

# Model Development for Lattice Properties of Gallium Arsenide using Parallel Genetic Algorithm

Mehdi Salmani-Jelodar, Sebastian Steiger, Abhijeet Paul and Gerhard Klimeck  
School of Electrical and Computer Engineering and Network for Computational Nanotechnology,  
Purdue University, West Lafayette IN 47906 USA  
{msalmani, steiger, paul1, gekco}@purdue.edu

**Abstract**—In the last few years, evolutionary computing (EC) approaches have been successfully used for many real world optimization applications in scientific and engineering areas. One of these areas is computational nanoscience. Semi-empirical models with physics-based symmetries and properties can be developed by using EC to reproduce theoretically the experimental data. One of these semi-empirical models is the Valence Force Field (VFF) method for lattice properties. An accurate understanding of lattice properties provides a stepping stone for the investigation of thermal phenomena and has large impact in thermoelectricity and nano-scale electronic device design. The VFF method allows for the calculation of static properties like the elastic constants as well as dynamic properties like the sound velocity and the phonon dispersion. In this paper a parallel genetic algorithm (PGA) is employed to develop the optimal VFF model parameters for gallium arsenide (GaAs). This methodology can also be used for other semiconductors. The achieved results agree qualitatively and quantitatively with the experimental data.

**Keywords** - gallium arsenide, GaAs, phonon dispersion, elastic constants, sound velocity, parallel genetic algorithm, valence force field model.

## I. INTRODUCTION

COMPUTATIONAL nanoscience is attracting ever more attention as the power of computers and clusters is increasing. The ability to accurately model nano-sized structures and their constituting materials is pivotal to understand and improve the state-of-the-art semiconductor materials and devices technology. Many modeling approaches use experimental and mechanical data to adjust required parameters for their models. These methods are termed semi-empirical. The underlying mathematical expressions are based on physical concepts such as specific types of interactions or symmetries. While the fundamental interactions are well understood, they can be extremely hard to quantify from ab-initio models. The interaction strengths are therefore treated as fitting parameters. Usually such approaches are based on regulating the model's input parameters to fit the model's output with measured experimental values or higher-order mechanical models. In some cases the number of inputs may be very few (two or three) and scientists find them by trial and error. However, it is more typical that the models are very complex and it is hard if not impossible to solve them analytically. The semi-empirical tight binding method for the

material's electronic structure, for example, has between 16 to 200 parameters to fit [1]. In the case of many input parameters, an optimizer is needed to fit the inputs for specific experimental target values. The authors employed evolutionary computing approaches for semi-empirical tight binding successfully in the past [1][2]. In these models the parameters have a physical meaning and the range of permitted values is usually constrained. The fitting process is also used to tweak and fine-tune the final model itself. The semiconductor device simulation tools which implement the models are monolithic and need several tenths of a second to several hours of computation time.

Developing accurate models for lattice properties is essential for the design of nanoscale electronic and optoelectronic devices [3]. The development of a model based on an atomistic representation of the crystal is still challenging. One of these approaches is the semi-empirical Valence Force Field (VFF) model [4][5]. Based on accuracy and complexity different types of VFF models have been proposed in the literature [5][7]. These models are comparatively simple and have deficiencies in capturing the physics. By adding additional physical interaction terms to the model and using genetic algorithm to find the related parameters, a more precise model can be constructed. Here, an 8-parameter VFF model is developed which includes all nearest-neighbor as well as the coplanar second nearest-neighbor interactions. The model is explained in the next section.

For fitting the VFF model with experimental data three issues need to be considered: a) objectives must be met to obtain a variety of physical characteristics of the material, b) model inputs have constraints in order to retain their physical meaning, and c) the dependence of the model results on the 8 input parameters is very complex and nonlinear. These issues and the complexity of the fitness landscape enforced us to use an evolutionary computing approach to solve this multi-objective problem [6]. Genetic algorithms (GAs) have been employed in the past to produce reasonable results for such problems. Each chromosome's evaluation takes a few tens of a second. For these reasons a parallel genetic algorithm approach (PGA) is employed over an eight-core cluster to speed up the optimization process.

