Analysis of Photoluminescence measurement data from interdiffused Quantum Wells by Real coded Quantum inspired Evolutionary Algorithm

Ashish Mani and C. Patvardhan

Dayalbagh Educational Institute, Agra, India

Outline

ALOGRITHM

- Evolutionary Algorithms
- Quantum Inspiration
- Existing QiEA
- Proposed Adaptive QiEA
- Adaptive Crossover

APPLICATION

- PL Experiment
- Problem Formulation
- Solutions
- Testing and Results
- Conclusions and Future Work

- References
- Questions???

Evolutionary Algorithms

Population based stochastic search and optimization techniques inspired by nature's laws of evolution.

Application

Large Search Space

Near Optimal Solution is acceptable

Efficient Deterministic Solutions are not available

Evolutionary Algorithms

Population of individuals which represents solutions.

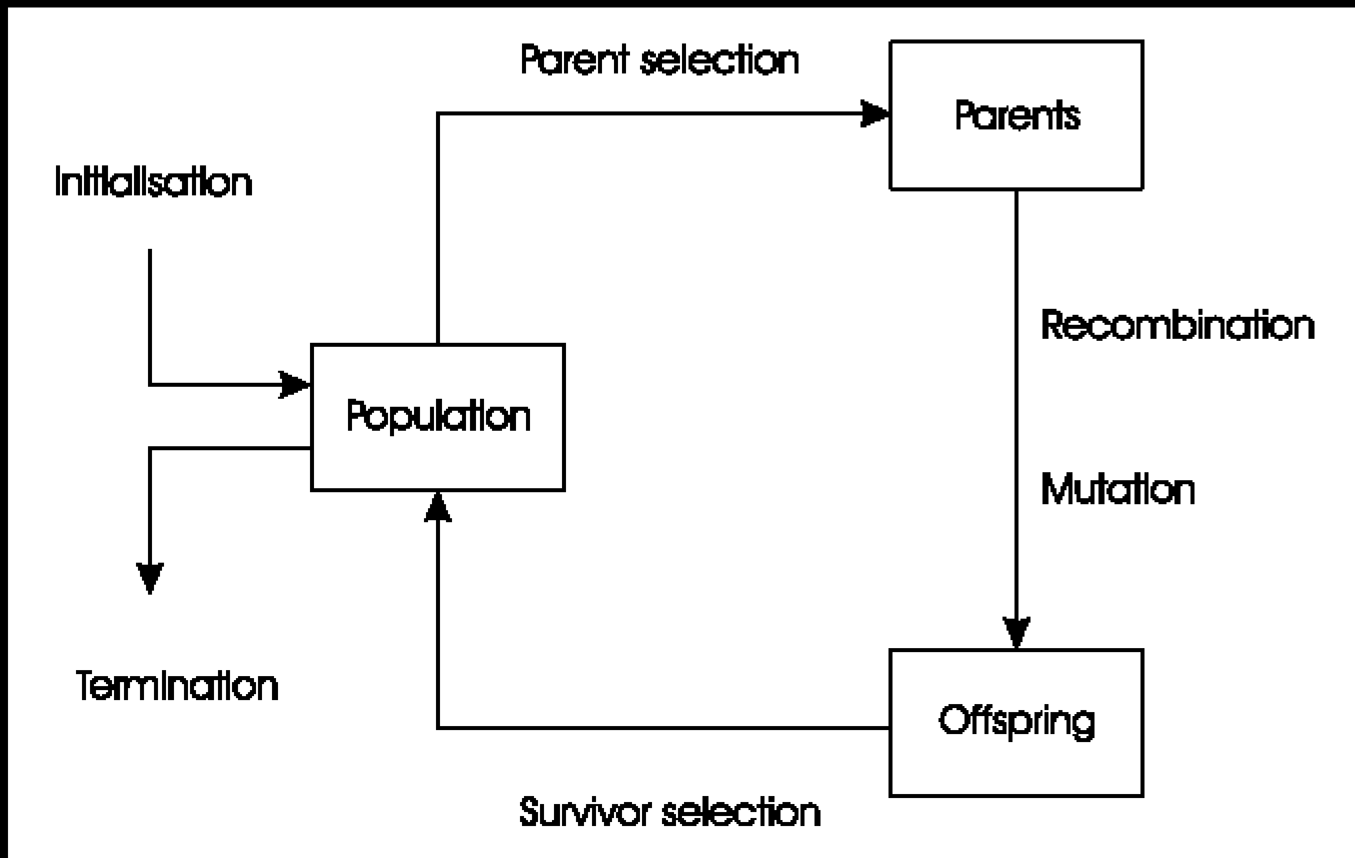
Individuals Compete against each other.

New individuals are generated from old ones through recombination and mutation.

New individuals compete (possibly also with parents) for survival.

Natural selection leads to improvement in the fitness of the population.

General Scheme of EAs



Ref: www.cs.vu.nl/~gusz/ecbook/slides/What_is_an_EA.ppt

Pseudo-code for typical EA

```
Initialize
Evaluate
Do  {
        Select Parents
        Recombine
        Mutate
        Evaluate
        Select Individuals for next Generation
        } While (!Termination_Criteria)
```

