing (Lowess) Linear (Type I):

Lowess Linear is selected on the curve fitting tool. The graphic and results are:

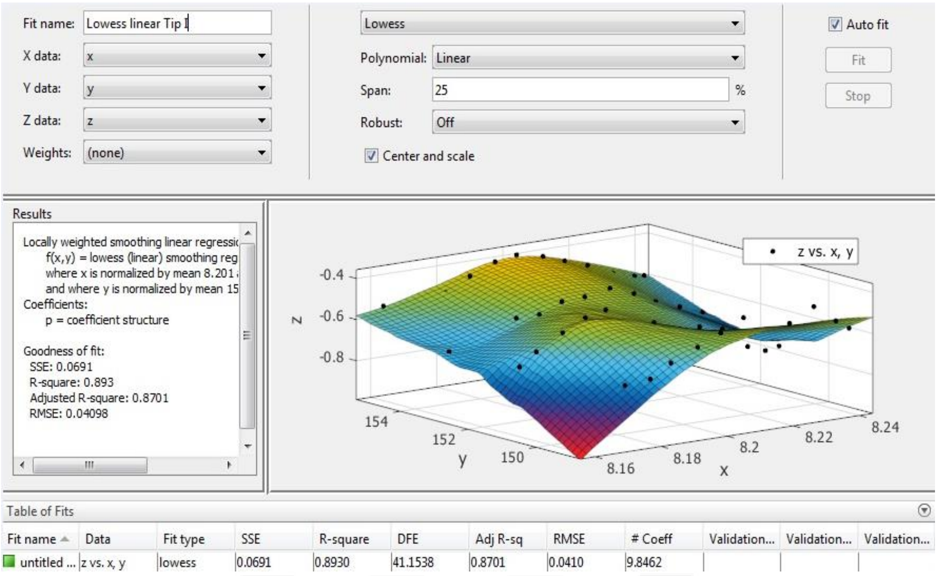


Figure 15 Surface of type I QCLs characteristics after lowess linear

f(x,y) = lowess (linear) smoothing regression computed from p where x is normalized by mean 8.201 and std 0.02634 and where y is normalized by mean 152 and std 2.276 Coefficients: p = coefficient structure

Goodness of fit:SSE: 0.0691 R-square: 0.893 Adjusted R-square: 0.8701 RMSE: 0.04098

2.3.3. Applying Locally Weighted Smoothing Quadratic(Type I) :

Lowess Quadratic is selected on the curve fitting tool. The graphic and results are:

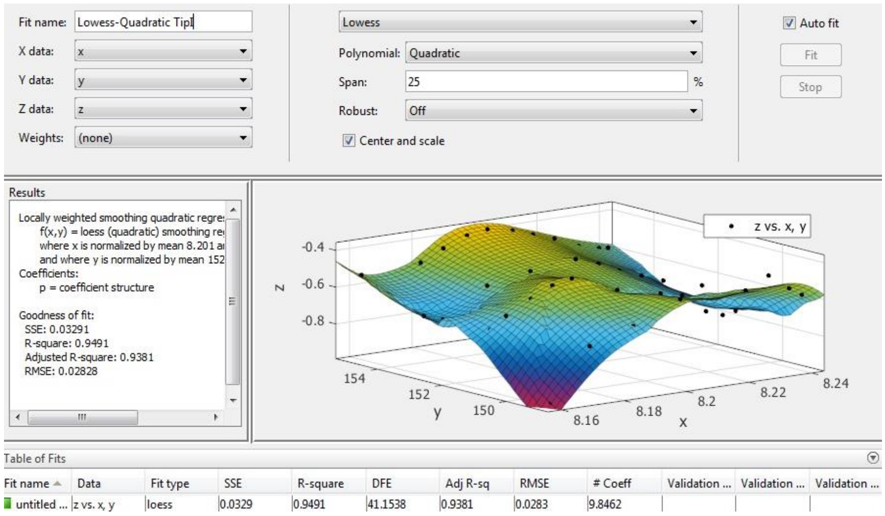


Figure 16 Surface of type I QCLs characteristics after lowess quadratic

f(x,y) = loess (quadratic) smoothing regression computed from p where x is normalized by mean 8.201 and std 0.02634 and where y is normalized by mean 152 and std 2.276

Coefficients: p = coefficient structure

Goodness of fit:

SSE: 0.03291 R-square: 0.9491 Adjusted R-square: 0.9381

RMSE: 0.02828

2.3.4. Applying Polynomial Degrees 2 Type (I)

Polynomial degrees 2 for x and y is selected on the curve fitting tool. The graphic and results are:

