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GLOBAL OPTIMIZATION OF OPTICAL NONLINEARITIES IN SEMICONDUCTOR QUANTUM-WELL STRUCTURES

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Abstract. *A procedure is proposed for finding the globally optimal semiconductor quantum-well profile in respect to specified nonlinear optical properties, e. g. second and third order susceptibilities. It relies on the variational calculus, i. e. the optimal control theory, combined with the method of simulated annealing in the initial phase of optimization. The largest nonlinear optical effects are obtained under resonance conditions but they still depend on transitions matrix elements between relevant quantized states, i. e. via the wave functions, on the potential shape which may be varied. The proposed method does not depend on the choice of input potential and includes the variation of a continuous function instead of a set of scalar parameters, so it should lead to the globally optimal quantum-well profile for a particular application, unconstrained to any particular class of functional forms. For purpose of illustration, the procedure is applied to the optimized design of $Al_xGa_{1-x}As$ based quantum wells, with $\hbar\omega = 116$ meV (CO_2 laser radiation), the objectives being the largest nonlinear susceptibilities achievable with chosen material.*

INTRODUCTION

The advances in sophisticated methods of semiconductor structures growth have enabled the fabrication of devices carefully tailored to a particular application. By varying the profile of a semiconductor quantum well (QW), both the bound state energies and their wave functions change, and so do various physical properties depending on them. Taking the linear or nonlinear intersubband optical properties of QW's, these depend on spacings between relevant quantized states and the transition (dipole) matrix elements between them. The largest effects are obtained under resonant conditions, when the spacing between some states coincides with the input photon energy. Having obtained the resonance in a QW structure, however, the effects of interest still depend on the

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matrix elements, i.e., via the wave functions, on the potential shape, which may be varied to optimize the structure. A few different approaches to such constrained optimization of QW profile have been described in the literature, covering the cases of asymmetric step QW's [1]-[3], electric field biased QW's [4,5], asymmetric coupled QW's [6]-[8], or continuously graded QW's, the family of their forms being derived from some chosen initial potential by applying to it the methods of supersymmetric quantum mechanics (SUSYQM) or inverse spectral theory (IST) [9]. In all these approaches the QW profile optimization was constrained not only by the requirement for resonance conditions, as it should be, but also by limiting the search to some class of potential shapes. This second type of constraints, which may be intrinsic to the optimization method itself, or is introduced for the simplicity of calculation or of the final design, implies that the obtained optimal QW shape may not be globally optimal.

In this work we propose another procedure for the QW profile optimization, which may perform a *global*, that is unconstrained, optimization (by which we mean *with no unnecessary constraints*). It relies on the variational calculus (optimal control theory), combined with the method of simulated annealing. In some more detail, using the roughly preoptimized, step graded QW profile, prepared by the simulated annealing, the profile is then variationally "polished" towards the globally optimal, smooth function. No unnecessary constraints are imposed anywhere in the procedure, i.e. the QW profile is completely freely varied. The procedure is here applied to find the best QW profile for the maximal second harmonic generation, and the expressions are largely specific to this case, but changing the objective of optimization is rather straightforward.

THEORETICAL CONSIDERATIONS

We consider an *n*-doped QW structure based on direct band gap semiconductors, and take the band gap throughout it to be large enough that interband transitions, caused by radiation present in the structure, may be neglected. The polarization response of the structure to the pump field with photon energy $\hbar\omega$ is then mainly governed by intersubband transitions between quantized conduction band states E_i. Nonlinear polarization at twice the frequency of the pump field, acting as the source of second harmonic field is described by the second order susceptibility $\chi^{(2)} \equiv \chi^{(2)}_{zzz}$ which, in the double-resonance regime, $\hbar\omega = \Delta E_{21} = \Delta E_{32} \equiv \Delta E$ (i.e. with strictly equispaced states), takes the maximal value [1]

$$\chi^{(2)}_{zzz} = \frac{e^3 \rho_{11}}{L_z \varepsilon_0} \frac{M_{12} M_{23} M_{31}}{(\hbar\Gamma)^2} \tag{1}$$

