

# EPITAXYproject®

v.2.9.8 © 2010

Software manual

## Overall description

The *EPITAXYproject*® software is designed as basic tool supporting epitaxial growth of semiconductor materials and structures. The package goal is to assist epitaxy of number of III-V ternaries, quaternaries, other user-defined compounds and device stacks in following applications groups.

- First one is the flows maintenance utility and processes database function. These features are especially valuable for quaternaries or higher order compounds growth, where control of flow parameters is not as simple as in case of ternaries. Results for MOCVD growth of InGaAsP/InP for example are excellent and efficiently allow to obtain desired material. Beside calculations for prefixed compounds available is also definition of arbitrary ternary, quaternary or quinary compound. Related software module includes band-gap, lattice constants calculators and the compounds database.
- Second feature of the software concentrates on structures with quantum well by simulation of inter-band transitions with choice of preset barrier/well systems. Applicable is more advanced option for analysis of any multi-layered semiconductor quantum well structure. Included is the algorithm for QW parameters determination. It solves the thickness only or - in more sophisticated option - both thickness and QW material band gap. The algorithm allows to obey costly TEM measurements and is very useful for strained QWs.
- Within frames of structure characterization available is next program aim spotted on 1-dimensional photonic structures like Bragg reflectors by estimation of reflectance spectra. It allows determinate structure thickness parameters and uniformity. Beside application for resonant structures the module can be helpful for any non resonant structure analysis by reflectivity.
- The fourth package feature delivers sample survey on electrical potential profile in structures. The calculation can be for example oriented toward assigning of depletion regions or consideration of quantum well profile.
- Attached are also few calculators making everyday life with semiconductor epitaxy easier.

The software is being developed, inclusion of next materials and functions should process in the future.

The software creation and tests were inspired by everyday needs of the epitaxy laboratory in the [Institute of Electronic Materials Technology](#) and [Epi-Lab.com](#).

*EPITAXYproject*®

[support@epitaxyproject.com](mailto:support@epitaxyproject.com)

<http://www.epitaxyproject.com>

# Contents

1.11. Introduction.....	2
2. Physical constants data of compounds.....	3
3. Flows maintenance.....	4
3.1 Flows recalculation.....	4
3.2 “Custom compound” calculation.....	8
3.3 “EPlearning” feature.....	11
3.4 “Find flows” function.....	11
4. Compounds database.....	11
5. Quantum well structures.....	13
5.1 “Simplified” option.....	13
5.2 “Advanced” option (QWproject®).....	14
5.3 QW thickness algorithm.....	16
6. 1-dim photonic structures.....	18
6.1 “Simplified” option.....	18
6.2 “Advanced” option (BRproject®).....	18
7. Heterojunction structures analysis (Jproject®).....	20
8. Calculators.....	22
8.1 XRD calculator.....	22
8.2 Partial pressures calculator.....	22
8.3 Other calculators.....	22
9. System requirements.....	23

## 1. Introduction

The EPITAXYproject® software package is designed as basic tool supporting epitaxial growth of semiconductor compounds as quaternary InGaAsP/InP, InGaAsP/GaAs, InGaAlP/GaAs, InAlGaAs/InP, InGaAsN/GaAs, InAlGaN/GaN and ternary InGaAs/InP, InGaAs/GaAs, AlGaAs/GaAs, GaAsP/GaAs, InAlAs/InP, InGaN/GaN, AlGaN/GaN, GaAsN/GaN or other III-V, II-VI and “user-defined”. The software is helpful in epitaxy of single layers and also in development of device structures. There are five main parts of the program:

1. Flows maintenance for epitaxy reactors (with compounds database). This function is accessible through “Materials” button in the main EPITAXYproject® taskbar.
2. Analysis of quantum well structures. (“Quantum wells” button).
3. Calculation of reflectance spectra and analysis for Bragg reflector and other 1-dimensional photonic structures. (“Reflectors” button).
4. Analysis of electrical potential in semiconductor heterostructures. (“Junctions” button).
5. Set of calculators for typical epitaxy-related problems. (“Calculators” button).



Fig.1. EPITAXYproject® taskbar.

## 2. Physical constants data of compounds

Almost all *EPITAXYproject*<sup>®</sup>'s units applies physical constants of semiconductor compounds, such values of band-gaps, lattice constants and other parameters of most important III-Vs are used in accordance to following data sources (T=300K):

- InGaAs/InP, InGaAs/GaAs: "Properties of Indium Gallium Arsenide" Edited by Pallab Bhattacharya, INSPEC, 1993.
- AlGaAs/GaAs: "Properties of Aluminium Gallium Arsenide" Edited by Sadao Adachi, INSPEC, 1993 .
- InGaAsP/InP, InGaAsP/GaAs, InAlGaAs/InP, InGaAsP/GaAs: "Indium Phosphide and Related Materials: Processing, Technology and Devices" Edited by Avishay Katz, Artech House, Boston, London, 1992. , by E. Kuphal, J. Cryst. Growth, Vol. 67, 1984, p. 441.
- InGaP/GaAs: "The MOCVD Challenge Volume2" Manijeh Razeghi, IOP Publishing Ltd 1995.
- InGaN/GaN, AlGaN/GaN, InAlGaN: "Gallium Nitride (GaN)" I , J.I. Pankove, T.D. Moustakas, Academic Press San Diego, San Francisco, New York, Boston, London, Sydney, Tokyo, 1998.
- InGaAlP/GaAs: I. Vurgaftmana, J. R. Meyer, R. Ram-Mohan, J. Appl. Phys. 66, 11 p. 5815-5874.
- InGaAsN, GaAsN, InAsSb: I. Vurgaftmana, J. R. Meyer, R. Ram-Mohan, J. Appl. Phys. 66, 11 p. 5815-5874.

All III-V data were compared to the review by I. Vurgaftmana, J. R. Meyer, R. Ram-Mohan, J. Appl. Phys. 66, 11, (2001) p. 5815-5874 and other data published in the literature and the internet.

Parameters of other III-Vs and also II-VI compounds which became included in the software were introduced on the basis of their values presented in the literature and the internet.

Dependencies of factors on composition are usually derived for both strained and relaxed crystals.

The most commonly used in *EPITAXYproject*<sup>®</sup> physical parameters are lattice mismatch ( $\Delta a/a$ ) and energy gap ( $E_g$ ). Because, when consider XRD of strained compounds, these values can be incorrectly applied, below presented is the specification of both terms for needs of software environment.

**The  $E_g$  and  $\Delta a/a$  parameters in case of relaxed layer should be understood as follows:**

- the wavelength value for maximum of PL signal in micron unit - as a measure of  $E_g$ .
- value of parallel mismatch  $\Delta a/a$  for relaxed crystal.

For cubic crystals this  $\Delta a/a$  is equal to measured by XRD (x-ray diffraction) difference of relaxed crystal perpendicular lattice constant relative to the substrate's value divided by the substrate's value in ppm unit. Simply: whole value of perpendicular  $\Delta a/a$  directly measured by x-ray.

**The  $E_g$  and  $\Delta a/a$  parameters in case of strained layer should be understood as follows:**

- the wavelength value for maximum of PL signal in micron unit - as a measure of  $E_g$ .
- value of parallel mismatch  $\Delta a/a$  for relaxed crystal.

