Determination of the complex refractive index of compound semiconductor alloys for optical device modelling

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Abstract

In this paper a method is presented to accurately and quickly interpolate a dataset of the complex refractive index of arbitrary compound semiconductors. The method is based on a parameter morphing algorithm which maps critical points of two endpoint materials with known optical parameter sets onto each other. Every desired intermediate material composition can be interpolated if the composition dependence of the band gap is known for the given material system. The accuracy and stability of the proposed procedure is validated experimentally using spectral ellipsometry and reflection measurements. Test samples of two III–V semiconductor material systems, AlGaAs and GaInAsP, with various compositions were grown using metalorganic vapour phase epitaxy and the morphed parameter sets are compared to corresponding measurement results. Modelling the absorption of a solar cell device and comparing it to the external quantum efficiency is presented as an application example of this method. The interpolation method is demonstrated to be a powerful tool for optical and electro-optical modelling of semiconductor structures if parameters of the complex refractive index are not available for the exact material composition.

Key words: complex refractive index, III–V semiconductor, dielectric function, interpolation, device modelling, spectral ellipsometry, solar cell

1. Introduction

Compound semiconductors, which consist of III–V or II–VI semiconductor alloys, e.g. GaAs, InP etc, are widely used in various fields of electronic device engineering [1]. Thanks to the possibility of mixing various elements to ternary or quaternary alloys they offer flexibility in optimising their electrical properties exactly for the needs of the application at hand. Many of these applications are optical devices such as solar cells, light emitting diodes (LED), solid-state lasers etc. Performance simulations of the device to be designed at an early stage of development are essential for high innovation rates and for saving costs of unsuccessful prototypes [2, 3]. With the freedom of alloying almost arbitrary material combinations comes the challenge to accurately model the optical properties of the used materials. Designing, building and measuring test samples for each material composition that could potentially be used is mostly not an option considering that there is an infinite set of gradually changing configurations. The solution to this problem proposed in this paper is the empirically motivated generation of a dataset for the complex refractive index, which describes dispersion, diffraction, and absorption inside a material, based on the known optical parameter data of two related materials.

The basic idea for optical parameter morphing was first suggested by Aspnes et al [4]. They determined the pseudoelectric functions of $\text{Al}_x\text{Ga}_{1-x}$As from fits to spectral ellipsometry data for $x = 0 - 0.8$ in steps of 0.1 and commented that these data could be used to calculate the optical parameters for composition values close to the reference compositions.
Later, Snyder et al [5] compared the results of this approach to an effective-medium approximation and a discrete harmonic oscillator model with analytic dependence on composition. They found superior performance of this interpolation model. So far, an empirical dependence of the so called critical points on composition was required and the model was applied only for the interpolation of data in a narrow sampling range [6]. In this paper we generalise that method by showing that with datasets of just two endpoint materials and a known compositional dependence of the band gap, excellent agreement with spectral ellipsometry and absorption measurements is obtained. Additionally, we also extend the method by applying it to material systems that do not share a common group-V element as is the case for AlGaAs. We demonstrate that this morphing algorithm even works for quaternary materials such as GaInAsP lattice matched to GaAs.

Besides phenomenological approaches for the determination of the optical parameters there exist a number of models which approximate the complicated band structure of a semiconductor by a parabolic band along with transitions at critical points (CPPB models) [7, 8]. Also hybrid models which combine CPPB calculations with higher energy harmonic oscillators were suggested [9]. More complicated models such as the one by Kim et al [10] are capable of accurately fitting not only the dielectric function of a certain semiconductor but also its first three derivatives. The downside of these models is the amount of free parameters, up to 21, that are required for them to work properly. As a consequence, in order to avoid overfitting of the data a large number of input datasets first have to be provided experimentally which renders these models unsuitable for novel and scarcely studied material systems. With the presented algorithm of this work neither precise knowledge of the exact band structure nor fitting of analytical model parameters are needed. This allows to still apply this method to material systems that have not yet been extensively investigated and understood.