where $M_{ij} = \langle \Psi_i | z | \Psi_j \rangle$ are the transition matrix elements, L_z the length of the structure, ρ_{11} the electron sheet density in the ground state (assumed to be the only populated state) and the off-diagonal rates are taken to be equal $\Gamma_{12} = \Gamma_{13} \equiv \Gamma$ (though this is not essential). In order to maximize $\chi^{(2)}$ one should clearly maximize the corresponding product of dipole matrix elements in numerator of Eq. (1), by appropriate tailoring of QW profile (and hence the wave functions) while preserving the levels spacing. Clearly, the presence of M_{31} rules out symmetric QW's because of definite parity of wave functions, so one should consider asymmetric structures only.

In previous treatments of the problem of QW profile optimization we have employed some kind of the profile (potential) variation, via the SUSYQM or IST, in which the variation was controlled via one or more scalar parameters. In the variational approach, however, a continuous function $U(z)$ is varied. It is now necessary to define the target function, to be maximized. Here we take it as

$$J = \frac{\Pi^{(2)}}{C} = \frac{M_{12}M_{23}M_{31}}{(\Delta\omega_{21}^n + \Gamma^n)(\Delta\omega_{32}^n + \Gamma^n)} \tag{2}$$

where the denominator $C = (\Delta\omega_{21}^n + \Gamma^n)(\Delta\omega_{32}^n + \Gamma^n)$ is introduced in order to favour structures with resonance conditions fulfilled. Normally one should set $n = 2$ and Γ equal to the linewidth, but other even powers of n and values of Γ may be tried to speed up the convergence (the optimum will not depend on this choice). The potential $U(z)$ may take arbitrary shape in the segment $[-z_L, z_R]$ in which it is optimized, and is constant outside it. Furthermore, we assume the envelope wave functions to satisfy the boundary conditions $\Psi_i(-z_L) = \Psi_i(z_R) = 0$ and $\Psi_i'(-z_L) = \Psi_i'(z_R) = 0$, $i = 1,2,3$. The maximization of the functional J is clearly a constrained type optimization, because the functions ψ_i satisfy the effective-mass Schrödinger equation

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m^*(z)}\frac{d\Psi}{dz}\right) + [U(z) - E]\Psi(z) = 0, \qquad i = 1,2,3 \tag{3}$$

where $m^* = m(z)m_0$ is the position-dependent electron effective mass, and m_0 the free electron mass. The constrained optimization is performed in the usual way, by introducing Lagrange multipliers, λ_i, [10]. The new functional, for unconstrained optimization, then reads:

$$J^* = J - \sum_{i=1}^{3}\int_{-z_L}^{z_R} \lambda_i(z)\left[\frac{\Psi_i''}{m} - \frac{m'}{m^2}\Psi_i' + b_i\Psi_i\right]dz = J - \sum_{i=1}^{3} J_i \tag{4}$$

where $b_i(z) = (2m_0/\hbar^2)[E_i - U(z)] = q[E_i - U(z)]$, and the constant q amounts to 0.2625 (in $\mathrm{eV}^{-1}\ \text{Å}^{-2}$ units). The conditions for the extremum of Eq. (4) are obtained by equating its variation δJ^* to zero, i.e.,

$$\delta J^* = \delta\left[(K_1M_{12} + K_2M_{23} + K_3M_{31} - \sum_{i=1}^{3} J_i)\right] = \delta\int_{-z_L}^{z_R}\Phi(\Psi_1, \Psi_2, \Psi_3, U, z)dz = 0 \tag{5}$$

where

$$\begin{aligned} K_1 &= M_{23}^{\circ}M_{31}^{\circ}/C \\ K_2 &= M_{12}^{\circ}M_{31}^{\circ}/C \\ K_3 &= M_{12}^{\circ}M_{23}^{\circ}/C \end{aligned} \tag{6}$$