For cubic crystals this  $\Delta a/a$  is also equal to the difference of relaxed crystal perpendicular lattice constant relative to the substrate's value divided by the substrate's value in ppm unit. It is typically about half of it's value for strained crystal directly measured by x-ray diffraction. Simply: corrected (typically about half) perpendicular  $\Delta a/a$  value measured by XRD.

This definition is easy to apply with XRD for cubic crystals. For non-cubic crystals it can bring some work, however in case of wurzite nitrides above specification related to cubic crystals is still quite applicable.

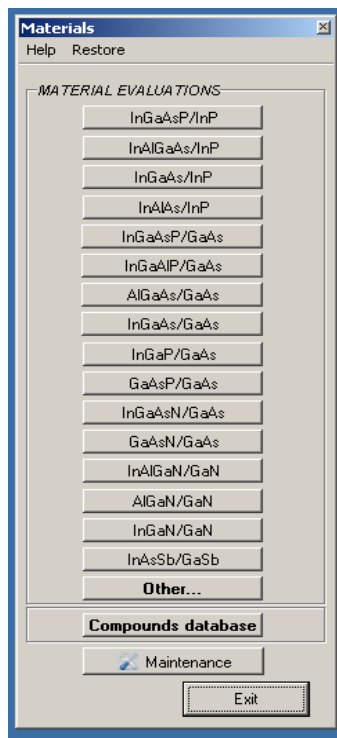
The energy gap of relaxed material is used to derive energy gap of strained crystal, in such cases correction of a few nanometers in photoluminescence per each 1000ppm of strain to evaluate appropriate energy-gap is applied. This correction can be obtained from deformation potential constants.

Occurring for strained semiconductors heavy hole – light hole separation is evaluated on the basis of it's known values for ternaries (InGaAs/GaAs, GaAsP/GaAs, InGaAs/InP). The evaluation error is estimated as 0-30% of separation energy value.

Band-gap calculators are accesible in two different options:

1. "*Materials*" button - specific compound button - "*B. gap. calc.*" button.
2. "*Materials*" button - "*Compounds database*" button.

### 3. Flows maintenance



The flows maintenance module is accessible through "*Materials*" button in the main taskbar.

In practice, the precursors flows evaluation for epitaxy of multiple compounds may be processed in two ways. The first one is data interpolation on the basis of a file of collected past process parameters. This first way in simplest form suffer from epitaxial system drift - mainly due to maintenance: source exchange, controllers exchange and other. This drift is a reason of development the second way which has a form of flows correction calculation, where basically only last one (or two) process with material's parameters as close to desired one as possible is used as a base of extrapolation.

This *EPITAXYproject*<sup>®</sup>'s module primary aim is the second of these choices: the evaluation of precursors flows corrections as a function of desired compound parameters (Chapter 3.1-3.3). The first choice also finds its place (Chapter 3.4).

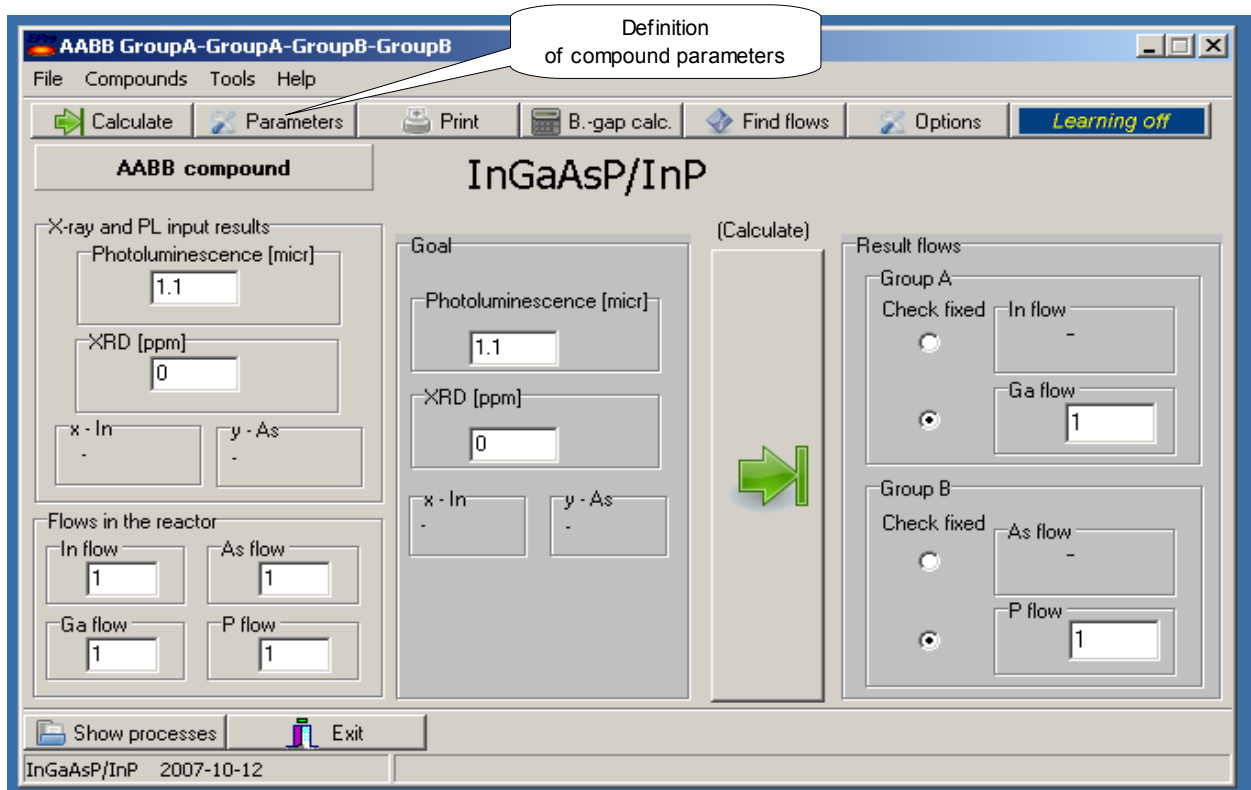
Additionally provided is the process database.

**Fig.2.** The flows maintenance module main form.

### 3.1. Flows recalculation

The *EPITAXYproject*<sup>®</sup> is capable to calculate corrections of elemental (precursors) flows in epitaxy reactors for adjustment of produced material composition. The calculation is processed under established all other than precursors flows reactor parameters. The execution of flow recalculation requires a test sample with as close composition to desired one as possible, the values of Eg or  $\Delta a/a$  and corresponding flows for this sample are input parameters. Other input parameters are Eg or  $\Delta a/a$  values of desired material.

For example, process with Gallium flow equal 5[arb. units - can be ccm/min, shutter angle or any other linear unit] and Arsenic flow 30[arb. units] produced the InGaAsP layer with measured by x-ray diffraction perpendicular lattice constant 1000ppm larger relative to InP and energy gap corresponding 1.35 $\mu$ m photoluminescence. All this parameters may be used to obtain InGaAsP lattice matched to InP with energy gap corresponding to 1.55 $\mu$ m. Corrections of flows are subject of this part of program.



**Fig.3.** Flows maintenance form (flows correction calculation) for InGaAsP/InP compound.

The calculation is available through clicking "Materials" button in the main taskbar and

then clicking desired compound button.