Limitations of EAs

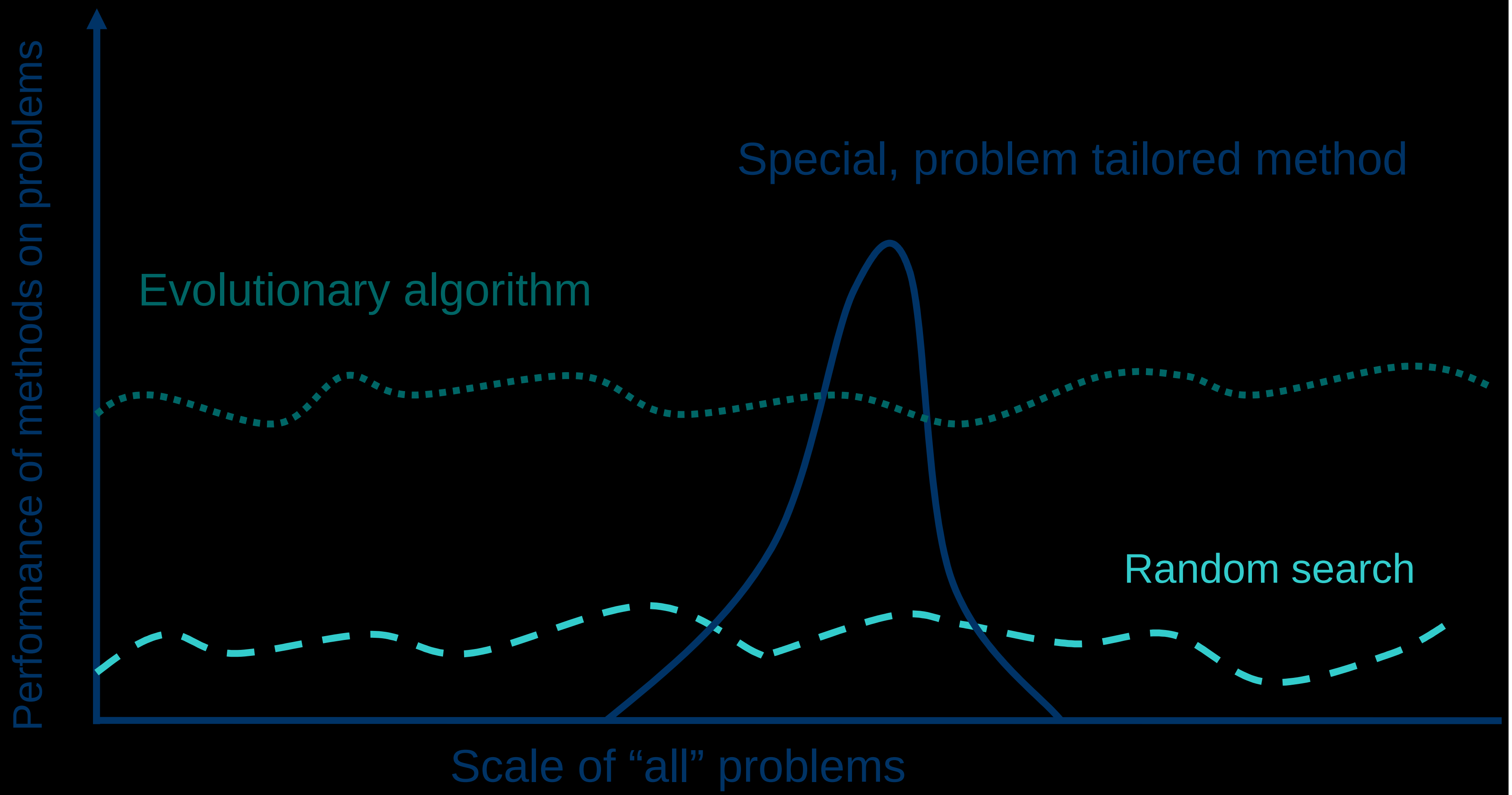
Premature convergence

Slow convergence, stagnation

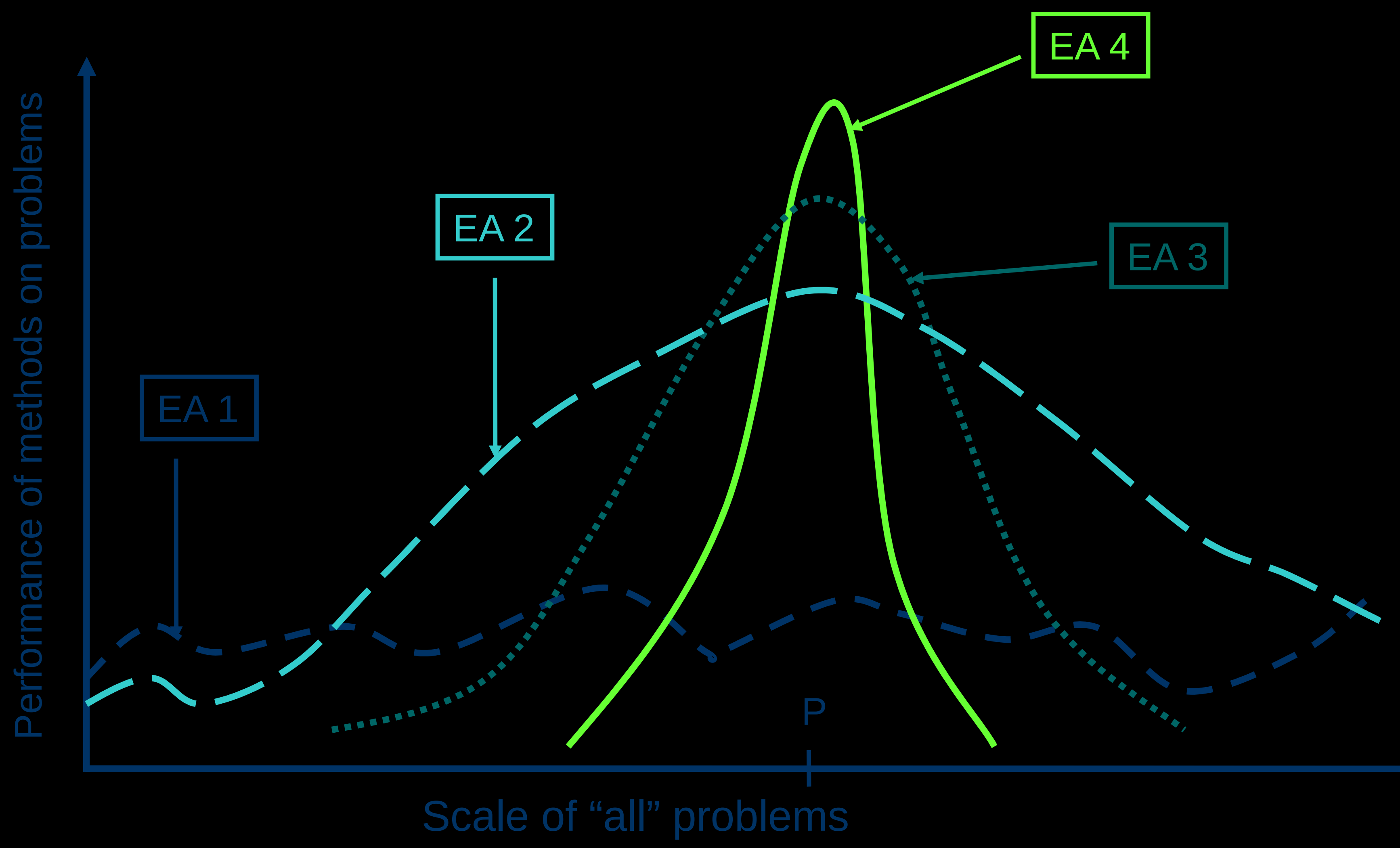
Sensitivity to choice of parameters

Efforts have been made to understand and overcome such limitations.