The quantities M_{12}°, M_{23}°, M_{31}° are taken as constants in finding the variation (5), because these are evaluated with fixed functions $\Psi_i^{\circ}(z)$ and $U^{\circ}(z)$, which give the

optimized value to the functional J^*. The unknown functions y_i (in this case $\Psi_i(z)$ and $U(z)$) maximizing Eq.(4) are to be obtained by solving the system of Euler-Lagrange equations:

$$\frac{\partial\Phi}{\partial y_i}-\frac{d}{dz}\left(\frac{\partial\Phi}{\partial y_i'}\right)+\frac{d^2}{dz^2}\left(\frac{\partial\Phi}{\partial y_i''}\right)=0 \tag{7}$$

the function Φ may, using Eqs.(5) and (6), be written as:

$$\Phi=K_1\Psi_1 z\Psi_2+K_2\Psi_2 z\Psi_3+K_3\Psi_1 z\Psi_3-\sum_{i=1}^{3}\lambda_i(z)\left[\frac{\Psi_i''}{m}-\frac{m'}{m^2}\Psi_i'+b_i\Psi_i\right] \tag{8}$$

The variation of J^* over the functions λ_i always equals zero, by the very way of writing Eq. (4). In the problem considered, Eq.(7) becomes

$$\begin{aligned}
&\lambda_1''-\frac{m'}{m}\lambda_1'+\lambda_1 b_1 m=mz(K_1\Psi_2+K_3\Psi_3)=F_1(z)\\
&\lambda_2''-\frac{m'}{m}\lambda_2'+\lambda_2 b_2 m=mz(K_1\Psi_1+K_2\Psi_3)=F_2(z)\\
&\lambda_3''-\frac{m'}{m}\lambda_3'+\lambda_3 b_3 m=mz(K_2\Psi_2+K_3\Psi_1)=F_3(z)\\
&G=q[\lambda_1\Psi_1+\lambda_2\Psi_2+\lambda_3\Psi_3]-\frac{1}{mU}[\lambda_1'\Psi_1'+\lambda_2'\Psi_2'+\lambda_3'\Psi_3']=0
\end{aligned} \tag{9}$$

In writing the system (9), and in particular when varying the potential, we take account of the fact that in ternary alloys of the general type $A_xB_{1-x}C$ the potential and the effective mass are related via: $U(z)=[\Delta E_c/\Delta m]m(z)\equiv\theta m(z)$, where ΔE_c is the conduction band offset between materials AC and BC, and $\Delta m=m_{AC}-m_{BC}$ is the difference of the corresponding electron effective masses. The solutions for the Lagrange multipliers may be written as:

$$\lambda_i(z)=\left[C_{1i}-\int_{z_0}^{z}\frac{y_{2i}(z')F_i(z')}{W(z')}dz'\right]y_{1i}(z)+\left[C_{2i}+\int_{z_0}^{z}\frac{y_{1i}(z')F_i(z')}{W(z')}dz'\right]y_{2i}(z) \tag{10}$$

where y_{1i} and y_{2i} are the solutions of the homogeneous system of differential equations for λ_i (9), i.e. the solutions for the case $F_i\equiv 0$ and $W(z)$ is the Wronskian. Since these homogeneous equations have the form of the Schrödinger equation, the two linearly independent solutions may be written as $y_{1i}(z)=\Psi_i(z)$ and $y_{2i}(z)=\Psi_i(z)[\widetilde{C}+\int_{z_0}^{z}(m(z')/\Psi_i^2(z'))dz']$, where $\widetilde{C}$ is a constant, and the Wronskian then amounts to $W(z)=m(z)$. The constants C_{1i} and C_{2i} are determined so that the boundary conditions for the potential correction are satisfied, i.e. $G(-z_L)=G(z_R)=0$ and $G'(-z_L)=G'(z_R)=0$. The last equation of the system (9) is the variation of the functional J^* in respect to the potential $U(z)$. Finding the optimal QW profile thus amounts to finding such $U(z)$ which will make this variation equal to zero, subject to the condition that all the equations of the systems (9) and (3) have to be satisfied. This set of coupled equations cannot be solved analytically. Instead, we employ an iterative algorithm that will be described below.

(1) Choose a starting potential $U^{(i=0)}(z)$ in the segment $-z_L \le z \le z_R$ (out of which the potential is taken constant).