In the following sections, first, the theoretical background of the parameter morphing algorithm is presented and a comparison to existing analytical methods of optical parameter modelling is drawn. Then, in section three the working principle of the algorithm and its mathematical formulation are explained in detail. In section four, the application of the algorithm to two different material systems is illustrated and its functionality is validated experimentally by spectral ellipsometry and comparison between morphed and known refractive index data. Furthermore, a strategy is explained to use such experimental data if available to increase the accuracy of the obtained refractive index dataset and ensure Kramers-Kronig consistency of the dielectric function. The suitability of the algorithm to model device performance is finally demonstrated by successfully simulating the absorption within a solar cell device and comparing it to the measured external quantum efficiency as one possible application example.

2. Theoretical background

When light waves are incident on a semiconductor they interact with the atoms that constitute the crystal lattice. During this interaction photons may be absorbed upon excitation of electrons to previously unoccupied states. Photons also experience a delay because of the finite interaction time and continue to propagate with a lag. For an individual photon the probability and quantitative description of these processes are determined by quantum-field theoretical calculations. Considering a large number of photons, though, the complex index of refraction \( n(\lambda) = n(\lambda) + ik(\lambda) \) of a material, a function of the photon wavelength in vacuum \( \lambda \) or correspondingly the photon energy \( E = hc/\lambda \), is an appropriate quantity to describe the effects of light propagation through matter. Its real component \( n \) describes how the propagation speed of light \( c(\lambda) = c_0/n(\lambda) \) changes leading to diffraction and dispersion where \( c_0 \) is the speed of light in vacuum. The imaginary component \( k \) is a measure of absorption as defined by the attenuation factor

\[
\alpha(\lambda) = 4\pi k/\lambda. \tag{1}
\]

A simple but powerful approximation for the interactions between photons and electrons in a crystal is the assumption of a general oscillator \( A(E; a, \gamma, E_u) \). The oscillator is characterised by its strength given in terms of the amplitude \( a \), by its broadening in terms of the damping coefficient \( \gamma \) and by its spectral position in terms of the resonance frequency \( E_u = E_c/h \) where \( h \) is the Planck constant. The overall dielectric function \( \epsilon(E) = \epsilon_1 + i\epsilon_2 = \sum_{i=1}^{N} A_i(E) \) is thus the sum of a finite number \( N \) of general oscillators and can be used to calculate the refractive index using

\[
n = \sqrt{\frac{1}{2} \left( \sqrt{\epsilon_1^2 + \epsilon_2^2 + \epsilon_1} \right)}, \quad k = \sqrt{\frac{1}{2} \left( \sqrt{\epsilon_1^2 + \epsilon_2^2 - \epsilon_1} \right)}. \tag{2}
\]

There exist different models implementing the general oscillator idea which differ in some details [11]. The Cody-Lorentz oscillator model, developed by Ferlauto et al [12], extends the general oscillator approach by including a parameterisation of the absorption threshold or optical band gap \( E_g \) of a semiconductor and additionally accounting for an Urbach tail inside the band gap due to defect states close to the band edge. The Urbach tail is modelled by an exponential decay constant \( E_u \) and a starting energy \( E_c \). The dissipative or imaginary part of the Cody-Lorentz oscillator can be written as

\[
\text{Im} \left( \hat{A}_{\text{CL}}(E) \right) = \begin{cases} \frac{E - E_u}{E_c} \exp \left( \frac{E - E_u}{E_c} \right) G(E) L(E), & 0 < E \leq E_t \\ G(E) L(E), & E > E_t \end{cases} \tag{3}
\]

where the variable band edge function

\[
G(E) = \frac{(E - E_g)^2}{(E - E_g)^2 + E_p^2} \tag{4}
\]

features a weighting factor \( E_p \) between the Lorentz model, for \( E_p = 0 \), which is ignorant of the existence of a band gap, and
the total amount of parameters is given by

\[ L(E) = a E \gamma (E^2 - E_i^2) + \gamma^2 E_i^2. \] (5)