**Summary:**

*must be known:* energy gap **and (or)** lattice mismatch  
**and** precursors flows for test material

*will be obtained:* precursors flows for desired material

("or" – in case of ternaries)

The flow recalculation is provided with the use of **compounds physical data described in chapter 2. The Eg and  $\Delta a/a$  input parameters should be set as follows:**

- The wavelength value for maximum of PL signal in microns (as a measure of Eg).
- value of parallel mismatch  $\Delta a/a$  for relaxed crystal.

For cubic crystals this  $\Delta a/a$  value is also equal to measured by XRD difference of relaxed crystal perpendicular lattice constant relative to the substrate's value divided by the substrate's value in ppm unit (so typically about half of directly measured value for strained layer and whole value for relaxed layer). For no-cubic layers the evaluation of parallel from perpendicular mismatch is formally not so simple, however often maintaining them as cubic does not lead to serious differences.

Basically calculations assume not relaxed strain in input and output sample (means typical layer thickness below 0.2-2 $\mu$ m when lattice mismatch on the level of 3000ppm or lower). Relaxed condition can be also set, it can be marked in specific compound's "Options" form. Similarly as in band-gap calculators, problem of composition-bandgap relations for strained compounds is resolved by the correction of few nm in photoluminescence per each 1000ppm of strain. In default data configuration, for simplicity of relation to XRD measurement, wurzite nitrides lattice mismatch corresponds to c-axis.

---

**To provide calculations do as follows:**

**For ternaries:**

1. Set measured photoluminescence maximum wavelength **or** lattice mismatch of the test sample in the "input values" frame.
2. Set two values of applied carrier flows for the test sample in the "applied flows" frame.
3. Set value for desired material: stoichiometry or lattice mismatch or energy gap - in the "results" frame.
4. Run calculations - stoichiometry of input sample and evaluated carrier flow for desired one will be displayed.

**For quaternaries:**

1. Set measured maximum wavelength **and** lattice mismatch of the test sample in the "input values" frame.

2. Set four values of carriers flows for the test sample in "applied flows" frame.
2. Set desired maximum wavelength and lattice mismatch for desired material in "Goal" frame.
4. Run calculations - all stoichiometries, and evaluated carriers flows for desired material will be displayed.

---

The composition difference between test sample and desired one is a source of error. For majority of compounds typically the 5% difference in composition factor (factors) allows to obtain desired sample with accuracy of 0.5% in one or two processes (the first result should be then used as an input set of values for the second process e.t.c.).

The flow recalculation for InGaAsP/GaAs in the region of its miscibility gap and compositions close to InGaP lattice matched to GaAs meets some problems in the sense of barrier in arsenic adsorbing. In such a case the first order approximation used initially for the flow correction is not efficient enough. Similar problems can occur for other materials within miscibility gaps (as antimonides) and also for InGaN/GaN, InAlGaN/GaN (saturation of Indium compounding) and other highly strained layer, these events are rather comparatively rare. The "EPLearning" (chapter 3.3) feature can help to resolve analogous difficulties.

Through application of "EPLearning" function experimental data are collected and problem with no linear flows-composition relations is efficiently reduced by application of higher order approximation. If the "EPLearning" corrections are not enabled, calculations are using first order approximation. Usually, if all reactor parameters except flows are fixed, this approximation will be evaluation good enough. Mentioned relatively rare miscibility or saturation regions can bring difficulties in such configuration. If the "EPLearning" feature and corrections are enabled the software collects process data and provides more careful data analysis for flows evaluation.

The possibility of direct solution of composition-flow relations of course exists but such analysis requires a file of parameters, complicates the evaluation and makes it case specific. This analysis is not the EPITAXYproject's method. Applied empirically evaluated relations between compositions ratios and flows ratios are quite efficient, at worst require one (or exceptionally two) secondary attempt to obtain desired sample and in principle lead to success for strong majority of practical cases.

The flow correction calculation for ternaries requires only one parameter of the material - instead of two,  $E_g$  and  $\Delta a/a$ , needed for quaternaries.

#### **Some details for few most important III-V compounds:**

- InGaAsP/InP

The flow correction calculation function with default parameters considers values of direct band-gap  $E_g$  transitions.

Inaccuracy of flow correction calculation with first order approximation is not significant in whole range of typical MOCVD growth of InGaAsP/InP and allows to obtain desired sample in one or two processes in case of compositional distance of a few percent. In case of MBE the vicinity of miscibility gap may affect results.

- InGaAsP/GaAs

The flow correction calculation function with default parameters considers values of direct band-gap  $E_g$  transitions.

Inaccuracy of flow correction calculation with first order approximation is low enough to obtain desired sample by MOCVD except the region of InGaAsP/GaAs miscibility gap where barriers for arsenic compounding may occur. Application of *Elearning* feature can be helpful.

- GaAsP/GaAs, GaAs/InP, AlGaAs/GaAs, InGaP/GaAs

The flow correction calculation function with default parameters considers values of direct band-gap  $E_g$  transitions.

Typically compositions-flows ratios relation is close to proportionality, so first order approximation works well and application of *Elearning* feature is not obligate.

- InAlGaAs/InP, InGaAlP/GaAs

The flow correction calculation function with default parameters considers values of direct band-gap  $E_g$  transitions.

Typically compositions-flows ratios relations are close to proportionalities, so first order approximation works well and application of *Elearning* feature is not obligate.

- InGaN/GaN, InAlGaN/GaN

The lattice mismatch value corresponds to c-axis.

Typically for higher Indium compositions proportional compositions-flows ratios relations do not work well. Application of *Elearning* feature can be helpful.

- AlGaN/GaN

The lattice mismatch value corresponds to c-axis.

Typically compositions-flows ratios relation is close to proportionality and first order approximation works well.

- Antimonides

Problems with saturation of Ga and Sb compounding occur, so proportional compositions-flows ratios relations sometimes do not work well. Application of *Elearning* feature can be helpful.

### 3.2. “Custom” compound calculations.

Flow correction procedure can be applied not only for prefixed but also for any arbitrary ternary, quaternary or quinary compound.

---

**To define “Custom” compound calculations do as follows:**

**1. Prepare following values:**

- Energy gaps (in eV unit) for related binary compounds. For instance in case of InGaAsP/InP which corresponds to quaternary AABB (GroupIII-GroupIII-GroupV-GroupV) sequence prepare direct energy gap values of InAs, InP, GaAs, GaP.
- Lattice constants (in Angstrom unit) for related binary compounds and substrate. As above.
- Energy gap bowing parameters for related binary pairs (in eV unit). For instance in case of InGaAsP/InP prepare direct energy gap bowing parameter “b” values of InAs-GaAs, InP-GaP, GaAs-GaP, InAs-InP pairs (default value is “0” and for majority of cases those values are not significant).
- Strain correction (in meV/1000ppm unit) when compound is strained but energy gaps correspond to relaxed one. Default value is “0” – typically flow correction will work (less correctly) with “0” value for close – to lattice matched materials.
- Light hole – heavy hole strain correction (in meV/1000ppm unit) that will be applied when compound is compressively strained (default value is “0”).