(2) Solve Schrödinger equation (3) and find the wave functions $\Psi_j^{(i)}$ for the relevant states, satisfying the boundary conditions $\Psi(-z_L) = \Psi(z_R) = 0$, and $\Psi_j'(-z_L) = \Psi_j'(z_R) = 0$ (the superscript (i) is the iteration counter, and subscript denotes the state index).

(3) Substitute the calculated Ψ_j's into the system (9), and, taking into account the boundary conditions for Lagrange multipliers λ_i (that is, $G(-z_L) = G(z_R) = 0$ and $G'(-z_L) = G'(z_R) = 0$), find the variation with respect to the potential $G^{(i)}$.

(4) Update the potential, using the steepest descent method

$$U^{(i+1)}(z) = U^{(i)}(z) - \alpha^{(i)} G^{(i)} \tag{11}$$

where $\alpha^{(i)}$ is a constant which gives the largest value of the functional J^*, i.e. is chosen so that $J^*(U - \alpha \frac{\partial J^*}{\partial U}) = J^*(U - \alpha G)$ takes maximal value.

(5) Return to step (2), using the updated potential $U^{(i+1)}(z)$, and repeat these iterations until obtaining sufficiently converged results, i.e. $J^*(U^{(i+1)}(z)) - J^*(U^{(i)}(z)) < \gamma$, where γ is a small positive number.

By performing a few "numerical experiments", using the iterative procedure described above, with different starting potentials, one immediately finds that it gets easily trapped in a "local minimum", nearest to the starting potential, with the optimized target function strongly depending on it. Therefore, absent the fully analytic solution of the problem, the variational iterative procedure alone is not enough to perform the global optimization of the potential. It clearly has to start with some potential, to be provided by other means, that is already "sufficiently" close to the final optimized potential. The task of preparing the starting potential is here done by the simulated annealing (SA). This is an iterative stochastic optimization method, nowdays in widespread use, with readily available algorithms. While always accepting a step (random change of values of variables) which improves the target function, it also sometimes accepts steps degrading the target function, and thus avoids being trapped in local minima. This is essential for the problem we consider, which appears to be of highly multivalley type. The SA is here applied to multilayer QW's (i.e. stepwise constant potentials), with some reasonably small number of layers, of the order of 10. Each layer brings in two independent variables – its width and potential height, and an additional free variable is the height of "outer" barriers. The variables may vary within some limits, imposed physically or technologically: minimal constraints, employed in this work, are that the width of any single layer cannot be less than one crystalline monolayer, and the mole fraction of any of the alloy constituents may be between zero and one (this effectively limits the maximal excursion of the potential within the structure). We have therefore used the SA algorithm [11] which can handle box-type constraints. The state energies, wave functions, and matrix elements, i.e. the target function (2) for this type of structures may be conveniently evaluated using the transfer matrix method, and SA will vary the discrete set of layers parameters until it finds the globally optimal structure with prescribed total number of layers. In principle one might apply SA to a QW structure with very large number of layers and obtain an almost smooth globally optimized potential, thus avoiding the variational part altogether.

However, this would be quite costly, because the computation time of SA scales at least quadratically with the number of variables (or worse, depending on the cost of the target function evaluation). Therefore, we have here adopted a mixed approach, employing SA to provide a rough approximation to the globally optimal potential, which will then be further improved by the variational method.

NUMERICAL RESULTS

The proposed optimization procedure was used to find the absolutely best profile of QW's based on the $Al_xGa_{1-x}As$ alloy, so to provide the maximal value of the nonlinear susceptibility $\chi^{(2)}$. We have first found the optimal step QW by the SA method, with the target function given by Eq.(2), in order to provide a good starting point for the variational method. The material parameters used in calculation are [12]: $E_{g\,GaAs} = 1.42$ eV, $E_{g\,AlAs} = 2.67$ eV, $m_{GaAs} = 0.067m_0$, $m_{AlAs} = 0.15m_0$, and the conduction band offset $\Delta E_c = 0.75$ eV, and Vegard's law (linear interpolation) was applied for the alloy. The incident photon energy was $\hbar\omega = 116$ meV, corresponding to the CO_2 laser radiation. We have chosen the QW with 8 "internal" layers (not counting the two outer barriers), i.e., having 17 parameters, for the SA optimization, as a tradeoff between the computation speed and achieving a reasonably good approximation to continuously graded QW.