In related work, Kane used a weighted least squares

approach to fit six input parameters of his model against a few selected points of the dispersion relation [7]. Martin's model has only two parameters that are fitted against the elastic constants – a single objective [8]. Lazarenkova et al. proposed three additional parameters where one of them was derived analytically and the remaining two were found by trial and error [9]. All these approaches had a single objective and few input parameters. This paper features a more complex model with 8 input parameters which is fitted against three different objectives. Due to this complexity GA is employed. The model is applied to the semiconductor gallium arsenide (GaAs) [3], but the methodology can also be used for other zincblende materials like InAs and InP.

The paper is organized as follows: Section II provides an overview on the lattice dynamics and the Valence Force Field (VFF) model. Section III is a brief introduction to standard GA and PGA. Readers who are familiar with these approaches can skip this section. In Section IV we explain the fitness function and the used parameters for the PGA and then show implementation results for fitting parameters of the VFF model to different objectives. Section V concludes with finishing remarks and future work.

## II. LATTICE DYNAMICS AND THE VALENCE FORCE FIELD METHOD

This section gives a brief introduction to the valence force field model and its connection to the vibrational modes, or phonons, of a semiconductor crystal.

Static and dynamic lattice dynamics of semiconductors play a decisive role in electronics. They determine the thermal conductivity, which is a limiting factor in the performance of today's transistors. Scattering between electrons and phonons typically deteriorates the speed of the device and introduces dissipation and heating, the latter being the main limiting factor in the operation frequency of today's transistors.

### A. Valence Force Field Model of the Crystal Energy

The valence force field (VFF) model provides a fundamental and microscopic description of lattice properties [5]. Semiconductor devices are typically made of materials like GaAs where atomic bonds are to a large extent covalent. This makes the interaction short-range, as opposed to ionic crystals like NaCl where the bond is largely based on long-range Coulomb interactions. The VFF method expresses the total crystal energy as a functional of the bond angles and bond lengths, as depicted in Figure 1. The functional reads [10]:

$$\begin{aligned}
 U = & \frac{3}{2 \cdot 8} \sum_{i,j \in NN(i)} \left[ \alpha_{ij} (\delta r_{ij})^2 + \sum_{\substack{k \neq j \\ k \in NN(i)}} \left( \beta_{jik} (\delta \theta_{jik})^2 \right. \right. \\
 & \left. \left. + \gamma_{jik} \delta r_{ij} \delta \theta_{jik} + \delta_{jik} \delta r_{ij} \delta r_{ik} + \sum_{\substack{COP(j-i-k-l) \\ l \in NN(k)}} \nu_{jikl} (\delta \theta_{jik}) (\delta \theta_{ikl}) \right) \right] \\
 & + \frac{1}{2 \cdot 4\pi\epsilon_0} \sum_{i,j \neq i} \frac{Z_i Z_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{1}
 \end{aligned}$$

$$\delta r_{ij} \equiv \frac{(r_{ij}^2 - d_{ij}^2)}{d_{ij}}, \quad \delta \theta_{jik} \equiv \frac{(\mathbf{r}_{ij} \cdot \mathbf{r}_{ik} - \cos \theta_0 d_{ij} d_{ik})}{\sqrt{d_{ij} d_{ik}}}$$

Here  $NN$  denotes nearest neighbors,  $COP$  stands for coplanar bonds,  $i, j, k, l$  are atom indices,  $r$  and  $\theta$  are bond lengths and angles, and  $\alpha, \beta, \gamma, \delta, \nu$  are empirical force constants.  $d$  is the equilibrium bond length and  $Z$  are fractional point charges. The most commonly used description, known as Keating model [4], neglects all but the first two contributions [5][12].