**2.** Click “*Materials*” choice in main taskbar.

**3.** Click “*Other..*” button.

**4.** Click “*Custom..*” button.

**5.** Select compound sequence.

**6.** Set all prepared values (as in point 1.), check if the layer is strained.

The “*A/B correction*” or similar fields correspond to justification that can be done via experiment (default value is “1”).

**7.** Click “*OK*” button.

The “*Custom..*” button (point 4.) will correspond to pre-set entered values.

---

**To Run “Custom” compound calculation do as follows:**

**a)** In case of **ternaries** and **quaternaries** do as described for prefixed compounds (chapter 3.1).

**b)** In case of **quinaries**:

- 1.** Prepare first sample - “Sample I” – results of PL, XRD and corresponding flows of all five carriers. This sample should be close to desired in composition factors.
- 2.** Prepare second sample – “Sample II”. This sample should be produced in the

same reactor parameters except one or two carrier flows - one of groupA elementals and one of groupB elementals. The difference in mentioned flows between both samples should be on the level corresponding to few percent difference in composition. It typically means:

- 100% of relative flow difference when composition factor is on the level of x=2-5%
- 50% of relative flow difference when composition factor is on the level of 5-10%
- 20% of relative flow difference when composition factor is on the level of 10-30%
- 10% of relative flow difference when composition factor is on the level of 30-60%
- 30% of relative flow difference when composition factor is on the level of 60-80
- 60% of relative flow difference when composition factor is on the level of 80-90%
- 100% of relative flow difference when composition factor is on the level of 90-96%

Prepare PL, XRD results and all five flows values.

3. Click "*Materials*" choice in main taskbar.
4. Click "*Other..*" button.
5. Click corresponding earlier preset button. (pages 8.-9.).
6. Set PL and XRD values of sample I in "*PL and XRD results – sample I*" frame.
7. Set five flows in "*Flows in the reactor – sample I*" frame.
8. Repeat steps 6.-7. for sample II.
9. Click "Calculate compositions – sample I and II" button – compositions of both samples should be displayed.
10. Set desired PL and XRD values of the "*Goal*" sample in "*Goal*" frame.
11. Select and set one composition factor to leave fixed (use values obtained in point 9.) – this value should be in low difference relative to sample I or II - on the level of 0-5% of "x".
12. Select and set two flows – one of groupA and one of groupB to leave fixed in "*Result flows*" frame.
13. Run calculations clicking "*Calculate*" button. Composition and required flows (in "*Result flows*" frame) of "*Goal*" sample should be displayed.

---

### 3.3 "EPlearning" feature.

This function provides monitoring of samples parameters for justification of flow corrections.

If function is enabled (*“Learning on”*), each time the calculation is processed and confirmed, sample parameters will be saved. Next time form is shown, it will be possible to enter parameters of sample grown according to previous calculation. This pair of results is used for estimation of corrections. Gradual collection of data within certain composition range allows to estimate compositions-flows dependencies with higher accuracy.

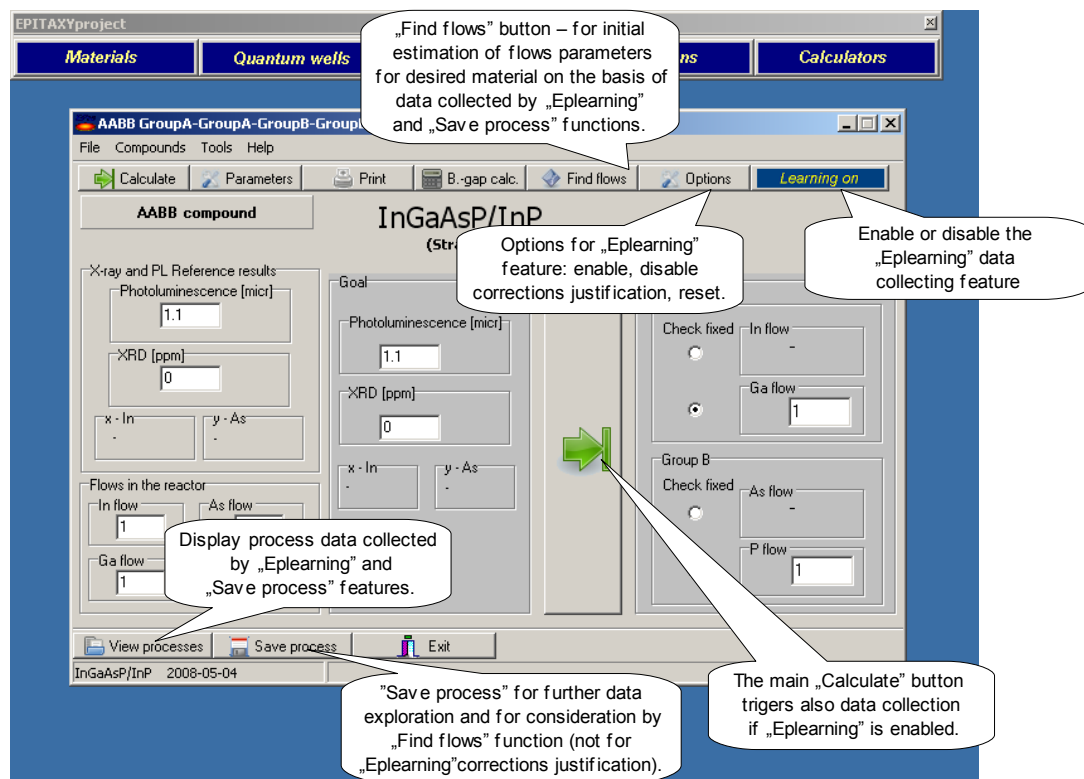
To disable learned corrections click the *“Options”* button in the specific compound form and check appropriate option. Corrections values will be then used as single values according to initially set. To change these values pursue the sequence according to *“To define “Custom” compound calculations do as follows: “* topic.

Saved corrections can be cancelled by *“Options”*, *“Reset corrections”* buttons sequence. If the learning function is on, the learning function will collect further data and ignore data previously stored.

Data are stored in *“elearning.ini”* file in the *EPITAXYproject’s* directory (typically *C:/Program Files/EPITAXYproject/“* directory). This file provides also process database function. The process data can be stored clicking *“Save process”* button.

**Remark:** If any problem that can be related to corrections adjustment system occur disable this function as follows:

select material – click *“Options”* button – select *“Disable learned corrections”* - click *“OK”*.



**Fig.4.** Epitaxial flows maintenance form for InGaAsP/InP compound. Described are buttons

responsible for data analysis: initial flows estimation, justification of computed flows corrections, process data storage.

### 3.4 “Find flows” function.

This function uses data stored by “*Eplearning*” feature. Function is accessible by “*Find flows*” button in specific compound form. It evaluates initial absolute flows for desired compound parameters. The interpolation is based on polynomial fitting to experimental data by smallest squares method. Stored data are time-weighted:  $\exp(-\text{days}/365)$ .

“Show processes” button allows to present saved process data, “*Edit*” button opens for edit the text log file.

## 4. Compounds database

The Compounds database is accessible through “*Materials*” - “*Compounds Database*” buttons. It offers information on basic parameters of binary and higher order III-V and II-VI (or user-defined) compounds.