Once the imaginary part is analytically fixed for all photon energies, the real part can be readily obtained using the Kramers-Kronig relationship [13, 14]

\[
\text{Re}\left(\hat{\alpha}_{\text{CL}}(E)\right) = 1 + \frac{2}{\pi} \int_0^\infty \frac{E' \text{Im}\left(\hat{\alpha}_{\text{CL}}(E')\right)}{E'^2 - E^2} \, dE',
\] (6)

which ensures that the model is physically sensible. \( \text{P} \) denotes the Cauchy principal value of an integral.

Relations among physical entities are continuous multidimensional functions of certain control variables \( x \). This allows such relations to be approximated using a Taylor expansion around a point of interest \( x_0 \). In the case of III–V semiconductor alloys \( A_xB_{1-x} \) one can choose the control variable to be the composition of the alloy. This is not limited to ternary semiconductors such as AlGaAs with \( A = \text{Al} \) and \( B = \text{GaAs} \) but can also be extended to quaternary semiconductors such as GaInAsP lattice matched to GaAs with \( A = \text{Ga}_{0.51}\text{In}_{0.49}\text{P} \) and \( B = \text{GaAs} \). In general nothing is known about the compositional dependence of the entire general oscillator parameter set

\[ \text{P} = \{ \ldots, \rho_i(x), \ldots \} = \{ \ldots, a_i(x), \gamma_i(x), E_i(x), E_i, (x), \theta_i(x), \theta_i, (x), \ldots \}. \] (7)

What is known, though, is the variation of the band gap energy with composition. It is described by a simple relationship

\[ E_g(x) = xE^A_g + (1-x)E^B_g - x(1-x)C \] (8)

with an empirical bowing factor \( C \) which has been determined experimentally for many ternary and quaternary alloys [15–18].

3. Methods and materials

3.1. Morphing algorithm

The total amount of parameters \( p_i \) from a phenomenological oscillator model of a single material needed to satisfactorily describe its optical parameters is typically very high. The vast number of parameters and the exponential dependence of some of the parameters make a direct interpolation \( P(x) = (1-x)P(0) + xP(1) \) too prone to inaccuracies. As for the analytical CPPB models apart from the large number of free parameters and consequently the even larger number of input datasets, they require sound input knowledge for instance on the identity of the critical points e.g. from low-temperature electoreflectance measurements. While such models are advantageous for studying well established semiconductors such as GaAs or InP, it can become very challenging or even impossible to apply them to material systems for which the needed input data are not yet available.

The algorithm described here overcomes this problem by an empirical morphing scheme for which only the refractive indices and the dependence of the band gap energy on the material composition must be known. It is inspired by morphing methods from computer graphics [19]. Such algorithms are typically used to create animation sequences that provide a smooth transition e.g. from one human face to another. The idea is to identify several critical regions in the two input images and find a morphing function that transforms these regions from the first to the second image.

Here, these critical positions are identified with the features in the complex refractive index functions of the input materials corresponding to the critical points [20]. This process defines a morphing function, which allows to map the energy-dependent complex refractive index to any material composition that is in between the compositions of the starting materials.

The process flow of the morphing algorithm is sketched in figure 1. The spectrally dependent optical parameters are first split into intervals according to the positions of the critical points which are labelled \( \epsilon_i \) for the low-band gap endpoint material, e.g. GaAs, and \( E_i \) for the high-band gap endpoint material, e.g. \( \text{Ga}_{0.51}\text{In}_{0.49}\text{P} \). The critical points are given by the positions of absorption resonances, i.e. general oscillator peaks, and the band gap energies of the interpolated materials. An example is shown in figure 2 for the case of GaAs and \( \text{Ga}_{0.51}\text{In}_{0.49}\text{P} \). The critical features can occur in the real or in the imaginary part but in either case the so defined intervals are used for the interpolation of both parts. Then, a piecewise linear mapping function

\[ M_i(E) = \left( E_{i-1} + (E_i - E_{i-1}) \frac{E - E_{i-1}}{\epsilon_i - E_{i-1}} \right) \theta(E - E_{i-1}) \theta(\epsilon_i - E) \] (9)
between the endpoints GaAs and Al.