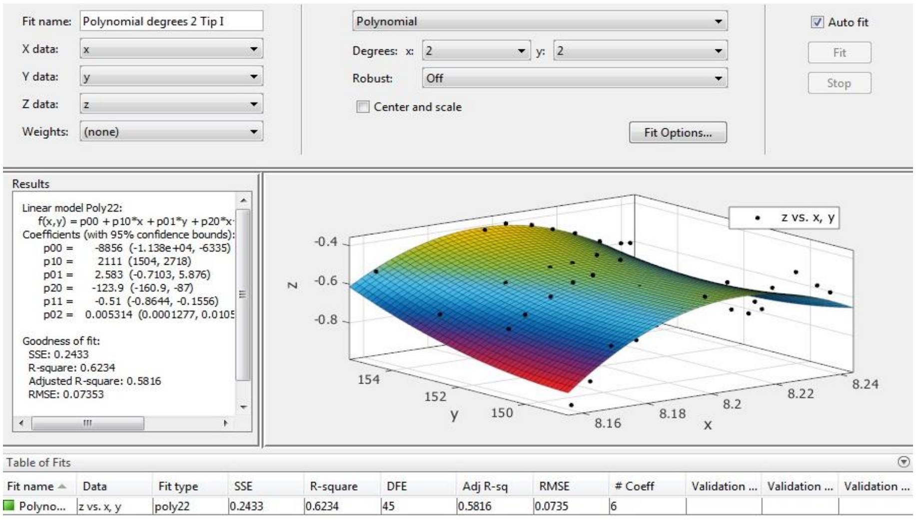


Figure 17 Surface of type I QCLs characteristics after polynomial degrees 2

Linear model :

f(x,y) = p00 + p10*x + p01*y + p20*x^2 + p11*x*y + p02*y^2

Coefficients (with 95% confidence bounds):

p00 = -8856 (-1.138e+04, -6335)

p10 = 2111 (1504, 2718)

p01 = 2.583 (-0.7103, 5.876)

p20 = -123.9 (-160.9, -87)

p11 = -0.51 (-0.8644, -0.1556)

p02 = 0.005314 (0.0001277, 0.0105)

Goodness of fit:

SSE: 0.2433 R-square: 0.6234 Adjusted R-square: 0.5816 RMSE: 0.07353

2.3.5. Applying Polynomial Degrees 3 Type (I):

Polynomial degrees 3 for x and y is selected on the curve fitting tool. The graphic and results are:

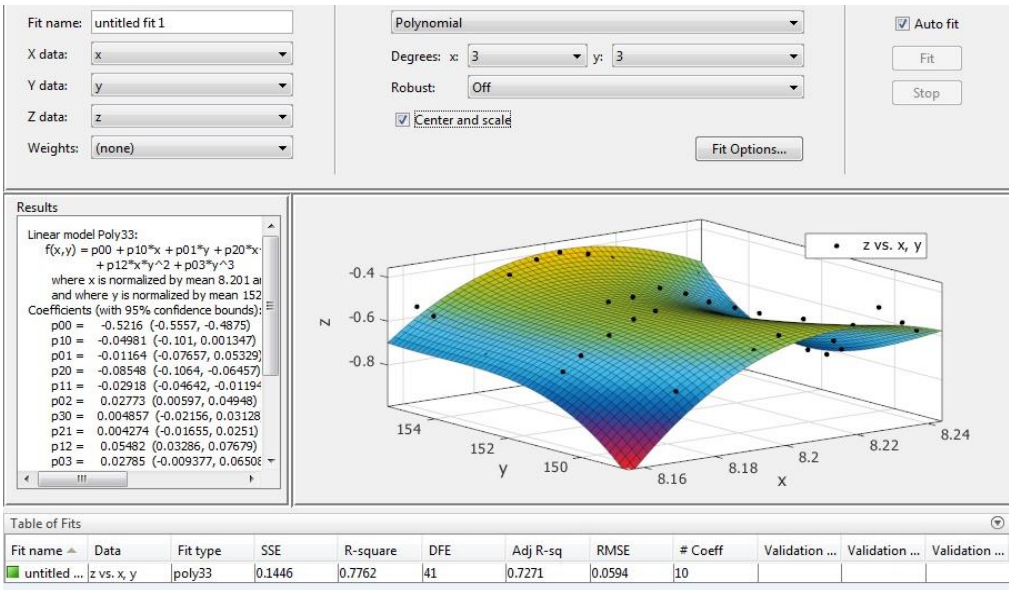


Figure 18 Surface of type I QCLs characteristics after polynomial degrees 3

Linear model :

f(x,y) = p00 + p10*x + p01*y + p20*x^2 + p11*x*y + p02*y^2 + p30*x^3 + p21*x^2*y

+ p12*x*y^2 + p03*y^3 where x is normalized by mean 8.201 and std 0.02634 and where y is normalized by mean 152 and std 2.276

Coefficients (with 95% confidence bounds):

p00 = -0.5216 (-0.5557, -0.4875)

p10 = -0.04981 (-0.101, 0.001347)

p01 = -0.01164 (-0.07657, 0.05329)

p20 = -0.08548 (-0.1064, -0.06457)

p11 = -0.02918 (-0.04642, -0.01194)

p02 = 0.02773 (0.00597, 0.04948)

p30 = 0.004857 (-0.02156, 0.03128)

p21 = 0.004274 (-0.01655, 0.0251)

p12 = 0.05482 (0.03286, 0.07679)

p03 = 0.02785 (-0.009377, 0.06508)

Goodness of fit:

SSE: 0.1446 R-square: 0.7762 Adjusted R-square: 0.7271

RMSE: 0.05938

2.4. Determining coordinates of points for type II:

According to Ungraph 5 program; 1st, 2nd and skew points are determined for real world coordinate system initially. (Figure)