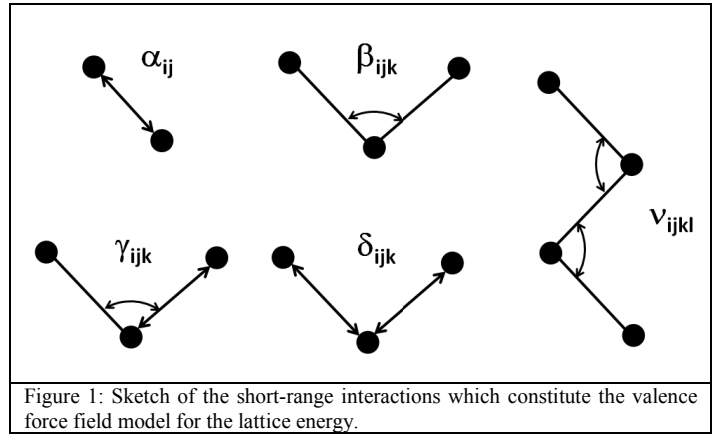


Figure 1: Sketch of the short-range interactions which constitute the valence force field model for the lattice energy.

In monoatomic crystals like Si the model's inputs are 5 parameters including  $\alpha, \beta, \gamma, \delta$  and  $\nu$ . In diatomic crystals like GaAs two different values of  $\beta, \gamma$  and  $\delta$  are possible depending on what atom sits at the apex of the two bonds, bringing the number of parameters up to 8.

It is well-known that the bonds in zincblende-type semiconductors like GaAs, which are binary compounds consisting of atoms with different radii, do exhibit a partially ionic character. To account for this, the Coulomb interaction between point charges fixed at the mean atomic positions was added (rigid ion model), which is represented by the last term in Eqn. (1). In 3D-periodic lattices this long-range interaction can be evaluated using Ewald summation [11].

### B. Elastic Constants

Nanostructures, i.e. structures at the size of few to hundreds of nanometers which are composed of different materials, typically comprise some lattice mismatch because the natural bond lengths of crystals differ. Structures consequently exhibit *strain* where the atoms are distorted from the natural positions they would take if only a single material was present. The microscopic description of the VFF model allows finding these

atomic positions by writing down the energy functional for the structure and minimizing with respect to the atomic coordinates, a process known as *strain relaxation*.

Calculations of strain in macroscopic materials, such as buildings or vehicles, are commonly performed using continuum elasticity theory. The model parameters for this theory are the *elastic constants*, well-established material parameters that are easily accessible by experiment. Due to the symmetry of zincblende-type lattices, only three constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  suffice to describe zincblende nanostructures. A connection to the microscopic VFF model is established by performing a Taylor expansion of the energy in (1) for a bulk crystal around the equilibrium bond length. This expansion can be rewritten in terms of the strain tensor. Coefficient comparison yields analytical relations between the microscopic VFF parameters and the macroscopic elastic constants [12].

### C. Lattice Dynamics and Phonons

The elastic constants are at the center of the description of *static* lattice properties of crystals. *Dynamic* properties, i.e. vibrations, are typically classified by harmonic oscillations of the lattice called *phonons*. Knowledge of the so-called *dispersion relation*  $\hbar\omega(q)$ , where  $\hbar\omega$  is the phonon energy at the phonon wavevector  $q$ , then permits the calculation of manifold quantities ranging from thermal conductivities to phonon-limited electron mobilities. The *vibrational frequencies*  $\omega$  of the phonons are the eigenmodes of the *dynamical matrix*, which is closely related to the crystal energy: It is the Hessian (second derivative) of Eqn. (1) with respect to all atomic positions, augmented with a wavevector-dependent phase factor that reflects the periodicity of the structure. The details to solve such a dynamical matrix are outlined in Ref. [5].

Zincblende lattices are periodic continuations of two-atomic unit cells. Since every atom has three spatial degrees of freedom, the size of the dynamical matrix for any wavevector is consequently 6. The resulting six eigen-modes are classified as follows:

- Three modes are low-energy oscillations that have vanishing energy as  $q \rightarrow 0$ . The slope of  $\hbar\omega(q \sim 0)$  determines the speed of sound in the material. These *acoustic* modes dominate properties such as thermal conductivity.
- The three high-energy modes are called *optical* modes. They are characterized by out-of-phase oscillations of the two atomic Ga and As sublattices. In zincblende crystals these modes dominate the scattering between electrons and phonons.

For each type two out of three modes vibrate in directions perpendicular to the wavevector whereas the vibration of the third mode is in the same direction. This classifies into *transversal* and *longitudinal* branches. The crystal hence

exhibits TA(2), TO, LA (2) and LO phonons. This classification is illustrated in Figure 2.