Following parameters are considered (T=300K):

- Eg - energy gap in corresponding wavelength ( $\mu\text{m}$ ) unit,
- $\Delta a/a$  - lattice mismatch in (ppm) unit,  $\Delta a/a = (a - a_{\text{substrate}}) / a_{\text{substrate}} * 10^6$  (ppm),
- CBO, VBO – “absolute” conduction and valence band offsets (CBO - VBO = Eg) in (eV) unit,
- Ex – indirect X-valley band gap in corresponding wavelength ( $\mu\text{m}$ ) unit,
- me – electron effective mass in (me) unit,
- mhh – heavy hole effective mass in (me) unit,
- mlh – light hole effective mass in (me) unit,
- Ehh-Elh – heavy holes – light holes bands splitting (strain – related) in (eV) unit,
- a – lattice constant in (Angstrom) unit.

For compounds of higher order than binary all values are derived on the basis of parameters for binaries with multilinear approximation except:

1. energy gap  $E_g$ , where second order approximation is applied,
2. Ex energy gap and VBO and CBO band offsets, which values consider earlier calculated  $E_g$  value.

Beside calculation with defined composition the database offers oppositely calculation of composition on the basis of entered other parameters.

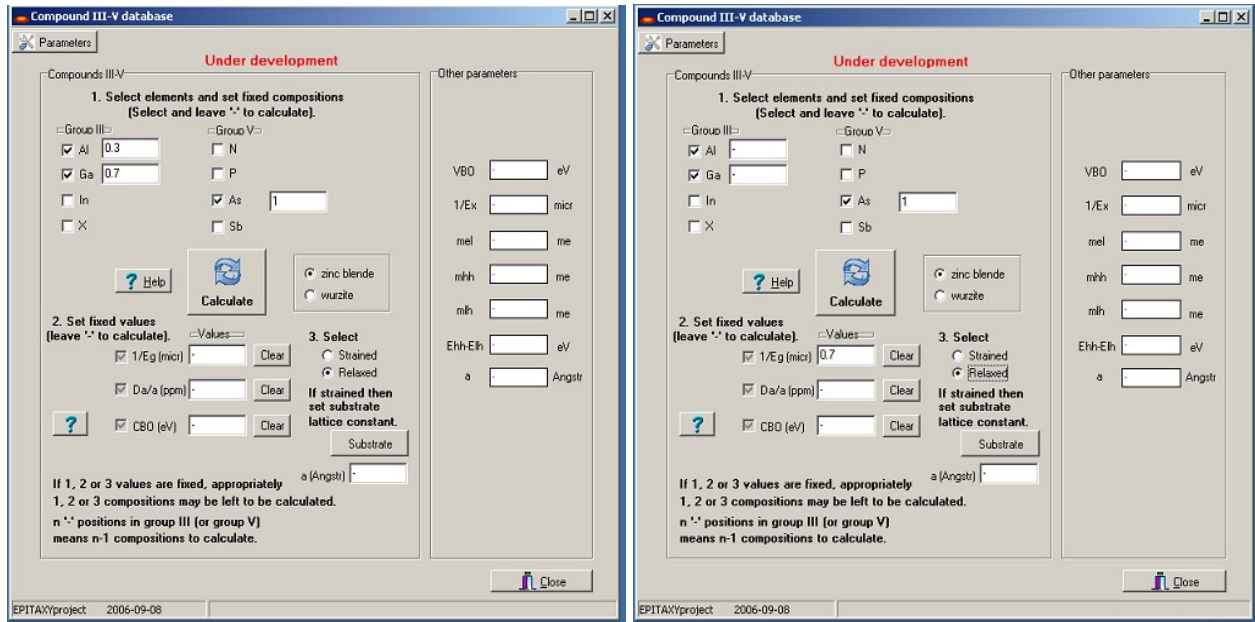
To calculate compound parameters (other than composition) on the basis of its composition do as follows:

- 
1. Select elements and set their compositions,
  2. Set substrate or select "*relaxed*",
  3. Run calculation.
- 

To calculate composition on the basis of known value (or values) of: Energy gap ( $1/E_g$ ), lattice mismatch ( $\Delta a/a$ ), band offset (CBO) do as follows:

- 
1. Set bounded value or values in "Values" group, leave sign '-' if value is unbounded.
  2. Select elements,
  3. Set bounded compositions if exist, leave sign '-' if composition is unbounded.
  4. Consider remark: Number of bounded values should be not greater then number of unbounded compositions. (Beware: '-' signs in two composition boxes typically assign one unbounded composition).
  5. Set the substrate or select "*relaxed*",
  3. Run calculation.
- 

**Remark:** In *EPITAXYproject*® v. 2.8... the main, described above, compound database does not directly maintain *QWproject*, quantum well resolving algorithm and *Jproject* modules, so data can slightly differ between them. The most careful data in customizable form is provided by the compounds database.



**Fig.5.** The compounds database form's configuration for calculation of Al(0.3)Ga(0.7)As parameters (left) and the configuration for calculation of composition x of Al(x)Ga(1-x)As having energy gap corresponding to 0.7 $\mu$ m wavelength (right).

## 5. Quantum well structures

### 5.1. "Simplified" option:

Provided is quantum well states calculation through resolving of the Schrödinger's equation for rectangular well potential with the use of effective mass approximation. There are a few barrier/well/barrier sets with prefixed values of energy gaps, effective masses and band offsets ratios according to data from sources pointed in "*Physical constants data of compounds*parameters of P". All values may be corrected by copying them to "other" fields.

**To execute the calculation please do as follows:**

1. Check appropriate barrier material in the "barrier" frame. If the material is not included in the list, please check "other" and set:
  - Bandgap wavelength (in micron unit),
  - electron effective mass (in electron mass unit),
  - heavy holes effective mass (in electron mass unit),
  - light holes effective mass (in electron mass unit).
2. Check appropriate well material in the "well" frame. If the material is not included

in the list, please check "other" and set:

- energy bandgap,
  - electron effective mass,
  - heavy holes effective mass,
  - light holes effective mass.
3. If anywhere above "other" option was checked please set the energy offsets ratio  $\Delta E_c/\Delta E_v$  (default is "1") and heavy holes - light holes splitting (default is "0"), data at the end of this topic may be useful. (optional)
  4. Set QW thickness (in angstrom unit).
  5. Run calculations – transition wavelengths (in micron unit) and indexes for heavy and light holes will be displayed (maximum ten lowest energies).

---

Applied band offsets ratios  $\Delta E_c/\Delta E_v$ :

InGaAsP/InGaAsP/InP	0.25/0.35
InGaAsP/InGaAs	0.26/0.34
InGaAs/InP	0.26/0.34
InGaAsP/GaAs	0.31/0.69
InGaP/GaAs	0.3/0.7
InGaP/InGaAsP	0.31/0.69
InGaP/GaAs	0.31/0.69
InGaAs/GaAs	0.6/0.4
InP/InAlGaAs	1/1
AlGaAs/GaAs	0.6/0.4
InGaN/GaN	0.72/0.8
AlGaN/GaN	67/33
AlGaN/InGaN	60/40

## 5.2. "Advanced" option:

This option uses "QWproject" module which allows to calculate energy levels in arbitrary defined quantum well. The well structure can be defined by selecting a number of different layers with specified band parameters. Available is set of standard semiconductor materials for simple selection.