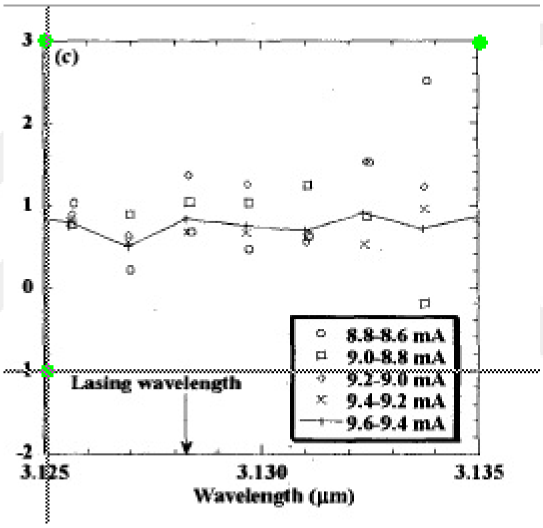


Figure 19 Points of coordinate system for type II QCLs properties

The 1st point (3.135,0), the skew point (3.125,3) and the 2nd point (3.125,-1) are figured out. Dataset that contains selected points coordinates is created by using scatter digitizing method.

Data between given currents are shown as the figures below.

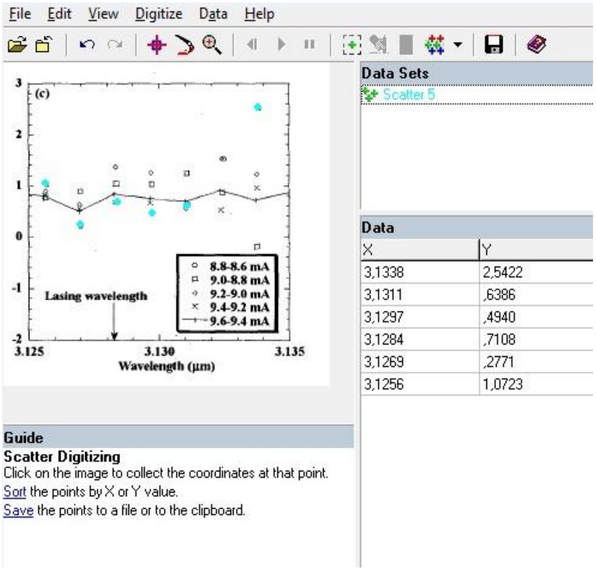


Figure 20 Points at current between 8.8-8.6 mA

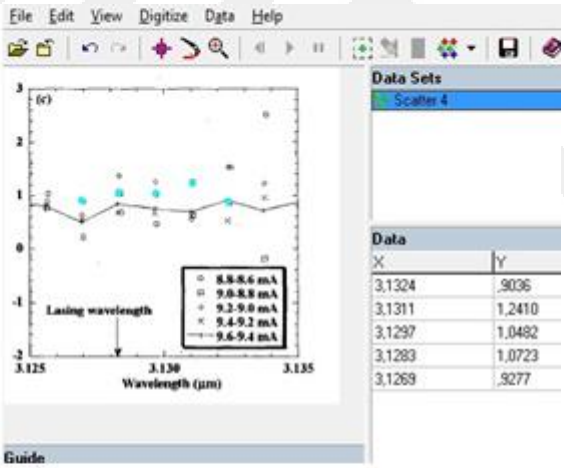


Figure 21 Points at current between 9,0-8,8 mA

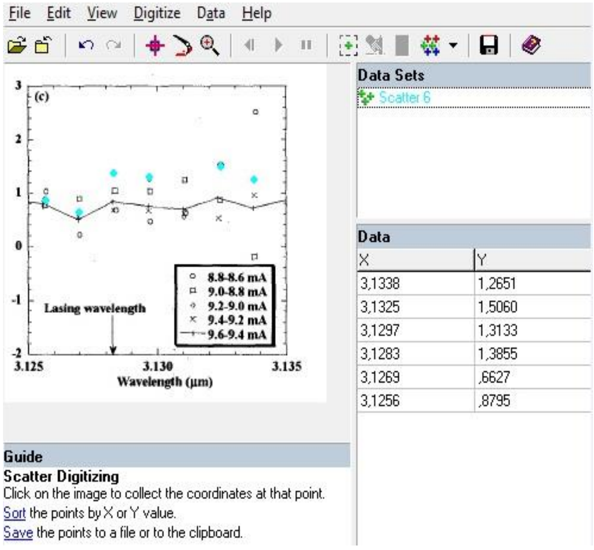


Figure 22 Points at current between 9,2-9,0 mA

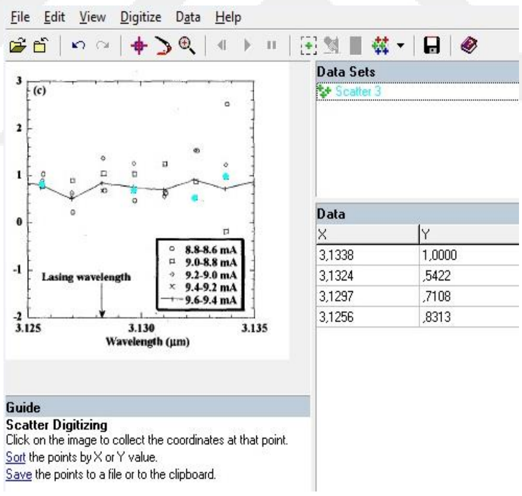
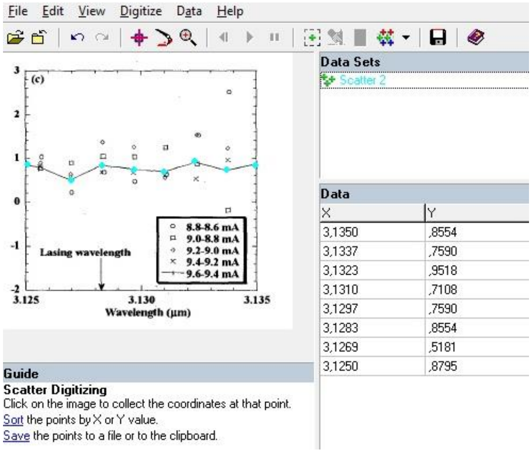


Figure 23 Points at current between 9,4-9,2 mA



X	Y
3,1350	,8554
3,1337	,7590
3,1323	,9518
3,1310	,7108
3,1297	,7590
3,1283	,8554
3,1269	,5181
3,1250	,8795

Figure 24 Points at current between 9,6-9,4 mA

2.5. Modelling parameters of type II QCLs by using surface fitting techniques

2.5.1. Planar Fitting of 3D Points of Form by Least Squared Method to Type II QCLs

$E(A,B,C)=\sum_{i=1}^{m}[(Ax_i+By_i+C)-z_i]^2$ is defined.

When the gradient occurs ∇ E = (0, 0, 0), the hyperparaboloid graph derived.

$$(0,0,0)=\nabla E=2\sum_{i=1}^{m}[(Ax_i+By_i+C)-z_i](x_i,y_i,1)$$

According to the formula the equation below is obtained.

$$\begin{bmatrix} \sum_{i=1}^{m} x_i^2 & \sum_{i=1}^{m} x_i y_i & \sum_{i=1}^{m} x_i \\ \sum_{i=1}^{m} x_i y_i & \sum_{i=1}^{m} y_i^2 & \sum_{i=1}^{m} y_i \\ \sum_{i=1}^{m} x_i & \sum_{i=1}^{m} y_i & \sum_{i=1}^{m} 1 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{m} x_i z_i \\ \sum_{i=1}^{m} y_i z_i \\ \sum_{i=1}^{m} z_i \end{bmatrix}$$