EAs as problem solvers: Goldberg's 1989 view



Michalewicz' 1996 view



No Free Lunch Theorem (1997)

"a general-purpose universal optimization strategy is theoretically impossible, and the only way one strategy can outperform another is if it is specialized to the specific problem under consideration"

Limitations of EA

1) Premature convergence
2) Slow convergence, stagnation
3) Sensitivity to choice of parameters

Many efforts have been made to overcome limitations 1) and 2) by establishing a good balance between the Exploitation and Exploration.

Limitation 3) can be overcome by Adaptivity (Hypothesis).

Latest Effort is **Adaptive QiEA**

Quantum Inspiration

Quantum inspired EA

- EA inspired by the principles of Quantum Mechanics.
- Improve the balance between exploration and exploitation.
- Quantum computing paradigm is conjectured more powerful.

Important principles of Quantum Mechanics are Superposition, Entanglement, Interference and Measurement.

Principles mostly utilized are superposition and measurement for improving diversity.

Quantum Principles:

- **Superposition**

  A particle can assume different positions, have different values of energy, spin and phase simultaneously, with each of them defined by a different probability amplitude.

- **Measurement**

  When a particle (or a quantum system) interacts with its environment, the superposition is destroyed and the system collapses into one single real state, as it is measured in the classical physics (Heisenberg).

- **Entanglement**

  Two or more particles, regardless of their location, define the same state, with the same probability function. The two particles can be viewed as "correlated", undistinguishable, "synchronized", coherent.

Quantum Computing

- The smallest information element in quantum computer is a qubit, which is quantum analog of classical bit.
- It is represented by a unit vector in Hilbert space with $|0\rangle$ and $|1\rangle$ as the basis states. The qubit can be represented by the vector $|\psi\rangle$, which is given by:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \qquad (1)$$

where $|\alpha|^2$ and $|\beta|^2$ are the probability amplitudes of the qubit to be in state $|0\rangle$ and $|1\rangle$ and should satisfy the condition:

$$|\alpha|^2 + |\beta|^2 = 1. \qquad (2)$$

- The qubits can store, in principal exponentially more information than classical bits.
- However, these qubits exist in quantum computing systems and are constrained by several limitations.
- The simulation of the qubits is inefficient on classical computers.

Existing QiEA framework

- Probabilistic nature of qubits has been widely used for maintaining diversity [4].
- A single qubit is attached to each solution vector and the solution is obtained by taking measurement in binary coded as well as real coded QiEA.
- The qubit associated with solution vector is also evolved by using quantum gate operators, which are influenced by phase rotation transformation used in Grover's Algorithm for searching unsorted database.
- Further, the past efforts have also used mutation operator and local heuristics [2].

QiEA for *global probability optimisation*

- QiEA use a q-bit representation of a chromosome of n “genes” at a time t:

$$Q(t) = \{q_1^t, q_2^t, \ldots, q_n^t\}$$

- Each q-bit is defined as a pair of numbers (α, β) – probability density amplitudes.

$$|\alpha_i|^2 + |\beta_i|^2 = 1$$

- A n element q-bit vector can represent probabilistically 2^n states at any time
- The output is obtained after the q-bit vector is collapsed into a single state
- Changing probability density with quantum gates, e.g. rotation gate:

$$U(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

- Evolutionary computing with q-bit representation has a better characteristic of population diversity than other representations, since it can represent linear superposition of states probabilistically .

N.Kasabov, Brain-, Gene-, and Quantum Inspired Computational Intelligence: Challenges and Opportunities, in: W.Duch and J.Manzduk (eds) Challenges in Computational Intelligence, Springer, 2007

Ref.: Patvardhan et. al. (2007)

QiEA

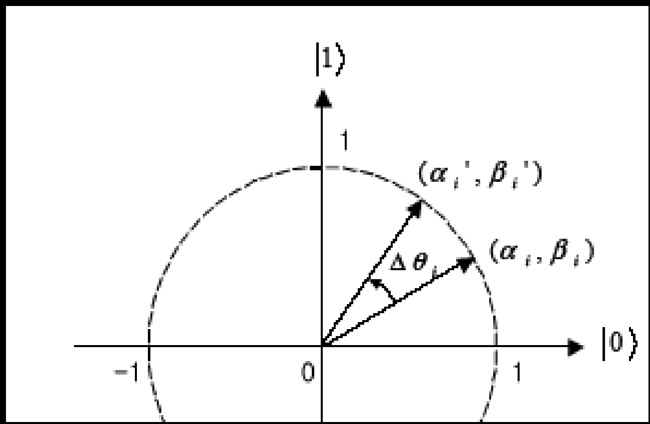
- Observation
  - Process of generating binary string by observing a qubit string

i =>	*1*	*2*	*3*	*4*	*5*	……..	*N*
Q ($\|\alpha\|^2$)	0.17	0.78	0.72	0.41	0.89	………	0.36
R	0.24	0.07	0.68	0.92	0.15	………	0.79
P	1	0	0	1	0	………	1

Alters the elements of Q such that , in subsequent iterations, there is a higher probability of generation of solution strings, which are similar to best solution.

- Updating qubit string

$$\begin{bmatrix} \alpha_i' \\ \beta_i' \end{bmatrix} = \begin{bmatrix} \cos(\Delta\theta_i) & -\sin(\Delta\theta_i) \\ \sin(\Delta\theta_i) & \cos(\Delta\theta_i) \end{bmatrix} \begin{bmatrix} \alpha_i \\ \beta_i \end{bmatrix}$$



Salient Points of Reported Efforts

- No direct correspondence between the solution vector and qubits especially in case of real coded QiEA [2].
- The quantum rotation gates / operators also behave independent of the information from the problem and the solution domain assuming that the quantum behavior would help in reaching the solution.
- However, it should not be forgotten that such algorithms are to be run on classical computers without simulating any quantum phenomena.
- Further, it can be argued that increasing the diversity by collapsing the solution qubit may affect the exploitation.