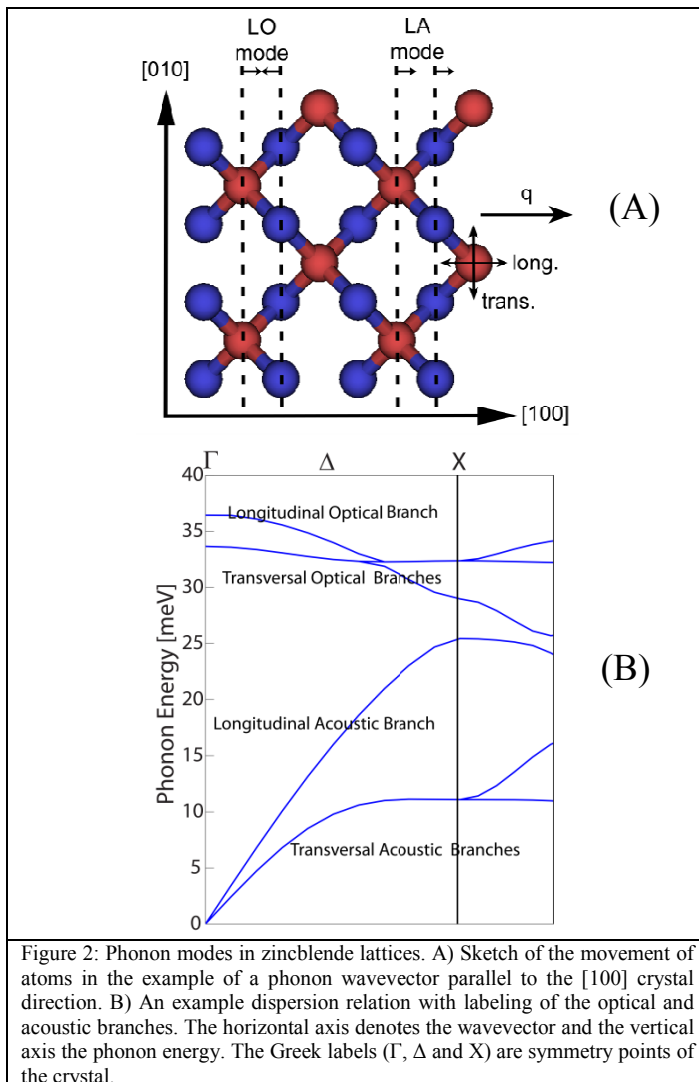


Figure 2: Phonon modes in zincblende lattices. A) Sketch of the movement of atoms in the example of a phonon wavevector parallel to the [100] crystal direction. B) An example dispersion relation with labeling of the optical and acoustic branches. The horizontal axis denotes the wavevector and the vertical axis the phonon energy. The Greek labels ( $\Gamma$ ,  $\Delta$  and X) are symmetry points of the crystal.

## III. GENETIC ALGORITHM

This section is a brief introduction to genetic algorithms and parallel genetic algorithms. Readers who are familiar to these algorithms may skip this part.

### A. Standard Genetic Algorithm

Genetic algorithms are adaptive heuristic search techniques which are inspired by the principles of evolution and natural selection. Due to this, they represent an intelligent exploitation of a random search within a defined search space to find solutions for a given problem. First pioneered by John Holland, they are widely used and experimented in the science and engineering area [13][14].

In the standard GA, candidate solutions are encoded as fixed-length binary strings (or vectors), where the bits of each string are considered to be the *genes* of an *individual chromosome* and where the tuple of these individuals called a *population*. The initial solution population is usually chosen randomly.

These chromosomes, which are candidate solutions, are allowed to evolve over a number of generations. In each generation, the fitness of each chromosome is evaluated. This is a measure of how well the chromosome optimizes the objective function. Subsequent generations are created through a process of *selection*, *recombination*, and *mutation*. A chromosome fitness measure is used to probabilistically select which individuals will recombine. Recombination (crossover) operators merge the information contained within pairs of selected “parents” by placing random subsets of the information from both parents into their respective positions in a member of the subsequent generation, or a child. Due to random factors involved in producing “children” chromosomes, the children may or may not have higher fitness values than their parents.