The SA-optimized QW, given in Fig. 1a, has a depth of $U_B = 523.6$ meV, and has a total of 4 bound states, though only the lowest three are relevant for our problem. The important matrix elements are: $M_{12} = -16.9$ Å, $M_{23} = -25.9$ Å, $M_{31} = -9.4$ Å. The product of matrix elements, relevant for the second harmonic generation is thus found to be $|\Pi^{(2)}| = |M_{12}M_{23}M_{31}| = 4114$ Å^3. Due to the properties of the SA algorithm this structure is (almost certainly) globally optimal in its class, that is among all the QW's with 8 internal layers. It was then further optimized (i.e. used as the starting potential) by the variational procedure. Approximately 57 iterations are necessary for satisfactory convergence, and this calculation is an order of magnitude less time-consuming than the SA one.

This fully optimized (globally optimal) potential is also given in Fig. 1b. Although the change of the potential shape may not seem too drastic, the target function is significantly improved over what was obtained in 8-layer QW, with $|\Pi^{(2)}| = 4685$ Å^3. Bound states in the fully optimized QW are positioned at $E_1 = -449.5$ meV, $E_2 = -333.5$ meV, $E_3 = -217.5$ meV, $E_4 = -73.1$ meV, (with the outer barriers potential taken as reference zero). The individual matrix elements here amount to: $M_{12} = -16.9$ Å, $M_{23} = -26.4$ Å and $M_{31} = 10.5$ Å. Finally, we note that the optimized potential $u^{opt}(z)$ given in Fig. 1b is accompanied with the variable effective mass given by $U^{opt}(z) = u^{opt}(z) + V_0$, with $V_0 = 1.194$ eV and $\theta = 9.036$ eV (because it was derived for the graded ternary $Al_xGa_{1-x}As$ alloy based QW).By comparing the result obtained here with those reported previously, e.g. $|\Pi^{(2)}| = 3090$ Å^3 for asymmetric step QW's [13], or $|\Pi^{(2)}| \approx 3300$ Å^3 (calculated using SUSYQM) [9], one can see an improvement by at least 25%.

The smooth potential from Fig. 1b can, in principle, be realized by continuous grading of alloy composition. Yet, the concept of the composition varying smoothly over a single crystalline monolayer may seem a bit ambiguous, so we attempted to discretize this optimal potential into a number of thin segments with fixed alloy composition, each

being at least one monolayer thick. Choosing wider segments would obviously make the realization easier, but would make the potential more remote from the fully optimal.

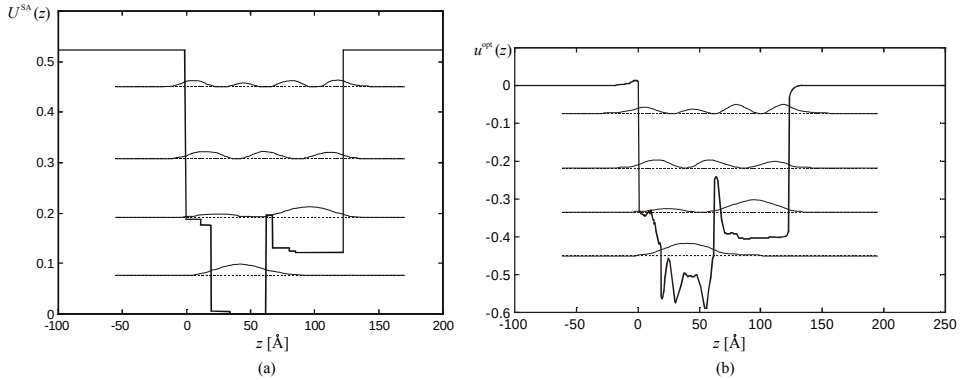

Fig. 1. (a) The stepwise-constant SA-preoptimized, and (b) the variationally fully optimized smooth potential, providing maximal second harmonic generation. Also displayed are the relevant bound state wave functions squared.