ternary and quaternary alloys. First, Al
to demonstrate the applicability of the method both for a reactor. Two material systems were investigated in order to phase epitaxy (MOVPE) on an AIX 2800G4-TM planet-

ary reactor. This end test structures were grown using metalorganic vapour phase epitaxy using the transfer matrix (TM) method. The morphed optical parameter sets were validated by com-

3.2. Samples and characterisation

Figure 2. The refractive index, shown here for GaAs and GaInP, as a function of photon energy features critical positions \( (e_i, E_i) \) both in its real and imaginary part. The energy mapping function \( M(E) \), c.f. equation (9), represented by the coloured arrows, projects the critical point energies of the low-band gap to the high-band gap material. These can be used for the definition of the morphing intervals.

is configured where \( \theta (x) \) is the Heaviside step function. This mapping fulfils the condition \( M(e_i) = E_i \) for all \( i \in \{0, \ldots, n\} \) and thus transforms the critical energies of the low- to the high-band gap material. In order to account for the non-linear dependence of the band gap energy on material composition given in equation (8), the composition parameter \( x \) is scaled according to

\[
x' = I(x) = \frac{E_E(x) - E_E(0)}{E_E(1) - E_E(0)}.
\]

Hence, the overall interpolation function \( \hat{n}(E, x) : [E_{min}, E_{max}] \times [0, 1] \rightarrow [\hat{n}_{min}, \hat{n}_{max}] \times C \) becomes

\[
\hat{n}(E, x) = (1 - I(x)) \left( \frac{E}{\hat{n}_0(E)} + I(x) \left( \frac{M(E)}{\hat{n}_1(M(E))} \right) \right)
\]

where \( \hat{n}_{0/1} \) are the complex refractive indices of the low- \( (x = 0) \) or the high-band gap material \( (x = 1) \), respectively.

3.2. Samples and characterisation

The morphed optical parameter sets were validated by comparison to measurements of corresponding III–V alloys. To this end test structures were grown using metalorganic vapour phase epitaxy (MOVPE) on an AIX 2800G4-TM planetary reactor. Two material systems were investigated in order to demonstrate the applicability of the method both for ternary and quaternary alloys. First, Al\(_{1-x}\)Ga\(_x\)As was morphed between the endpoints GaAs and Al\(_{0.49}\)Ga\(_{0.51}\)As and second, Ga\(_{1-x}\)In\(_x\)As\(_{1-y}\)P\(_y\) lattice matched to GaAs was morphed between GaAs and Ga\(_{0.51}\)In\(_{0.49}\)P. The experimental validation of the morphing algorithm is based on three different methods: direct measurement of the complex dielectric function, fitting of spectral ellipsometry data, and modelling of the external quantum efficiency and reflection of solar cell devices.

For AlGaAs a pn-junction test structure with a 2600 nm thick Al\(_{0.20}\)Ga\(_{0.80}\)As absorber was grown at a temperature of 640 °C and a V/III-ratio of 35. The Al-content was determined from an x-ray diffraction (XRD) rocking curve measurement. In the case of GaInAsP both double heterostructures with a 300 nm thick test layer and pn-junctions were grown at a temperature of 580 °C and a V/III-ratio of 25. The layer structures are shown in figure 3. This structure design allowed to determine the composition by combining measurements of the band gap energy and the out-of-plane lattice constant using spectral photoluminescence and XRD, respectively. The impact of strain on the band gap in these samples is considered by the application of the van-de-Walle formalism [21] and the ternary bowing parameters were taken from [22]. Different compositions resulting in band gaps of 1.50 eV, 1.61 eV, and 1.70 eV were investigated.