Nevertheless, because of the selective pressure applied through a number of generations, the overall trend is towards a generation of higher fitness chromosomes. Selection is a costly process which is usually based on the chromosomes' fitness. Mutations are used to help preserving diversity in the population. Mutations introduce random changes into the chromosomes[15]. The main objective of the mutation is exploring the solution space versus the main objective of the crossover which is exploiting. The pseudo-code of the canonical GA is depicted in Figure 3.

```

Begin
  INITIALIZE population with random candidate solutions;
  EVALUATE each candidate;
  REPEAT UNTIL (TERMINATION CONDITION is
  satisfied )
  Begin
    1 SELECT parents;
    2 CROSSOVER pairs of parents;
    3 MUTATE the resulting offspring;
    4 EVALUATE new candidates;
    5 SELECT individuals for the next generation;
  End
End

```

Figure 3: Pseudo-code of the canonical genetic algorithm.

### B. Parallel Genetic Algorithm

The parallel GA (PGA) is an algorithm used to accelerate computation using parallel and distributed computing. The PGA has the potential capability to solve problems much faster than simple GA. However, it was mainly used by the software. The parallel GA can be categorized into four types: global (or master-slave), coarse-grain (or island), fine-grain and hybrid [16] (Figure 4).

1) *Global parallel genetic algorithm*: The global (or master-slave or standard) model divides the fitness evaluator unit into multiple processing units. Each unit evaluates one or more chromosomes independently (their operations are similar to each other). After fitness evaluation, they pass the chromosomes and their corresponding fitness value to the next unit (genetic operators unit)[14]. In computation intensive fitness evaluations this model works very well and could speed up the evolution process up to near the number of

involved cores.

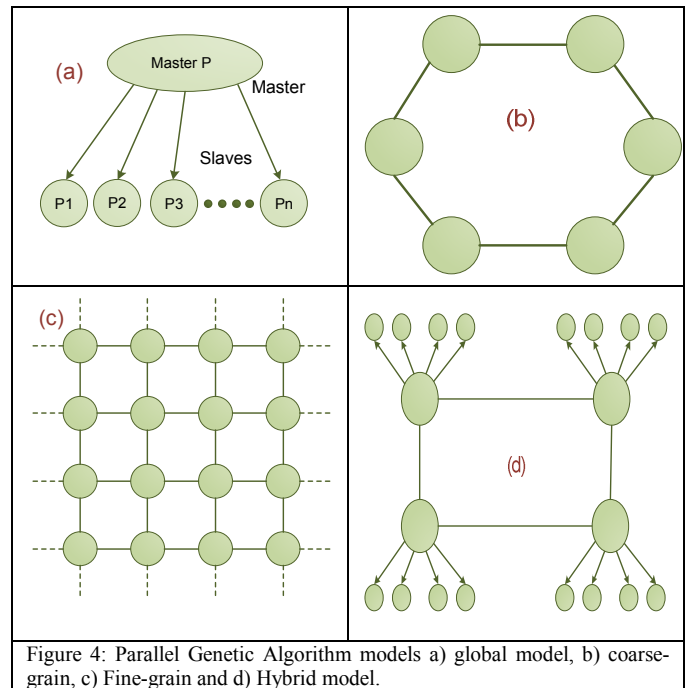


Figure 4: Parallel Genetic Algorithm models a) global model, b) coarse-grain, c) Fine-grain and d) Hybrid model.

2) *Coarse-grained parallel genetic algorithm*: The island (or coarse-grained) model divides the population in multiple sub-populations. The sub-populations evolve independently from each other for a certain number of generations (isolation time). After the isolation time, a number of individuals are distributed among sub-populations by the migration operator. This model also is more capable to find global optimum chromosome in complex fitness landscapes. Petty and Leuze studied a coarse-grain PGA in Ref. [18]. In this research we employed a coarse-grain PGA.

3) *Fine-grained parallel genetic algorithm*: Fine-grained PGA acts on each member of the population in parallel. Consequently, each chromosome of the population performs crossover with its immediate neighbors, where the neighborhood is defined by the topology and some distance parameter [19][20].