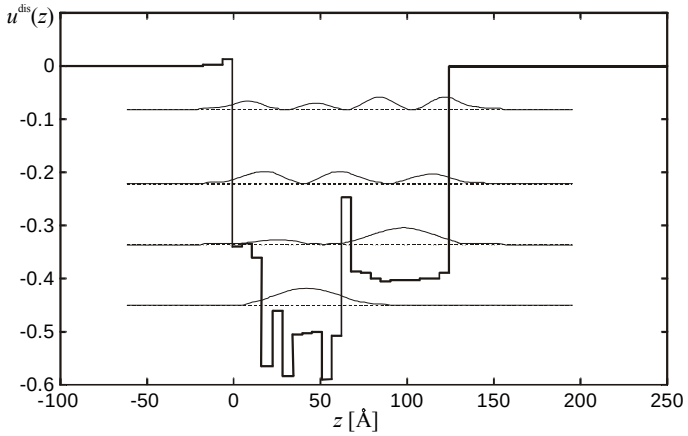

Fig. 2. The discretized, step-graded version of the optimal potential from Fig. 1b, with 2 monolayers wide steps.

Choosing e.g. the width of all the segments as 2×2.83 Å (i.e., 2 monolayers) we find that this discretized structure, displayed in Fig. 2, has its parameters somewhat changed from those of the optimal smooth one: $E_1 = -451.4$ meV, $E_2 = -335.7$ meV, $E_3 = -220.2$ meV, $E_4 = -81.5$ meV, $M_{12} = -16.7$ Å, $M_{23} = -26.2$ Å and $M_{31} = -10.3$ Å, and finally $|\Pi^{(2)}| = 4507$ Å^3. Clearly, the discretized potential could be obtained by SA, with no variational type optimization, but this would have been very time-consuming because of the large number of free variables (step widths and heights) involved. It is only the combined use of SA and the variational method that leads to efficient design of optimal QW profile.

CONCLUSION

The procedure was proposed for finding the globally optimal QW profile, in respect to a specified property, e.g. the second harmonic generation at resonance. To achieve both the speed and reliability (avoiding local minima) the procedure relies on the combined use of simulated annealing and the variational method. Unlike the optimization procedures we have used previously, this one does not depend on the choice of input ("seed") potential, and includes the variation of a continuous function instead of a set of scalar parameters, so it (almost certainly) leads to the globally optimal QW profile for a particular application. The results obtained with the resonant second order susceptibility relevant for second harmonic generation, as the target to be maximized, are considerably better than those previously stated in the literature. Certainly, the procedure may just as well be applied for the QW profile optimization in respect to optical rectification, third harmonic generation, electro-optical coefficients, intersubband laser gain, and similar.

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GLOBALNA OPTIMIZACIJA OPTIČKIH NELINEARNOSTI U POLUPROVODNIČKIM KVANTNIM JAMAMA

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Predložena je procedura za određivanje globalno optimalnih profila kvantnih jama u odnosu na specificirana nelinearna optička svojstva, npr. susceptibilnosti drugog i trećeg reda. Zasniva se na varijacionom računu, tj. teoriji optimalne kontrole, kombinovanim sa metodom simuliranog odgrevanja u inicijalnoj fazi optimizacije. Najveći nelinearni optički efekti se postižu u uslovima rezonancije ali i tada zavise od matričnih elemenata prelaza između relevantnih kvantnih stanja, tj. preko talasnih funkcija zavise i od oblika potencijala koji se može varirati. Predložena metoda ne zavisi od izbora početnog potencijala i uključuje varijaciju kontinualne funkcije umesto skupa skalarnih parametara, tako da bi trebalo da vodi ka globalno optimalnom profilu kvantne jame za konkretnu primenu, neograničenom na bilo koju specifičnu klasu funkcionalnih formi. U svrhu ilustracije, procedura je primenjena na optimizovani dizajn kvantnih jama baziranih na $Al_xGa_{1-x}As$ leguri, za $\hbar\omega = 116$ meV (zračenje CO_2 lasera), sa ciljem određivanja najvećih nelinearnih susceptibilnosti ostvarljivih sa datim materijalom.