Proposed Adaptive QiEA

- **Different approach**
- **Two Qubits**
- **Superposition as well as Entanglement Principle**
- **Quantum Rotation inspired Adaptive Crossover**

Two Qubits

- **Helps in overcoming limitations associated with the classical EA**
- **The first qubit,** $|\psi_1(t)>$ stores design variables **of solution vector**.
- **The second qubit,** $|\psi_{2i}(t)>$ **stores scaled and ranked objective function value of the solution vector.**
- **The second qubit is used as feedback in parameter - tuning free adaptive quantum inspired rotation crossover operator used for evolving the first qubit**

Entanglement Principle

The mathematical representation of the classical implementation of entanglement principle is as given below:

$|\psi_{2i}(t)\rangle = f_1(|\psi_{1i}(t)\rangle)$ (3)

$|\psi_{1i}(t+1)\rangle = f_2(|\psi_{2i}(t)\rangle, |\psi_{2j}(t)\rangle, |\psi_{1i}(t)\rangle, |\psi_{1j}(t)\rangle)$ (4)

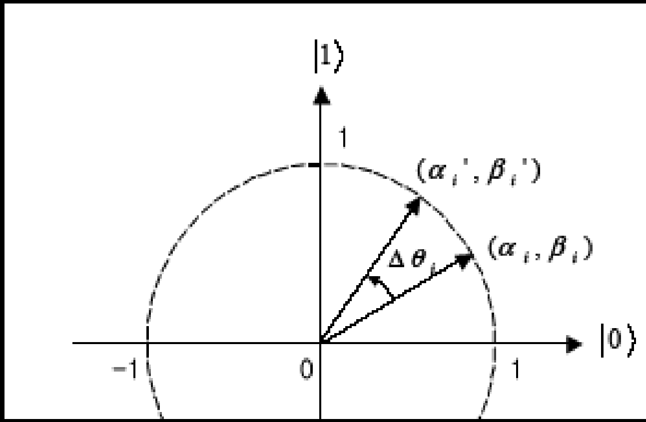
where $|\psi_{1i}\rangle$ and $\psi_{1j}\rangle$ are the first qubits associated with the i^{th} and j^{th} solution vectors respectively, $|\psi_{2i}\rangle$ is the second qubit associated with the i^{th} solution vector, t is iteration number, f_1 and f_2 are the functions through which both the qubits are classically entangled.

Quantum Rotation inspired Adaptive Crossover

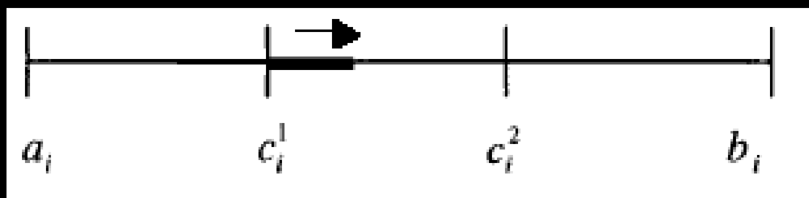
- **A quantum rotation inspired adaptive and parameter tuning free crossover operator is designed.**
- **The second qubits's amplitude is used for determining the angle of rotation for evolving the first qubit. The following equation is used for the purpose:**

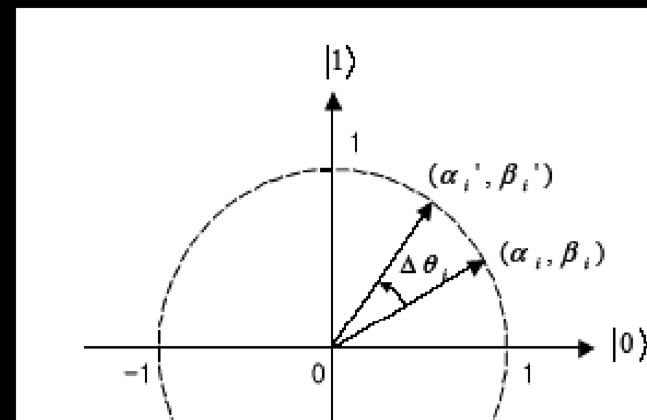
  $$\psi_{1i}(t+1) = \psi_{1i}(t) + f(\psi_{2i}(t), \psi_{2j}(t))*(\psi_{1j}(t) - \psi_{1i}(t)) \quad (5)$$

  where t is iteration number, ψ_{1j} can be the best solution vector or any other randomly or deterministically selected solution vector.



Rotations strategies





- **Rotation towards Best (R-I)**
- **Rotation towards Better (R-II)**
- **Rotation away from Worse (R-III)**

- **The rotation crossover operator balances the exploration and exploitation and converges the solution vector adaptively towards global optima.**

Adaptive Crossover

- The function $f(\psi_{2i}(t), \psi_{2j}(t))$ controls gross and fine search.
- Presently, $f(\psi_{2i}(t), \psi_{2j}(t))$ generates a random number either between $(0, |\alpha_{2i} - \alpha_{2j}|)$ or $(0, ||\alpha_{2j}|^2 - |\alpha_{2i}|^2|)$.
- Random_var$(0, |\alpha_{2i} - \alpha_{2j}|)$ is used for the gross search
- Random_var $(0, ||\alpha_{2j}|^2 - |\alpha_{2i}|^2|)$ is used for the fine search.
- The salient feature of the new quantum rotation inspired crossover operator is the adaptive change of each variable in the solution vector and at the same time, it is problem driven rather than being an arbitrary choice of the user.

Engineering Optimization Problems

Optimize $f(x)$,

Such that

$x_{il} < x_i < x_{ui}$ x_i – i^{th} variable, x_{il} and x_{ui} are lower and upper limits of x_i.

$g_j(x) \leq 0$; j - number of inequality constraints .

$h_K(x) = 0$; k - number of equality constraints.

where $x = (x_1, x_2, \ldots, x_N) \in R^N$.

f(x), g(x) and h(x) can be non-convex, non linear, non differential, multi-modal and of high dimension.

Such problems are in NP Hard complexity Class

Applications

- Mechanical Design Optimization
- Ceramic Grinding Optimization
- Wireless Sensor Networks (Localization)
- And also the….

Analysis of Photoluminescence measurement data from interdiffused Quantum Wells

Photoluminescence

- It is a contactless, nondestructive method of probing the electronic structure of materials.
- Light is directed onto a sample, where it is absorbed and imparts excess energy into the material in a process called photo-excitation.
- One way this excess energy can be dissipated by the sample is through the emission of light, or luminescence.
- The intensity and spectral content of this photoluminescence is a direct measure of various important material properties.

http://inventors.about.com/od/pstartinventions/a/Photoluminescen.htm

Measurement Principle

- PL used for measuring interdiffusion in semiconductor Quantum Wells
- Correlates changes PL peak energy into a characteristic diffusion length
- Interdiffusion process is assumed to be linear
- Linearity Assumption is tested by plotting the correlated diffusion lengths squared against anneal time.