$z=Ax+By+C.$

The equation is similar with the method applied in deriving type I QCLs. Only x , y and z values imported from data coordinates obtained from parameters dispersion related to given current intervals.

The equation is found as:

z=50.9625353071023710*x+-0.3605423368522338*y+-155.2717637140303900

A=50.9625353071023710 B=-0.3605423368522338 C=155.2717637140303900

The results of examined data in excel data analysiswith regression are:

Table 2.4 Regression statistics of type II

Regression Statistics	
Multiple R	0,41308727
R Square	0,170641092
Adjusted R Square	0,106844253
Standard error	0,394225069
Observations	29

Table 2.5 Regression results of type II

	Df	*SS*	*MS*	*F*	*Significance F*
Regression	2	0,831386438	0,415693	2,674757	0,08783198
Residual	26	4,040748549	0,155413		
Total	28	4,872134987			

Table 2 6 Regression statistics of type II- part 2

	Coefficients	*Std Error*	*t Stat*	*P-values*	*Lower %95*	*Upper %95*
Intercept	-155,2744923	80,56314569	-1,92736382	0,06492709	-320,87441	10,32542369
X	50,9634012	25,82662057	1,973289578	0,05918073	-2,1239772	104,0507796
Y	-0,360540467	0,247268034	-1,45809574	0,15678882	-0,8688072	0,147726251

2.5.2. *Applying Custom Equation (Type II)*

Custom equation is selected on the curve fitting tool. The graphic and results are:

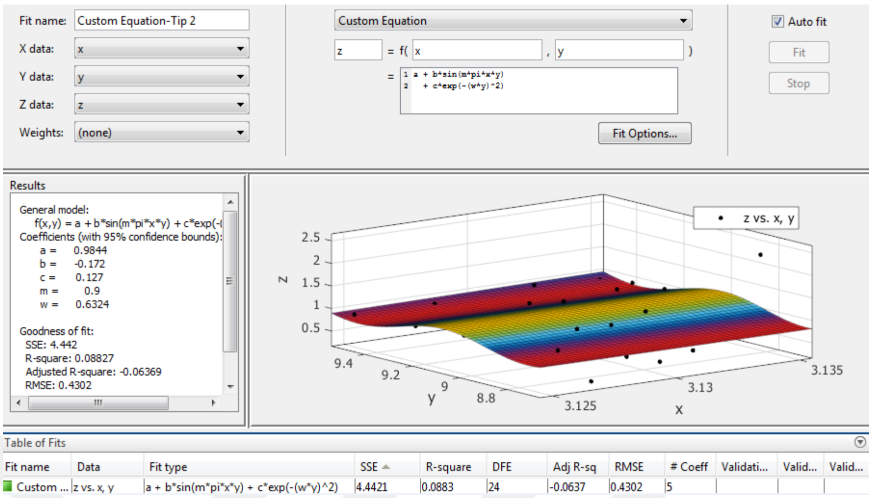


Figure 25 Surface of type I QCLs characteristics after custom equation

General model:

f(x,y) = a + b*sin(m*pi*x*y) + c*exp(-(w*y)^2)