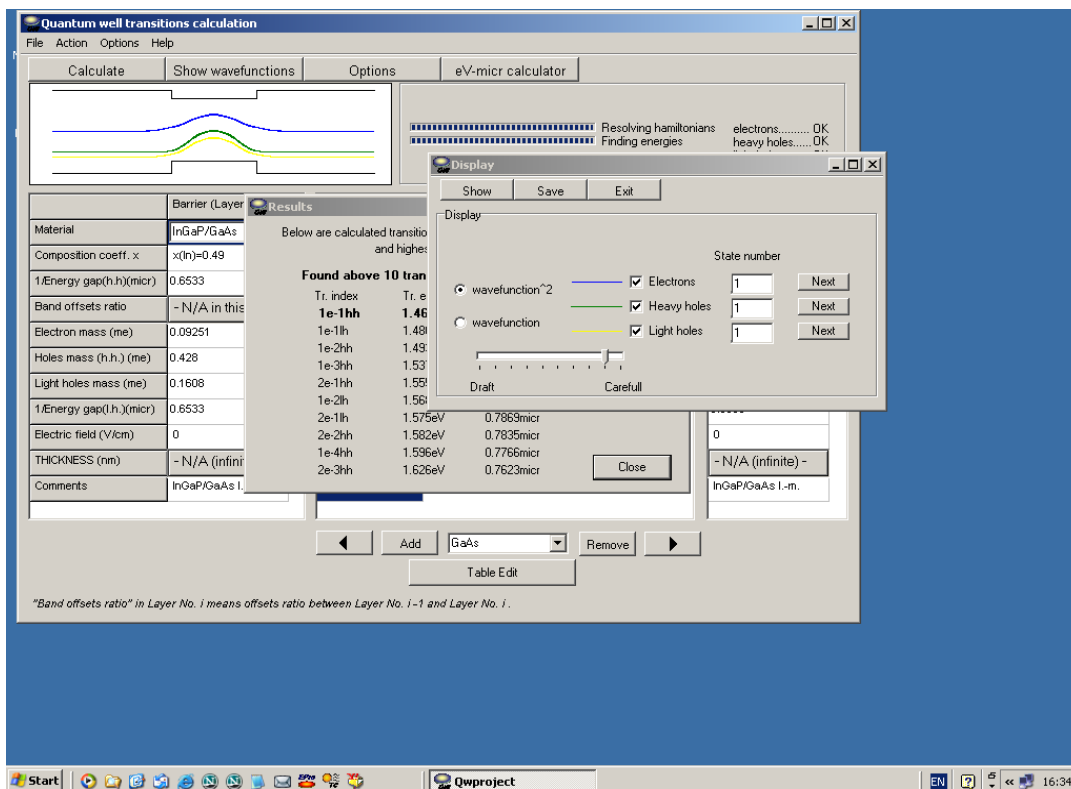
The finite-element calculation resolves directly 1-dimensional Schrödinger's equation with effective mass approximation for electrons, heavy and light holes. The structure table considers "built-in" electric field values making possibility for simple analysis of layers with high junction or piezoelectric field.

Calculated wavefunctions can be displayed and stored in ASCII file.

**To execute calculation do as follows:**

1. Select left barrier parameters
2. Select inner layer (layers)
3. Select right barrier parameters
4. Run calculations

If the compound is not available for direct selection from the choice list, helpful data can be found in the "Compound database". The database is accessible through "Materials"- "Compound database" buttons from main EPITAXYproject's taskbar.



**Fig.6.** QWproject® screen.

To display wavefunctions click "Show wavefunctions" button. Because calculations can be

time-consuming the “*Hamiltonian dimension*” value should be below 20 or alternatively the spatial resolution should be lowered. Those values are accessible by “*Options*” button in the main *QWproject* form. (Problem of time-consuming calculations should be resolved in future versions of the software.)

To save wavefunction click “*Save*” button in the “*display*” form after “*Show*” completion.

#### Limits:

- x The Hamiltonian dimension: below 200.
- x The number of layers in main table: below 100.
- x **Remark:** *Qwproject*® ver.1.1 does not consider junction electric field. The difference in transition energy between p-n structures with and without consideration of built-in junction field for QWs below 15nm in thickness with doping in the  $1E17\text{cm}^{-3}$  range is typically below 10nm in wavelength. This field can be often evaluated with *Jproject*® (“*Junctions*” button in main taskbar) and set manually in corresponding to QW layer “*Electrical field [V/cm]*” cell.
- x **Remark:** In current module version (V.1.1 ) calculations can be time-consuming and plot data can be not highly accurate.

### 5.3. QW thickness algorithm

This option is provided to evaluate quantum well thickness and depths by photoluminescence tests and is reachable by “*QW thickness algorithm*” button in the “*QW states calculation*” “*Simplified*” form. In current version of *EPITAXYproject*® (v.2.4.0) this algorithm is available for rectangular well potentials only.

The “*QW thickness algorithm*” form may be simply used for **determination of QW thickness** when both materials - barriers and well are known and the QW thickness is the only unknown parameter. The “*first test*” check-box should be only checked and proper parameters of barrier and well energy gaps and masses set.

---

#### For determination of QW thickness in this case of “*single test*” do as follows:

1. Leave only “*First test*” check-box checked
2. Set values of barrier material energy wavelength, in “*Barrier*” frame, (QW states form can be used by “*Import values*” button).
3. Set values of electron and holes effective masses for barrier and well materials in “*Barrier*” and “*Well*” frames, (QW states form can be used by “*Import values*” button). Set also offsets ratio  $\Delta E_c/\Delta E_v$  below (data in help file - QW states form can be used).
4. Set value of measured QW photoluminescence maximum in “*First test*” frame, (leave value “1” for “*thickness proportion*”).
5. Set value of well material energy gap in frame “*Limits*” (1/ $E_g$  “*down*”)

6. Run calculation, the "a.u. thickness" in "Results" frame is the calculated QW thickness. The accuracy of the evaluation may be calculated - "evaluate errors" button (it describes output value fluctuation under 5nm of fluctuation of input wavelength in "first test").

---

The form may be also used in more complicated case - when **both well material energy gap and thickness** are uncertain - that happens for strained QWs. The idea is closely related to the epitaxy technology, when the quantum well growth rate and composition may be in difference relative to thick layers growth rate and composition. Two test samples with exactly known QW thickness proportion and the same well material allows to evaluate the absolute thickness and well energy gap. The thickness ratio - for instance 1:2 – can be known on the basis of growth times ratio or flows ratio. The used experimental parameter is photoluminescence-measured transition energy.

**To evaluate the QWs parameters in this "double test" option prepare:**

1. Two samples for PL measurements of QW band to band 1e-1h transition. Time of QWells growth proportion or flows proportion should be at least about 1:2 to minimalise error, and suspected thinner well thickness 20-100angstroms - to make the well levels sensitive on this value, (thinner wells for semiconductors with heavier masses).

**Example I:** Sample I: AlGaAs/GaAs QW with GaAs well growth time 10s, Ga flow 4 (suspected QW thickness 4nm). Sample II: AlGaAs/GaAs QW with GaAs well growth time 20s, Ga flow 4 (suspected QW thickness 8nm).

**Example II:** Sample I: AlGaAs/GaAs QW with GaAs well growth time 10s, Ga flow 4 (suspected QW thickness 4nm). Sample II: AlGaAs/GaAs QW with GaAs well growth time 10s, Ga flow 8 (suspected QW thickness 8nm).