Calculations

Interdiffusion coefficient is determined from the plot according:

$$L_D^2 = 4*D(T)*t \qquad \text{(A)}$$

The interdiffusion parameters viz., activation energy, E_a, and the interdiffusion prefactor, D_o, are determined by using Arrhenius equation:

$$D(T) = D_o *\exp(-E_a/(kB*T)) \qquad \text{(B)}$$

where kB is Boltzmann Constant and T is annealing temperature in Kelvin.

Challenges

Uncertainty in Experimental Data

Multiple Data Set for a Single Set Parameter Estimation.

Existing Methods

- ❑ **Least Squared Analysis**
  - ➢ **Most Commonly employed**
  - ➢ **Needs Arrhenius Plot**
  - ➢ **Provides Best fit Line**
  - ➢ **Lines had non–zero intercepts on Y (Ea) Axis ???**
    - **Extrinsic Diffusion Phenomena !!!**
    - **Or merely error in data collection**
- ❑ **Evolutionary Algorithm**
  - ➢ **Recently proposed**
  - ➢ **Provides Line which matches theory**
  - ➢ **Can incorporate theoretical models through multiple objectives and constraints**
  - ➢ **Lines crossed through origin and erroneous data was highlighted.**

Problem Formulation

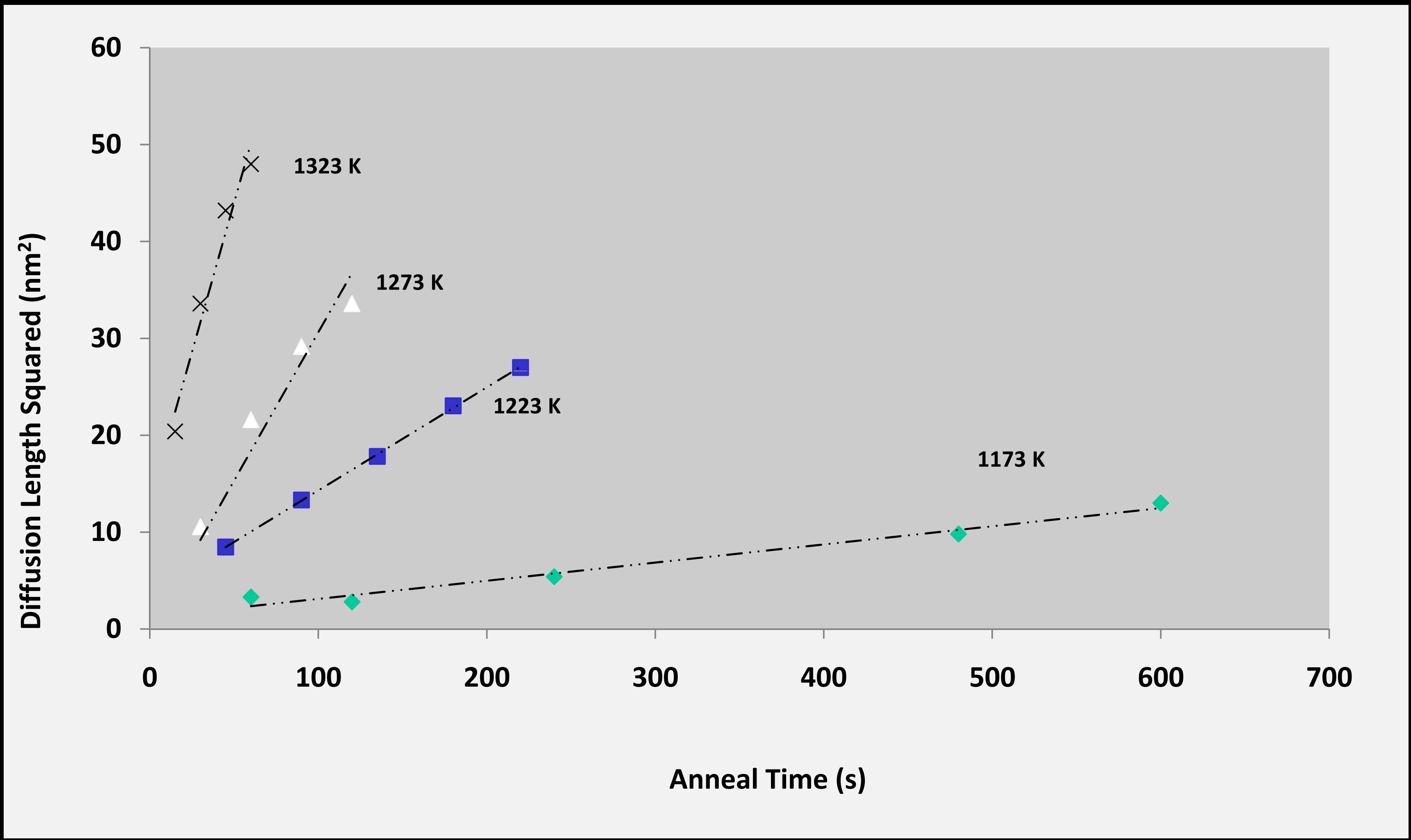
By combining (A) and (B), we have

$$L_D^2\,(t, T) = 4 * t * D_o * \exp(-E_a/(kB*T)) \qquad \text{(C)}$$

Fitness Function:

$$e = \sum_i \sum_j [L_D^2\,(t_j, T_i) - 4 * t_j * D_o * \exp(-E_a/(kB*T_i))] \qquad \text{(D)}$$

Graph of diffusion length squared as a function of anneal time for single quantum wells of $In_{0.2}Ga_{0.80}As/GaAs$ *[Gillin et al., 1993].*



Graph of diffusion length squared as a function of anneal time for single quantum wells of $In_{0.2}Ga_{0.80}As/GaAs$ [Gillin et al., 1993] and GA method [Khreis et al., 2005]