Coefficients (with 95% confidence bounds):

a = 0.9844 b = -0.172 c = 0.127 m = 0.9 w = 0.6324

Goodness of fit:

SSE: 4.442 R-square: 0.08827Adjusted R-square: -0.06369RMSE: 0.4302

2.5.3. *Applying Locally Weighted Smoothing (Lowess) Linear (Type II)*

Lowess Linear is selected on the curve fitting tool. The graphic and results are:

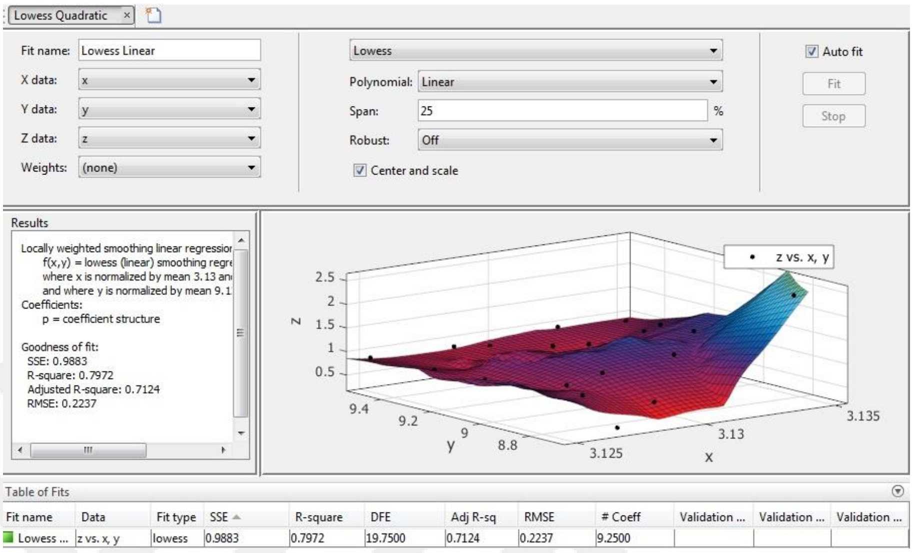


Figure 26 Surface of type II QCLs characteristics after lowess linear

f(x,y) = lowess (linear) smoothing regression computed from p where x is normalized by mean 3.13 and std 0.002911 and where y is normalized by mean 9.121 and std 0.304

Coefficients:

p=coefficient structure

Goodness of fit:

SSE: 0.9883 R-square: 0.7972 Adjusted R-square: 0.7124 RMSE: 0.2237

2.5.4. *Applying Locally Weighted Smoothing (Lowess) Quadratic (Type II)*

Lowess Quadratic is selected on the curve fitting tool. The graphic and results are:

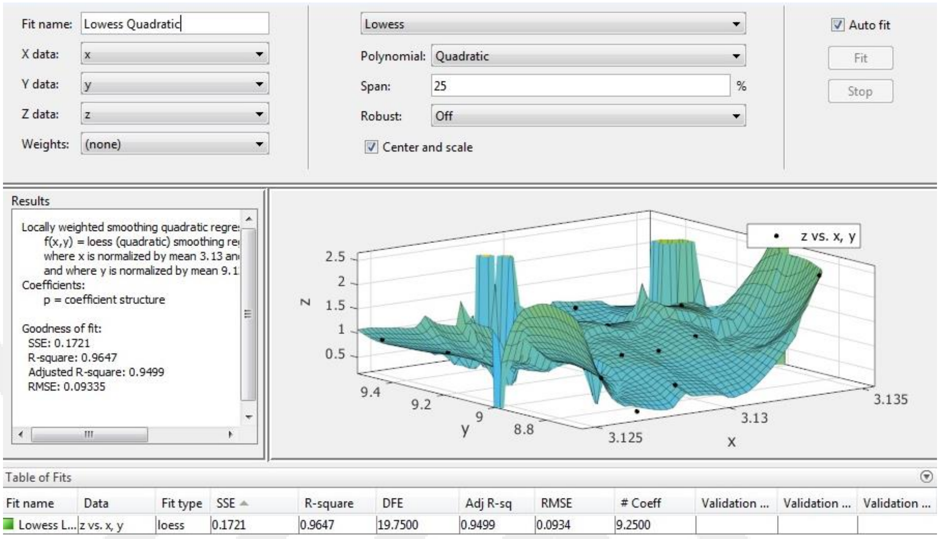


Figure 27 Surface of type II QCLs characteristics after lowess quadratic

f(x,y) = loess (quadratic) smoothing regression computed from p where x is normalized by mean 3.13 and std 0.002911 and where y is normalized by mean 9.121 and std 0.304

Coefficients:

p = coefficient structure

Goodness of fit:

SSE: 0.1721 R-square: 0.9647 Adjusted R-square: 0.9499 RMSE: 0.09335

2.5.5. Applying Polynomial Degrees 2 Type(II)

Polynomial degrees 2 for x and y is selected on the curve fitting tool. The graphic and results are:

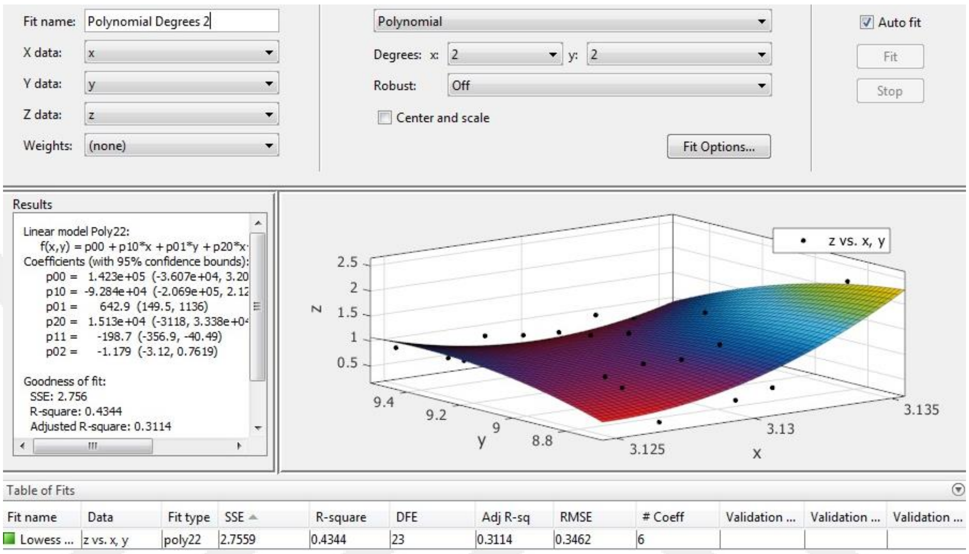


Figure 28 Surface of type II QCLs characteristics after polynomial degrees 2

f(x,y) = p00 + p10*x + p01*y + p20*x^2 + p11*x*y + p02*y^2

Coefficients (with 95% confidence bounds):

p00 = 1.423e+05 (-3.607e+04, 3.206e+05)

p10 = -9.284e+04 (-2.069e+05, 2.125e+04)

p01 = 642.9 (149.5, 1136)

p20 = 1.513e+04 (-3118, 3.338e+04)

p11 = -198.7 (-356.9, -40.49)

p02 = -1.179 (-3.12, 0.7619)

Goodness of fit:

SSE: 2.756 R-square: 0.4344 Adjusted R-square: 0.3114 RMSE: 0.3462

2.5.6. Applying Polynomial Degrees 3 Type(II)

Polynomial degrees 3 for x and y is selected on the curve fitting tool. The graphic and results are:

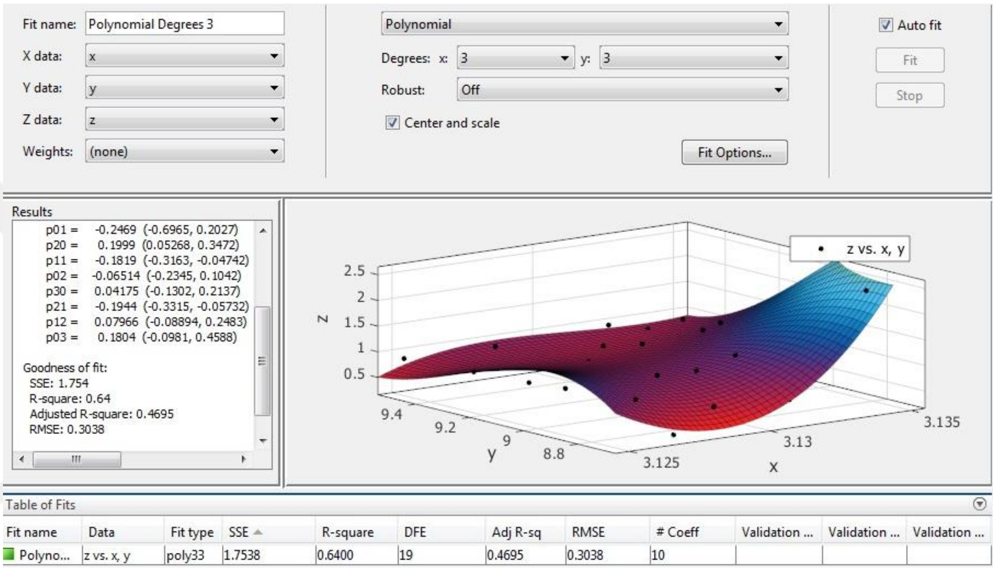


Figure 29 Surface of type II QCLs characteristics after polynomial degrees 3

f(x,y) = p00 + p10*x + p01*y + p20*x^2 + p11*x*y + p02*y^2 + p30*x^3 + p21*x^2*y

+ p12*x*y^2 + p03*y^3

where x is normalized by mean 3.13 and std 0.002911 and where y is normalized by mean 9.121 and std 0.304

Coefficients (with 95% confidence bounds):

p00 = 0.8793 (0.6414, 1.117)

p10 = 0.04685 (-0.2746, 0.3683)

p01 = -0.2469 (-0.6965, 0.2027)

p20 = 0.1999 (0.05268, 0.3472)

p11 = -0.1819 (-0.3163, -0.04742)

p02 = -0.06514 (-0.2345, 0.1042)

p30 = 0.04175 (-0.1302, 0.2137)

p21 = -0.1944 (-0.3315, -0.05732)

p12 = 0.07966 (-0.08894, 0.2483)

p03 = 0.1804 (-0.0981, 0.4588)

Goodness of fit:
SSE: 1.754 R-square: 0.64 RMSE: 0.3038

3. RESULTS

In this study, we present the relationship between characteristic parameters of type I and type II QCLs on their own and in terms of data given in this presentation, the best surface fitting method is found by comparing different approved methods.The main characteristics of QCLs as linewidth enhancement factor, refractive index and current which are related to each other and other external factors are modelled dimensionally.