For the ellipsometry measurements the top barrier of the double heterostructures was selectively removed by wet chemical etching using hydrochloric acid. The measurements were then carried out on a J. A. Woolam M-2000F spectral ellipsometer at incidence angles of 65°, 70°, and 75°, which are in the range of the Brewster angle for the materials under investigation.

From the pn-junction samples simple solar cell devices without anti-reflection coating were processed. The reflection and external quantum efficiency (EQE) were measured in a pvtools LOANA Solar Cell Analysis System. It is expected for such high quality crystals, that the EQE matches closely the absorption in the pn-junction material. In other words, for materials with sufficient diffusion length, every absorbed photon also contributes to the photocurrent. Under this assumption, the measured EQE can be compared to the simulated absorption, which was calculated using the transfer matrix (TM) method [23]. The wavelength dependent absorption coefficient given by equation (1) is computed from the morphed optical parameter set.
4. Results

4.1. Optical parameters

The input optical parameters of GaAs [16, 24] and Al$_{0.49}$Ga$_{0.51}$As [4] were taken from literature. Using a bowing coefficient of 0.55 eV for the direct band gap [15], the morphing algorithm yields a dataset for Al$_{0.32}$Ga$_{0.68}$As that is shown in figure 4. Both the real part and the imaginary part of the morphed parameters agree well to the data determined directly by spectral ellipsometry [4]. The average relative deviation

$$\langle \Delta n_{\text{rel}} \rangle = \frac{1}{\lambda_f - \lambda_i} \int_{\lambda_i}^{\lambda_f} \frac{|n_{\text{meas}}(\lambda) - n_{\text{morph}}(\lambda)|}{n_{\text{meas}}(\lambda)} \, \mathrm{d}\lambda$$  \hspace{1cm} (12)$$

in the entire energy interval from 1.0 eV to 4.1 eV amounts to 0.5%. The integral was replaced by a sum for the calculation because of the discreteness of the measurement sampling points. The deviation may only reach up to 2% in the surrounding of the critical points at 1.8 eV, 3.0 eV and 3.5 eV. The average deviation compares very well with relative deviations between measurement and model obtained for analytical models. For example Zheng et al reported a 0.4% deviation for their semi-empirical model for the refractive index of GaAs in the much smaller range between 1.3 eV and 1.8 eV [25]. Similarly for $k$ the average relative deviations amount to 1.7% for photon energies above 1.85 eV. Approaching the band gap, the morphing algorithm overestimates the measurement and the average deviation diverges as $k$ approaches 0.

For GaInAsP lattice matched to GaAs the two chosen endpoint materials were GaAs and Ga$_{0.51}$In$_{0.49}$P since to our knowledge no optical parameter data from an intermediate composition is published. This fact required to make an assumption on the merging of critical points as there are two critical points around 3 eV in the real part of $n_{\text{GaAs}}$ while there is only one such point in $n_{\text{GaInP}}$. We chose the more dominant point to correspond to the remaining point in GaInP as indicated by the green arrow in figure 2. The direct band gap bowing factor for the interpolation between GaAs and Ga$_{0.51}$In$_{0.49}$P was taken to be $-0.62$ eV [15]. The morphing results are shown in figure 5.