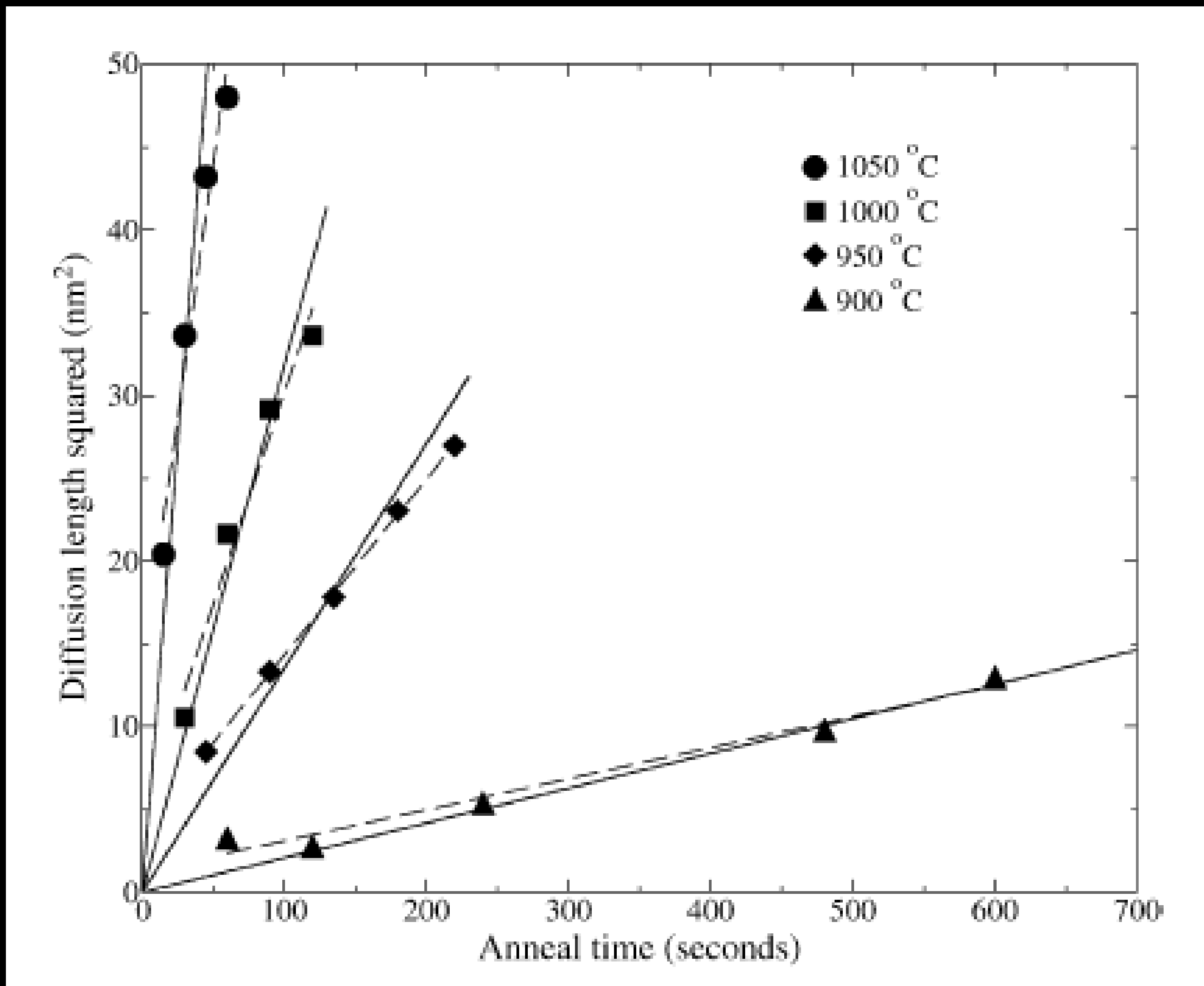


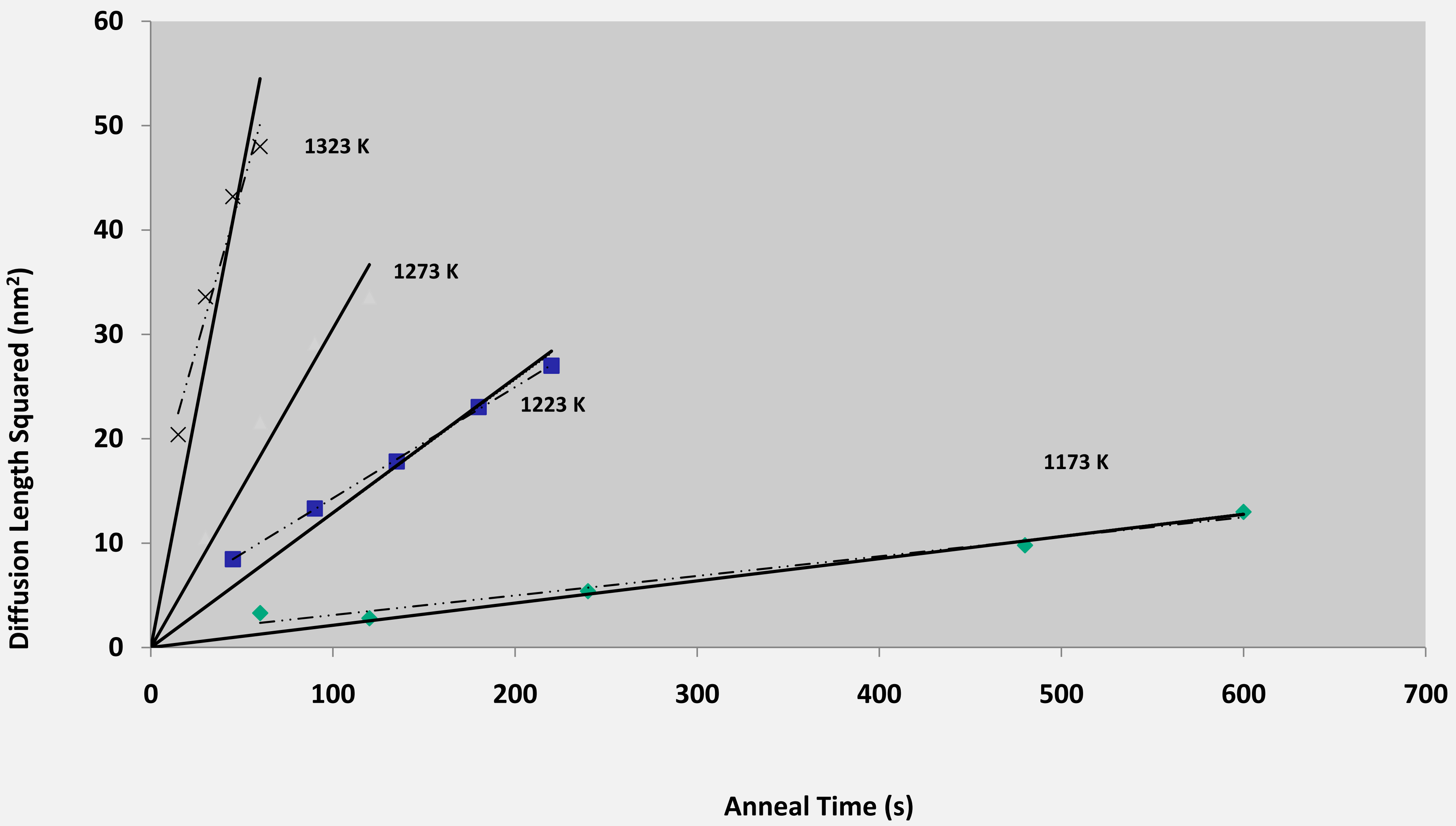
Table 1: Individual Run Comparison

Temperature (K)	RQiEA			GA			LSA
	D_o X 10^{-3} (cm^2/s)	E_a (eV)	D (T) X 10^{-16} (cm^2/s)	D_o X 10^{-3} (cm^2/s)	E_a (eV)	D (T) X 10^{-16} (cm^2/s)	D (T) X 10^{-16} (cm^2/s)
1173	**1.00**	**3.090**	0.744	1.06	3.099	0.536	0.46