4) *Hybrid parallel genetic algorithm*: A few researchers have tried to combine two of the methods to parallelize GAs, producing hierarchical parallel GAs. Some of these new hybrid algorithms add a new degree of complexity to the already complicated scheme of PGA, but other hybrids manage to keep the same complexity as one of their components. When two methods of parallelizing GAs are combined they form a hierarchy. At the upper level, most of the hybrid parallel GAs are multiple-population algorithms. Some hybrids have a fine-grained GA at the lower level (see Figure 4-d) [16].

Migration as a PGA operator increases the diversity among the individuals in every subpopulation and decreases the probability to stop in a local optimal solution. The number of exchanged individuals (migration rate), selection method and

migration topology determine how much genetic diversity can occur in the subpopulations and how the subpopulations exchange information [21].

To speed up the optimization process and improve the results, this work employs coarse-grain PGA over an 8-core cluster.

#### IV. IMPLEMENTATION AND EXPERIMENTAL RESULTS

To fit the model with experimental data using a PGA, a sophisticated multi-objective fitness function is defined to help the optimization method to find the optimum solution with minimum fitness evaluations. This section first describes how the fitness function is developed and what the used parameters were for PGA. Then the three-step parameter fitting for the objectives is explained: acoustic branches, whole dispersion relation, and at the end whole dispersion and elastic constants. The extracted parameters are displayed in Table 1.

This problem has an 8-dimensional vector of real numbers as a gene, where each of the genes is related to the model's inputs. The order of genes in the chromosomes was as follows:

$\alpha$	$\beta_{Ga}$	$\beta_{As}$	$\gamma_{Ga}$	$\gamma_{As}$	$\delta_{Ga}$	$\delta_{As}$	$v(Nu)$
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##### A. Fitness Function and PGA Parameters

We minimize the mean-squared-error between the model's simulation outputs and experimental data. Three objectives needed to be fit. The first objective was the dispersion relation. By this objective an attempt was made to match the acoustic (and optical) branches with experimental data points ( $F_1$ ). This is shown in the following equation:

$$F_1 = \sum_{\text{all } k \text{ points}} \text{range}(VFFOut - ExperVal)^2$$

At high symmetry points ( $\Gamma$ , X and L in Figs. 6-8) weight was added to push the evolution process to converge to a better match for these points, as they are particularly important ( $F_2$ ). The third objective, which was added to the third part of the fitting process, was the mean-square-error between calculated and target elastic constants ( $F_3$ ). The total cost value is then composed as follows:

$$\text{Cost Value} = W_1F_1 + W_2F_2 + W_3F_3,$$

where  $W_i$  is the weight of every distance function. These weights were assigned manually based on tolerable deviations from target values.

To handle the constraints over the range of input parameters, a very large cost value ( $10^6$ ) was applied when the inputs were out of the acceptable range. The acceptable ranges were  $0 < \alpha, v < 100$  and  $-100$  to  $+100$  for all other parameters.

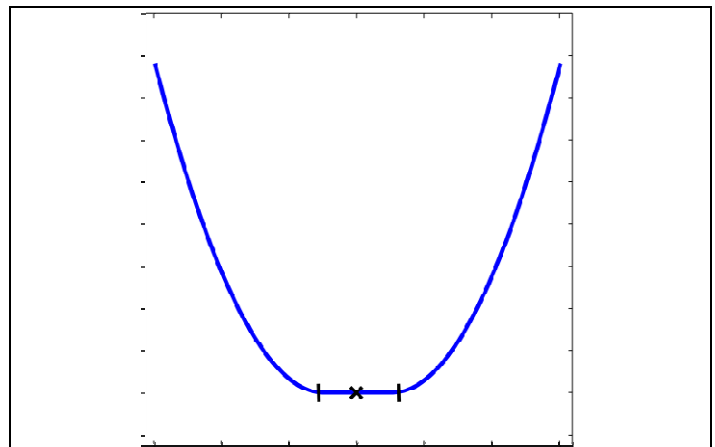


Figure 5: Fitness evaluation with variation around the target value. In this minimization problem the fitness value increases with the distance between a target range and the model's output.