4.2. Spectral ellipsometry

Due to the lack of known optical parameters for Ga$_{1-x}$In$_x$As$_{1-y}$P$_y$ lattice matched to GaAs, the morphed parameter set was used as input to model the results from spectral ellipsometry based on Maxwell’s equations. As can be seen from figure 6 it is indeed possible to describe both the magnitude $\tan(\Psi)$ and the phase $\Delta$ of the reflectivity ratio of p- and s-polarised light waves for all three compositions throughout the entire range of photon wavelengths. The results of the three different incidence angles are qualitatively the same.
so only the one for an incidence angle of 70° is shown representatively. For assessing the predictions of the morphed dataset for the ellipsometry measurement results, a forward calculation of $\Psi$ and $\Delta$ was performed with only taking the thicknesses of the bottom barrier, of the GaInAsP test layer, and of a thin native surface oxide layer as adjustable parameters. The mean squared error (MSE) increases from 11 to 20 when approaching the high-band gap endpoint but still stays below 25, a margin that is tolerable for ellipsometry data analysis of structures consisting of more than a single layer. The deviations are most prominent in regions where the oscillations in $\Psi$ and $\Delta$ are fastest. Despite a good overall agreement, these observations point out a shortcoming of the morphing algorithm if it is applied to endpoints that are far apart from each other in terms of composition and which have a different number of critical points. In such cases the combination of optical parameter morphing with general oscillator based modelling of the dielectric function is beneficial. In general the morphed dataset by itself does not obey the Kramers–Kronig relations. If however the dielectric function given by the morphed dataset is analytically described by a number of Cody–Lorentz oscillators, which are fitted to the morphed data, the resulting dataset will be Kramers–Kronig consistent by construction. Such an analytical model can then be fitted to the results obtained by spectral ellipsometry which will give a closer match to the real refractive index. Without morphing the dataset prior to the Cody–Lorentz fitting procedure, no sensible fit can be achieved because of the vast amount of fitting parameters and the large distance in parameter space between either of the endpoint materials and the composition of interest. Thanks to the morphing algorithm, the starting conditions of the fitting procedure are already initialised close to the desired local convergence point. Applying this procedure with four Cody-Lorentz oscillators to the data of the GaInAsP samples yields a significantly reduced MSE between 6 and 9 for all three compositions and a physically consistent dataset.

4.3. Application example: quantum efficiency of solar cells

As a third way to validate the suitability of the proposed morphing algorithm, its ability to describe solar cell characteristics was tested. To this end the measured EQE of a 550 nm thick Ga$_{0.92}$In$_{0.08}$As$_{0.66}$P$_{0.14}$ solar cell without anti-reflection coating are compared to the absorption (solid lines) and the reflection (dotted lines), respectively, as modelled by transfer matrix (TM) simulations using three different optical parameter datasets for the absorber layer.

![Figure 6. Phase angle (top) and magnitude angle (bottom) of the complex reflectivity ratio at an incidence angle of 70°. The results of the other incidence angles are not shown for the sake of clarity. The measured data for low (orange), medium (green), and high band gap (blue) are compared to the calculated curves which were based on the morphed parameter sets (solid black lines).](image)

![Figure 7. The measured external quantum efficiency (EQE, black dots) and reflection $R$ (black triangles) of a 550 nm thick Ga$_{0.92}$In$_{0.08}$As$_{0.66}$P$_{0.14}$ solar cell without anti-reflection coating are compared to the absorption (solid lines) and the reflection (dotted lines), respectively, as modelled by transfer matrix (TM) simulations using three different optical parameter datasets for the absorber layer.](image)
of the AlInP window rather than the GaInAsP absorber. The agreement of the measured and modelled reflection, however, is very good.

Also for the Al$_{0.20}$Ga$_{0.80}$As based solar cell the morphed parameter set is able to describe the measured reflection and EQE as can be seen in figure 8. There is a systematic deviation of around 1%$_{\rm abs}$ in the plateau region between the modelled absorption and the measured EQE. At wavelengths above 750 nm, the absorption edge of Al$_{0.20}$Ga$_{0.80}$As, photons are transmitted through the absorber layer and reflected at the interface to the GaAs substrate which results in interference fringes. These oscillations are not well resolved in the reflection measurement because of too scarce sampling.