1223	**0.99**	**3.031**	2.560	1.01	3.037	3.208	2.63
1273	**1.00**	**3.061**	7.995	0.98	3.062	7.656	6.34
1323	**1.00**	**3.057**	22.906	1.00	3.061	22.657	15.40

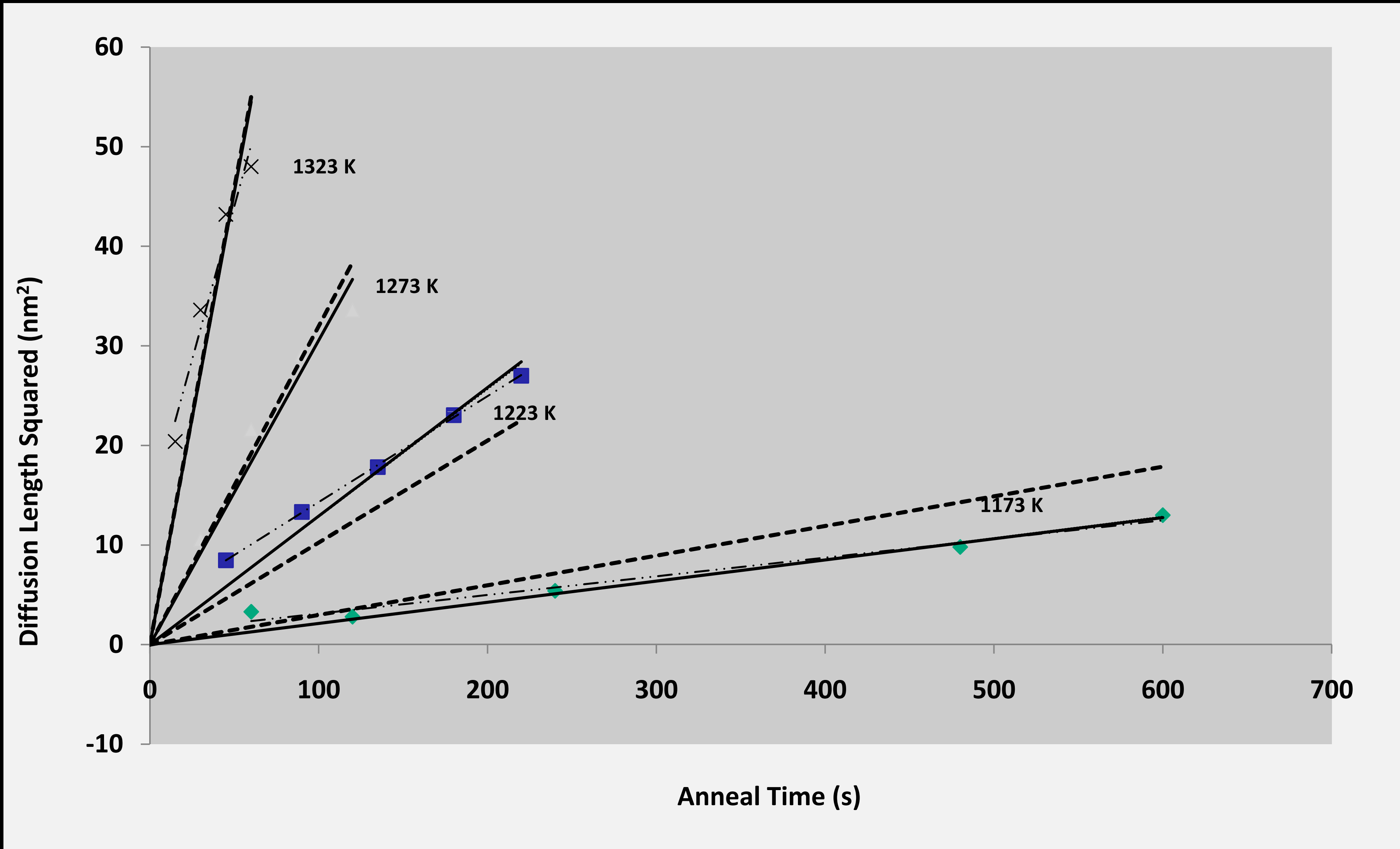
Collective Run Method

RQiEA : D_o = 1.00 X 10^{-3} (cm^2/s) and E_a = 3.056 eV
GA : D_o = 1.05 X 10^{-3} (cm^2/s) and E_a = 3.07 eV
LSA : E_a = 3.0 $\pm$ 0.3 eV