Before modelling surface of parameters for each type of QCLs, data was determined by using Ungraph 5 program. Data is collected by scatter digitizing method. All points were selected by user preference. 51 data points were chosen and processed. Least square method was applied to extracted data of QCLs as planar fitting of 3D modelling formula and the results were calculated with Excel data analysis program. The other methods were applied by using surface fitting techniques of Matlab R2013a version. These are custom equation, locally weighted scatterplot smoothing linear, locally weighted scatterplot smoothing quadratic, polynomial degrees 2 and polynomial degrees 3 methods.

Firstly we look at the results of modelling of type I QCLs. In the results least square method, R square is 0,127917051 which means data and regression line are not close to each other. Also it means that %12 of the variation can be explained by the independent variables. Adjusted R square which is the term gives more accurate information about analysis because of not being affected each added independent variables similarly is 0,09158. It is less than R square, that tells this modelling method is not very suitable. Significance of F is 0,037 which is a good value.It means there is only %3 probability that regression output could have been by chance. P values of intercept, x and y are not very high. P value for x variable is the highest of them that means there is %3 probability for the result to have been by chance. x variable has the lowest P value means the probability of the result to have been by chance is very low so it is meaningful for the result of regression.

In the results of applied custom equation method, sum of squares error has a higher values as 0,643 which affects R square negatively. R square is 0,0047 that defines %0,47 closeness between regression line and data. Adjusted R square is -0,081 and not meaningful for the regression model. The root mean square error is 0,1182; according to this result it can be said that the measure of the regression error rate is not high.

Lowess regression method consists two different polynomial choice in matlab program. One of them is linear and the other is quadratic form. In the linear form, it is realised that lowess quadratic analysis results are more significant than lowess linear analysis results. In the lowess linear method; R square is 0,893, meaning % 89 closeness between data and regression line, this ratio in lowess quadratic is % 94 (0,9491) . SSE is 0,0691 in lowess linear but it is 0,03291 in lowess quadratic. Adjusted R square is also higher in lowess quadratic (0,9381) than lowess linear regression (0,8701). In lowess quadratic method RMSE (0,02828) is closer to zero more than in lowess linear (0,04098).

In matlab polynomial regression analysis, the degrees of variables can be decided by user till finding optimal solution. In this study degrees 2 and degrees 3 were used in the analysis. R square in polynomial degrees 3 is 0,7762 and in degrees 2 this value decreases 1 percent and becomes 0,6234. Adjusted R square decreases 2 percent in polynomial degrees two and becomes 0,5816 while it is 0,7271 in polynomial degrees 3. RMSE and SSE whose littleness are more valuable are less in degrees 3 than degrees 2.

Table 3.1 Results of all methods applied on type I

	Least Square	Custom Equation	Lowess Linear	Lowess Quadratic	Polynomial-2 degrees	Polynomial-3 degrees
R-square	0,127917	0,004706	0,893	0,9491	0,6234	0,7762
SSE:	0,563410	0,643	0,0691	0,03291	0,2433	0,1446
Adjusted R-square	0,091580262	-0,08184	0,8701	0,9381	0,5816	0,7271
RMSE	0,105106	0,1182	0,04098	0,02828	0,07353	0,05938

As shown above , we can say that custom equation has the worst results and lowess quadratic method has the optimal results for the analysis of given data.