5. Discussion

The optical parameter morphing algorithm presented in this paper does not claim to yield \textit{ab-initio} theoretically calculated complex refractive index datasets which may be prone to errors because of the amount of fit parameters they require. Its main purpose is to offer a quantitative, reliable, empirically motivated, and simple approximation to the refractive index of a material with complicated alloy composition. It was shown to accurately describe experimental results from spectral ellipsometry, absorption, and reflection measurements. The error that is introduced by the morphing algorithm is largest halfway in composition space between the two endpoint materials. The main sources of this error are inaccurate input datasets of the endpoint materials, imperfect modelling of the band gap dependence on composition for example by not well known bowing parameters or deviations from a quadratic behaviour, and the impact of effects which are not considered in the morphing routine such as strain or atomic ordering; tensile (compressive) in-plane strain results in a reduction (an increase) of the band gap and atomic ordering of the CuPt-type is known to reduce the band gap for instance in GaInP [26].

This interpolation method assumes a locally linear dependence of the dielectric function on the band gap energy. Here, local dependence means that the dependence is linear for every energy-value pair of the mapping sequence. In particular, if one endpoint material is an indirect semiconductor and the other component is a direct semiconductor, such as the combination (AlAs/GaAs), the dependence of the dielectric function on the composition may change strongly near the point where the semiconductor switches from direct to indirect. It is possible to resolve this issue if the redundant characteristic energies converge to a single point in the other material, as is e.g. the case for the transition from direct Al$_{x}$Ga$_{1-x}$As with $x < 0.45$ to indirect Al$_{x}$Ga$_{1-x}$As with $x > 0.45$. In such a case, equation (9) can be modified to accept a mapping to this convergence point by adding another case decision, which handles the situation of identical mapping points. In general it is advisable to use three material compositions, where the third composition is located near the transition point from direct to indirect semiconductor. In this case, two mapping sequences are used: one to map from the indirect material to the intermediate composition and the other one to map from the intermediate composition to the direct material.

Due to the purely mathematical approach, the algorithm is not limited to interpolating between different alloy compositions. The approach can also be used to interpolate optical constants between two different versions of a material such as from an atomically ordered to a disordered state or from a strained to an unstrained state. Modelling the optical properties of a material using only one parameter for variation allows for an easy integration into numerical optimisation algorithms. This makes it possible to model whole layer systems of widely unknown materials. Introducing additional boundary conditions, such as lattice constant or strain, it even enables the possibility to optimise the layer system with respect to these boundaries paving the way for experiments in entirely new material systems.

Further promising domains of application for this method are all material classes for which there is an equivalent to the band gap bowing parameter. Examples could include organic semiconductors, perovskites, and III-nitrides such as AlGaN or InGaN. Both have limited availability of $n$ and $k$ data for intermediate compositions. So far, in these material systems the optical parameters are modelled by a general oscillator approach for a specific sample using spectral ellipsometry measurements [27]. The long-wavelength limit of the refractive index can then be deduced from the respective model for a known band gap [28]. With the proposed morphing algorithm one saves a significant amount of development time since a targeted device structure can be simulated without producing a large number of test samples. The necessary precondition, though, is that the wavelength range of the two measured input datasets is wide enough to include a minimum of two to three critical points. These critical points must be mutually identifiable and simultaneously present so that the energy mapping function is well defined. More detailed results
for these new material systems may be included in a future publication.

6. Conclusion

We presented a method for a quick determination of optical parameters for a variety of compound semiconductors. The only input data needed are first, the wavelength dependence of the dielectric functions of two semiconductor compounds and second, the dependence of the band gap energy on composition between them. An energy mapping sequence is defined by critical points in the imaginary and real part of the refractive index function of both endpoint materials. The morphing algorithm transfers these features from one endpoint material to the other assuming that the composition dependence follows the non-linear relationship for the band gap energy. The morphing algorithm was validated for a ternary, Al$_x$Ga$_{1-x}$As, and a quaternary, Ga$_{1-x}$In$_x$As$_1$P$_y$, material system. The experimental validation was done by comparing the interpolated datasets for Al$_{0.32}$Ga$_{0.68}$As with corresponding measurements of a test sample and predicting the results of spectral ellipsometry, EQE, and reflection measurements of Al$_{0.20}$Ga$_{0.80}$As and various GaInAsP samples.

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