2. Value of the energy-gap and effective masses of the barrier material and also estimated masses for the QW material (QW transitions calculation form can be helpful) .

3. Measured energies of the photoluminescence maxima.

**Summary:**

<i>must be known:</i>	thickness proportion for two samples barrier parameters photoluminescence maxima
<i>will be obtained:</i>	absolute QW thickness QW material energy-gap

---

**Please in case of this "double test" do as follows:**

1. Leave "First test" and "Second test" check - boxes only checked,
2. Set proper values of energy gap wavelength, electron effective mass and hole effective mass for barrier material in "Barrier" frame, (QW states form can be used by "Import values" button.

3. Set estimated values of electron effective mass and hole effective mass for well material in "*Well*" frame. Those may be only estimated values (as well is unknown) - the procedure is moderately sensitive on well masses so please don't care and set what is expected for well material - typical 8% error in electron mass gives about 8% error in thickness. (QW states form can be used by "*Import values*" button).

4. Set also band offsets ratio  $\Delta E_c/\Delta E_v$  (QW states form).

5. Set Values of measured photoluminescence maximums for both samples in "*First test*" and "*Second test*" frames.

6. Set values of relative thickness in "*First test*" and "*Second test*" frames. For instance "1" for first test and "2" for second test - when growth time was 20seconds for first sample and 40second for the second.

7. Set limits in "*Limits*" frame for both elemental thickness (1.a.u.) and well material energy gap wavelength. Limits windows usually can be quite wide - so please don't be very careful.

8. Run calculations and find results in "*Results*" frame. You can also evaluate errors to check how the result is sensitive on fluctuations of input wavelengths and thickness proportion.

---

The accuracy of evaluation can be calculated by clicking "*evaluate errors*" button, it describes output values fluctuations under 5nm input wavelength fluctuation in "*second test*" and 10% fluctuation of thickness ratio between "*first test*" and "*second test*" data.

To increase the evaluation accuracy analogous direct three-sample test can be used.

## 6. 1-dimensional photonic structures

Provided are simulations of reflectance spectra for Bragg reflector or other 1-dim photonic structures. Two options are available:

### 6.1. "Simplified" option:

Simulations are simplified by using fixed (wavelength - independent) refraction indexes, so checked values of indexes should be chosen to be exactly proper for the most important region of the spectra, typically the resonance region. Also for simplicity, the value of absorption coefficient is introduced as fixed, "effective" coefficient and basically average coefficient for the pair of Bragg layers at the resonant wavelength should be checked. The "0" value of absorption is set as default. Result spectra can be stored in ASCII text format file. The calculation is available for perpendicular and no-perpendicular beam-surface configurations. If set is no-perpendicular, appropriate polarisation option should be checked.

## 6.2. "Advanced" option (uses "BRproject®" module):

This option gives possibility to set arbitrary structure in details. Layers can be specified by single-value refractive indexes and absorption coefficients or by data sheets with (wavelength [nm], refractive index n) or (wavelength [nm], absorption coefficient [cm<sup>-1</sup>]) space separated pairs in two columns in text files form. Result spectra can be stored in the text file. The module provides also calculation of field amplitude profile, this profile can be displayed and stored in text file.

The option makes available also a "fitting session" to fit experimental and calculated spectra with estimation of selected thickness parameters.

---

### I. To calculate reflectance spectra:

1. Specify the structure details clicking "*Edit structure*".
2. Click the "*Plot spectra*" button in the main software form.

Spectrum can be saved in text file form. To save the spectrum click "*File*" menu.

---

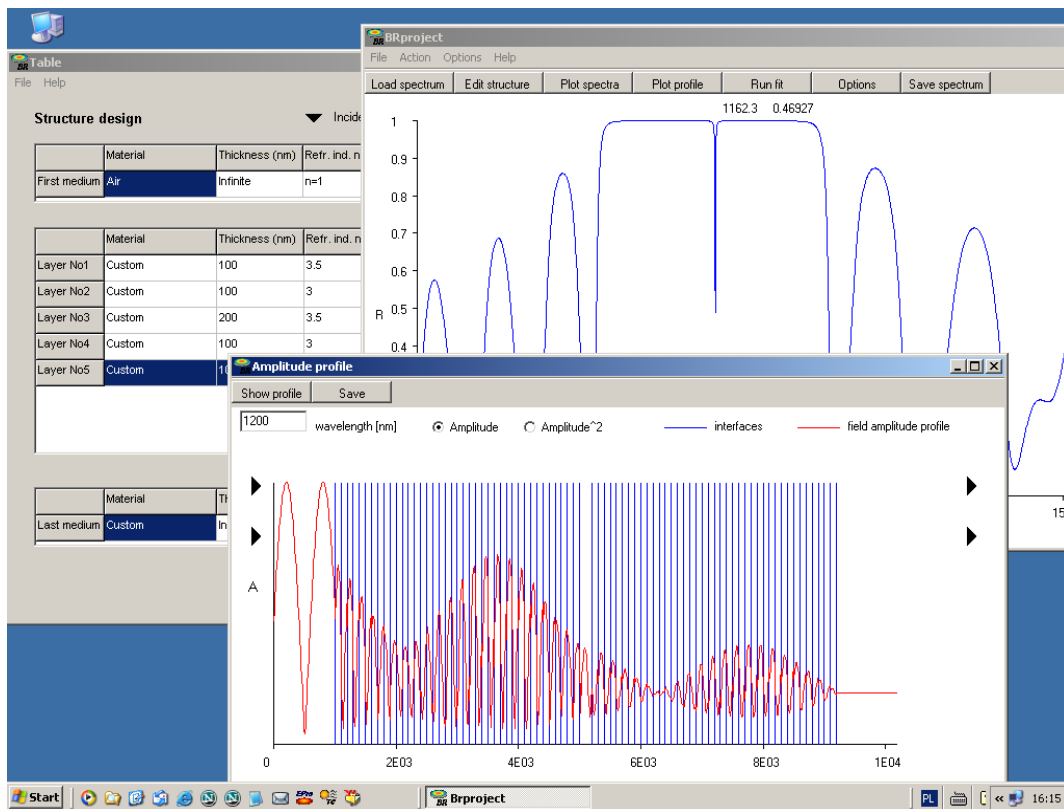


Fig.7. BRproject® screen.

---

## II. To fit structure to experimental data:

1. Click "*Load spectrum*" button in the main form to load experimental data file. This file should be in text file form with two columns - first one assigning wavelength (in micron), second one assigning measured absolute reflectance  $R$  ( $0 < R < 1$ ).

2. Click "*Edit structure*" and set structure details.

3. Choose thickness parameters to fit (maximum six thickness) - set for those thickness any arbitrary values in the table. Click "*Options*" button to specify thickness to fit. Click "*OK*" button.

4. Run the fitting by pressing "*Run fit*" button.

---

## III. To calculate field profile:

1. Calculate reflectance spectra according to above procedure I.

2. Click the "*Show profile*" button.

- To change wavelength set appropriate value and click "*Show profile*" button in the "*Amplitude profile*" form.
  - Spectrum can be saved in text file form. To save the spectrum click "*Save*" button.
- 

### Limits:

- x Number of lines in the structure design table is limited to 100.