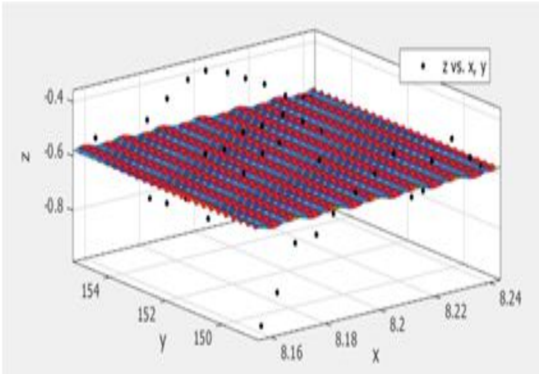


Figure 30 Custom Equation Model for Type I

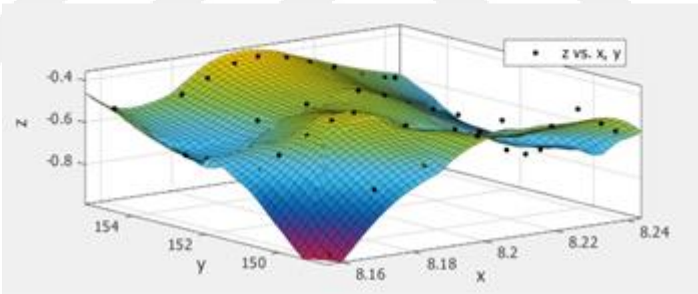


Figure 31 Lowess Quadratic Model for Type I

For type II QCLs, 29 data points were chosen and processed by Ungraph 5 program. According to applied least square method on these points, the results were calculated by Excel data analysis program, too. R square is calculated as 0,17064 by least square method. By this result it can be interpreted as independent variables can explain %17 of variation. Adjusted R square is less than R square as 0,106. Significance F is 0,08783 corresponding % 8,7 probability for regression to have been by chance. The number of observations affects the quantity of significance F. P values of intercept, x and y variables are given as 0.065, 0.059, 0.1567 sequentially. The highest p value belongs to variable y. The variable y has %15 probability on the result to have been by chance. The variable x has the least p value, corresponding more significance for the result.

After least square method, custom equation was applied and the results were calculated. The sum of square error has a value as 4.442 that causes R square to be less. R square is 0,08827 that defines %0.088 closeness between regression line and data. Adjusted R square is -0.06369. The results don't hold optimal and meaningful values. The root mean square error is 0.4302, regression error rate is very low and not close to zero.

The analysis and comparision of results of custom equation and least square method are similar as told in the comparision results of least square and custom equation methods in type I QCLs. Least square method has beter results than custom equation for the given data points.

In the linear and quadratic forms, analysis results are more significant than least square and custom equation analysis results. In the linear quadratic regression, % 96 closeness between data and regression line according to R square and this closeness decreases little in adjusted R square as the value % 95. Sum of square error of quadratic type is less than linear type's SSE which affects directly R square of analysis. RMSE in quadratic method is also less than RMSE of linear form considerably.

In polynomial regression analysis, degrees 2 and 3 are used in Type II QCL, too. Polynomial degrees 3 results make regression line and data closer than polynomial degrees 2. When the results are compared, it is realised that polynomial degrees 3 is more meaningful for user to acces right solution. The scores are not very approximate. While being % 43 access in polynomial degrees 2, it is % 64 in polynomial degrees 3. The difference between R squares seems like the difference between adjusted R squares. SSE of the polynomial degrees 2 is greater than the SSE of polynomial degrees 3 cauisng R square to decrease. RMSEs of analysis are closer as it is 0,3462 in polynomial degrees 2 and 0.3038 in polynomial degrees 3.

Table 3.2 Results of all methods applied on type II

	Least Square	Custom Equation	Lowess Linear	Lowess Quadratic	Polynomial-2 degrees	Polynomial-3 degrees
R-square	0.170641	0.08827	0.7972	0.9647	0.4344	0.64
SSE:	4,040748	4.442	0.9883	0.1721	2.756	1.754
Adjusted R-square	0.106844	-0.06369	0.7124	0.9499	0.3114	0.4695
RMSE	0,373277	0.4302	0.2237	0.09335	0.3462	0.3038

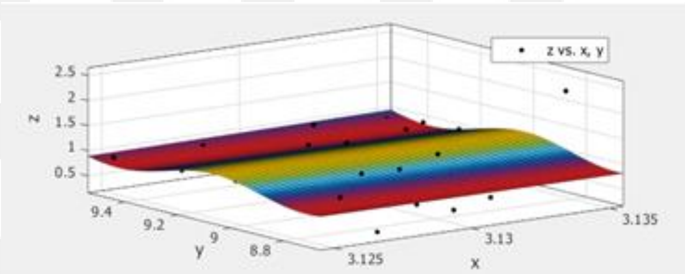


Figure 32 Custom Equation Model for Type II

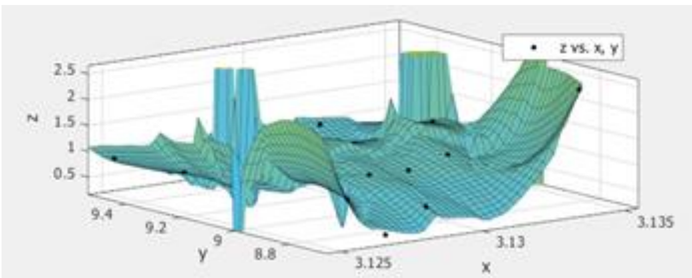


Figure 33 Lowess Quadratic Model for Type II

4. CONCLUSION

When we compare the results of least squares and custom equation method, we come to a conclusion as least square method is better than custom equation method in the analysis of given data. We can see that least square method has higher R square and adjusted R square, lower RMSE and SSE that cause higher performance. The results of type II are similar with the type I regression methods results. When analysed, it is seen that lowess quadratic regression method gives much more significant results than the others and custom equation is the worst method for the given data and it should not be chosen for modelling of the given type II data points.

There also studies about laser modelling. These studies are generally effect of temperature on the laser creation. One of them is “Modelling of temperature effects on the characteristics of mid-infrared quantum cascade lasers”. This study is used to improve increased output to design more effective devices. The temperature dependence of gain, current density and output power is analysed. Another study about laser modelling is “Complete rate equation modelling of quantum cascade lasers for the analysis of temperature effects”. On the Dynamics of GaAs-based quantum cascade laser (QCL), effect of temperature is analysed. The aim is to get better condition of threshold current density by the experiment at higher temperatures. (Chen, 1993)

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