In the semi-empirical methods experimental data are typically used as target values. In this paper we used experimental data from [22]. For some experimental points like Gamma this data was extended with generally accepted values (e.g. zero). Experimental data has some error which depends on the precision of the measurement devices. To include this issue in the minimizing process a "range" fitness function was used: if the model's outputs were within a certain range of the target values they would get the same high positive weight in fitness value. If the model's outputs are out of the range then the square of the distance to the target range enters the fitness value (see Fig. 5).

Other parameters for the island PGA are a population size of 2000, 100 for number of generations, crossover rate 0.7, crossover type was one-point, mutation rate 0.05, migration rate 1 per each island. The PGA ran on an 8 core cluster. Due to the random nature of evolutionary algorithms, we ran each optimization process about 10 times and reported the best achieved results. The model was developed in C++. Each optimization process takes about 10 hours to be done on an eight 2.5GHz cores shared memory cluster with 32 GB memory and 10 GibE (Gigabit Ethernet) connection.

##### B. Optimization for Acoustic Phonon Modes

In the first part model parameters were found which fit the acoustic branches of the target. Achieved results for the dispersion relation are depicted in Figure 6. Elastic constants from experimental data and VFF model are described in Table 2. Optimum parameters are shown in Table 1.

It is clear from Figure 6 that the experimental acoustic branches are fit very well. As it was expected, the optical branches are far above the experimental target values. The elastic constants are also far from the targets. This is due to the objective in the fitting process which only fits the acoustic branches.

Table 1: Achieved parameters for best fits in all cases.

Parameters optimized for	$\alpha$	$\beta_{Ga}$	$\beta_{As}$	$\gamma_{Ga}$	$\gamma_{As}$	$\delta_{Ga}$	$\delta_{As}$	$\nu(Nu)$
Acoustic Branches	54.2438	-8.7605	16.1228	4.2962	-3.4887	-45.6978	39.2157	1.7662
Whole Dispersion Relation	43.5859	14.4958	-6.2249	-11.3335	25.2914	-46.5666	46.4393	3.7995
Whole Dispersion Relation and Elastic Constants	39.4707	-15.1765	26.5749	22.5695	-20.8050	57.8911	-61.0179	3.7995

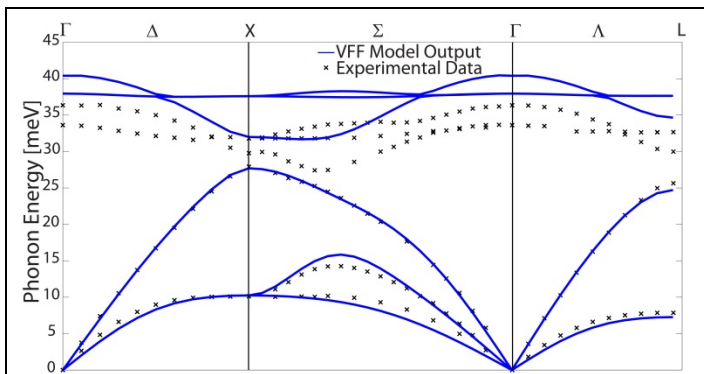


Figure 6: Achieved results for optimizing VFF model’s inputs for tuning acoustic branches with experimental data.

### C. Optimization for Dispersion Relations

Here the whole dispersion relation (optical and acoustic branches) is targeted to be fitted with experiment. Achieved results for dispersion relation are depicted in Figure 7. Elastic constants from experimental data and VFF model are shown in Table 2. Optimum model parameters are described in the Table 1.

From Figure 7 it can be seen that the optical branches are fit very close to experimental points. On the other hand the acoustic branches are not as close as during the previous optimization but still within a reasonable distance. As it was expected, the achieved elastic constants are far from the experimental values.