## 7. *Jproject*<sup>®</sup>

The *Jproject*<sup>®</sup> is accessible through "*Junctions*" button in the main task bar. It provides calculation of electrical potential for homo- or hetero-junction structures. This function can be applied for analysis of device structure, depletion regions or quantum well profile.

To pursue calculation define the structure in the main software form assigning at least three layers. First left and last right layers should be defined thicker than related depletion regions, default value is 200nm. To analyse 2-layer structure please set first or second as superposition of two pieces.

---

## Do as follows:

1. Set left layer parameters selecting material and defining doping. If the compound is not present in the combobox list please set following parameters manually.
  - Energy gap wavelength – in ( $\mu\text{m}$ ) unit,
  - Conduction band offset – in (eV) unit,
  - Built-in electric field – in (V/cm) unit,
  - N- and P- doping – in ( $\text{cm}^{-3}$ ) unit.
2. Set inner layers parameters as above. Set also layers thickness.
3. Set right layer parameters (as above).
4. Click “Calculate” button. The profile will be displayed.

If the compound is not available for direct selection from the choice list, helpful data can be found in the “Compound database”. The database can be accessed by “Materials”-“Compound database” buttons from main *EPITAXYproject*'s taskbar.

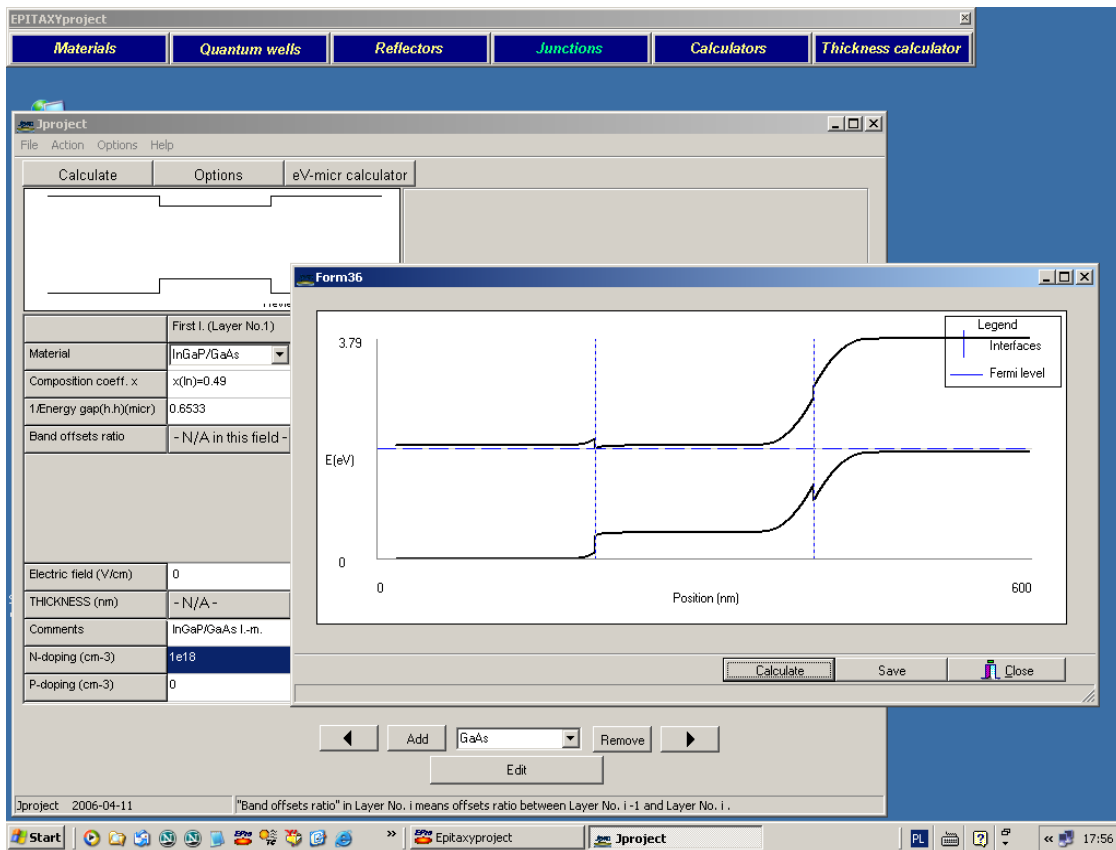


Fig.8. *Jproject*<sup>®</sup> screen.

The calculated profile can be saved in the three column – 1. position (in nm unit), 2. conduction band potential (in eV unit), 3. valence band potential (in eV unit) - text file by clicking “Save” button.

The option menu (in ver. 1.0.1) allows to set values of first left, last right layer thickness, value of dielectric constant, donors and acceptors levels.

### Limits:

- x Maximum number of layers in the main table: 100.
- x The number of separate junctions when separated by thick layers (above depletion thickness): below ~10. **Remark:** In case of multiple junctions calculation time may grow  $2^n$  times.
- x **Remark:** *Jproject*® ver. 1.0.1 is initial module version and may contain errors and generate exceptions.
- x **Remark:** The module in its initial form neglects some factors and provides only an evaluation of the potential profile. The most important of neglected factors is the dependence on band shape, which influences profile when Fermi level penetrates one of bands. The next is temperature dependence, calculation corresponds to about room temperature.
- x **Remark:** *Jproject*® ver. 1.1.0: first and last layers should have no-zero doping levels for appropriate boundary conditions.

## 8. Calculators

### 8.1. XRD calculator

This function provides calculation of the lattice mismatch value or lattice constant value on the basis of the XRD reflex (reflexes) in Theta/2Theta scan. The calculation is designed for arbitrary [k,l,m] reflex in case of cubic geometry or for [k,0,0], [0,l,0], [0,0,m] reflexes in case of no-cubic geometry.

#### Attention:

Output values are directly measured values, so please be careful when using "*Band-gap and lattice mismatch calculator*" or "*Flows recalculation form*" where relaxed values are required. When strained layer is measured, to apply obtained in "*XRD calculator*" value please divide it by appropriate factor (typically close to 2).

### 8.2. Partial pressures calculator

The partial pressures calculator allows to calculate the absolute pressures, absolute concentrations and pressures ratio in MOCVD reactors. Beside preset precursors available is

also definition of custom ones.

For calculation of the V/III ratio value only, "*Reactor temperature*" and "*Reactor pressure*" fields may be left unfilled.

### 8.3. Other calculators

- **Dilution calculator** - for calculation of diluted line flow.
- **r - m - n calculator** - for determination of one of: resistivity, mobility, carrier concentration.
- **eV -  $\mu\text{m}$  calculator** - energy versus radiation wavelength calculation.
- **Thickness calculator** - for determination of one of: growth time, growth rate, thickness.
- **Depletion layer calculator** - for evaluation of depletion layer thickness in p-n junction or metal - semiconductor junction.
- **Free carrier absorption and refractive index calculator** - for calculation of free carriers plasma absorption coefficient and free carriers - related change of refractive index.
- **Surface concentration and sheet resistance calculator** - for calculation of surface concentration versus bulk concentration and sheet resistance versus resistivity.

## 9. System requirements:

- MS Windows XP or Windows 2000 operating system,
- Minimum 1024x768 screen resolution.

[support@epitaxyproject.com](mailto:support@epitaxyproject.com)