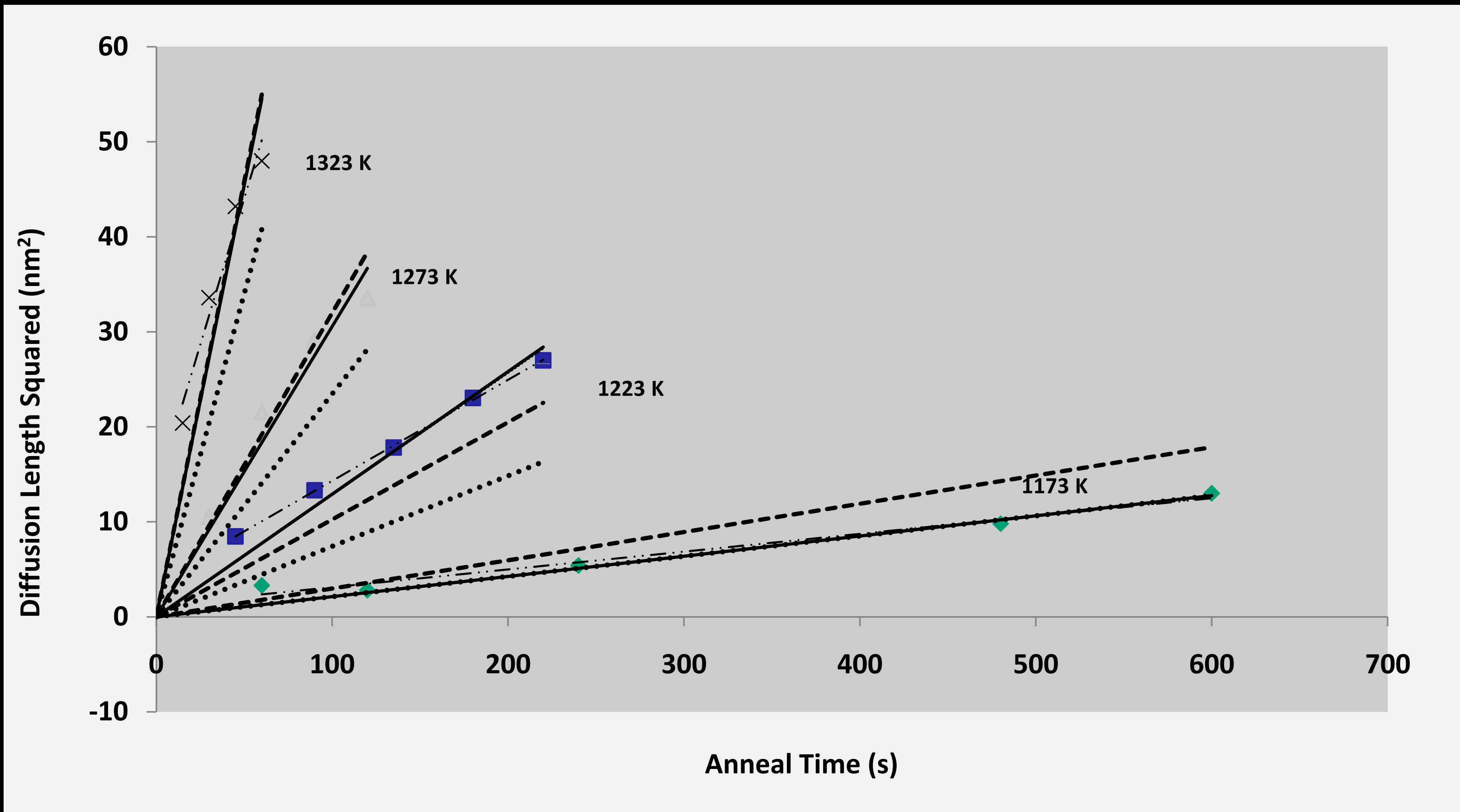
And with RQiEA (Individual Run)



With Collective Run Method



With RQiEA
(Min. Error Data set Ea and Do)



Discussion

- It is clear that the performance of the proposed algorithm as indicated by the quality of solution is superior to the existing techniques for this problem.

- The algorithm is Robust and Efficient .

Conclusions

- A new adaptive quantum inspired evolutionary algorithm is used for analyses of Photoluminescence measurement data from interdiffused Quantum Wells.
- The algorithm uses two qubits representation instead of one and utilizes the quantum entanglement and superposition principles hitherto not tapped.
- It does not require mutation or local heuristic for improving the solution quality but still provides better solutions than the state of the art approaches.
- Ability to quantify data deviation from theoretical predictions, which would lead reliable detection of extrinsic process.
- Future work would involve more applications of the proposed Algorithm for Analysis of HEP Data.

References

1. **Z. Michalewicz, *Genetic Algorithms + Data Structures = Evolution Programs*. Berlin: Springer-Verlag, 1996.**
2. **K.H. Han and J.H. Kim, "Quantum-Inspired Evolutionary Algorithms with a New Termination Criterion, Hε Gate and Two Phase Scheme," *IEEE Trans. Evo. Co.,* vol. 8, no. 2, 2004, pp. 156—168.**
3. **M.A. Nielsen and I.L. Chuang, *Quantum Computation and Quantum Information*. Cambridge: Cambridge University Press, 2006.**
4. **F.S. Alfares and I.I. Esat, "Real-coded Quantum Inspired Evolutionary Algorithm Applied to Engg. Optimiz. Problems," *2nd Int. Symp. On LAFMVV IEEE C S*, 2007, pp.169-176.**
5. **F. Herrera, M. Lozano and A.M. Sanchez, "A Taxonomy for the crossover operator for Real-coded Genetic Algorithms," *Int. J. Intelligent Systems*, vol 18, 2003, pp. 309--338.**
6. **O.M. Kheris and I.S. Al-Kofahi, A genetic algorithm analysis of photoluminescence experimental data from interdiffused quantum wells, Superlattices and Microstructures 37 (2005), pp 193-201.**
7. **W.P. Gillin, D.J. Dunstan, K.P. Homewood, L.K. Howard, B.J. Sealy, J. Appl. Phys. 73 (1993) 3782.**
8. **Ashish Mani and C. Patvardhan,** An Adaptive Quantum Evolutionary Algorithm for Engineering Optimization Problems, Accepted in IJFCA.
9. **Ashish Mani and C. Patvardhan, Solving Ceramic Grinding Optimization Problem by Adaptive Quantum Evolutionary Algorithm, In Proc. of ISMS-2010, pp. 43-48.**
10. **Ashish Mani and C. Patvardhan, An Adaptive Quantum inspired Evolutionary Algorithm with Two Populations for Engineering Optimization Problems, In Proc.** JOINT INTERNATIONAL CONFERENCE ON APPLIED SYSTEMS RESEARCH AND XXXIII NATIONAL SYSTEMS CONFERENCE (ASR-NSC 2009), pp. 43-47.

Before I say Thanking You

???

TAJ MAHAL, In Agra, Uttar Pradesh, India (N 27°10' E 78°03')


Dayal Bagh
Dayal Bagh Rd
Dayal Bagh Rd
Dayalbagh
Educational
Institute
Computer
Center