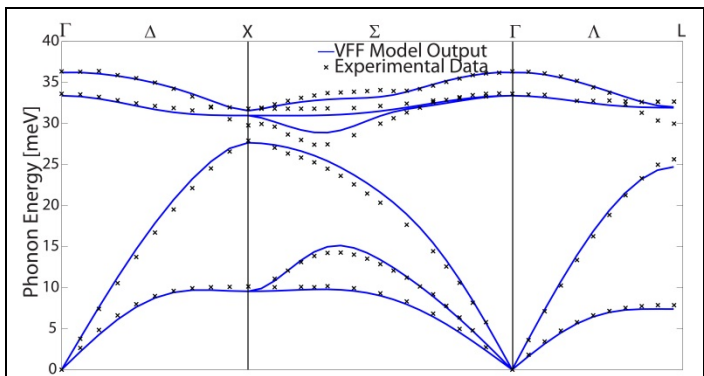


Figure 7: Achieved results for optimizing VFF model’s inputs to compare the whole dispersion relation with experimental values.

### D. Optimization for Dispersion Relation and Elastic Constants

For many atomistic modeling applications an accurate description of the elastic constants is essential. To achieve this goal another part was added to the objective function which gives a negative large weight to the distance between

calculated elastic constants and the experimentally values. Achieved results for the dispersion relation are depicted in Figure 8. Elastic constants from experimental data and VFF model with achieved parameters are shown in Table 2. Achieved parameters are described in the Table 1.

Comparing the optimization runs in Table 1, it is noted that the parameters  $\beta$ ,  $\gamma$  and  $\delta$  may change their signs. These changes are permitted since the interactions do not decouple and it is the interplay of all parameters rather than individual values which determines the physical properties. For example, only the average between the Ga and the As value of every parameter influences the elastic constants.

Comparing Figure 8 to Figs. 6 and 7, the whole dispersion relation is not as fit but the elastic constants (from Table 2) are now very close to the experimental values. On the other hand, the dispersion relation is still close to the target.

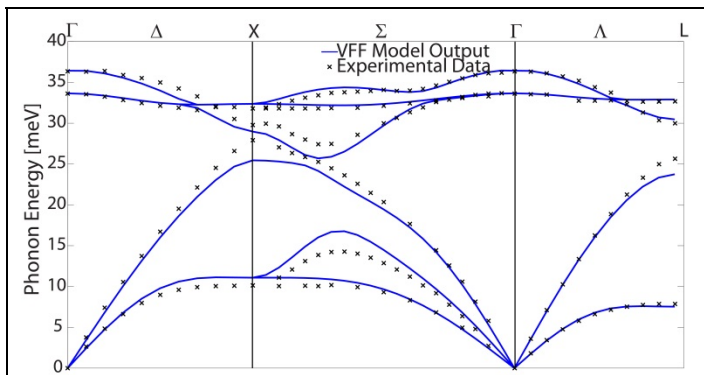


Figure 8: Achieved results for optimizing VFF model’s inputs to compare whole dispersion relation and the elastic constants with experimental values.

Table 2: Experimental and achieved elastic constants for all fitting cases.

Elastic Constants	$C_{11}$	$C_{12}$	$C_{44}$
Experimental Values	119.0	53.4	59.6
VFF for Acoustic	142.027	74.6006	44.1655
VFF for Dispersion	148.048	92.004	48.4741
VFF for Dispersion & Elastic Constants	118.622	52.6308	57.0678

## V. CONCLUSION AND FUTURE WORK

In this paper a parallel genetic algorithm was employed to develop a semi-empirical model for semiconductor lattice properties by fitting its constant parameters to experiment. Simple optimization methods fail due to the increasing complexity and number of parameters as multiple objectives need to be fit.

It is shown that the genetic algorithm finds sufficiently optimal parameters for the defined objectives. As a first step in

the optimization process the model's outputs were fitted to the acoustic modes, which yielded a good match to experimental values for the acoustic branches but not to the optical branches and the elastic constants. In a second step fitting with optical modes was added to the fitness function. The results were good for the entire dispersion relation but not for the elastic constants. In a third step, the elastic constants were added as an additional objective and both the achieved dispersion relation and elastic constants were close to experimental values (less than 2% discrepancy).

This model can be used for atomistic modeling of nanoelectronic devices and thermoelectricity, and it can be applied to other zincblende-type materials. An extended explanation of the model, the connection between the VFF parameters and the elastic constants, and the final parameter sets will be published elsewhere.

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