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OPTICAL PROPERTIES OF 3C-SiC/Si (001)

A Thesis
Submitted to the School of Graduate Studies and Research
in Partial Fulfillment of the
Requirements for the Degree
Master of Science

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May 2013
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With the continuous development of new optical materials using various experimental methods the need to find a way to characterize what a particular material is cost effectively becomes eminent. The most effective way to truncate cost is to have the ability to characterize materials nondestructively.

For the manufacturing requirement of semiconductor materials there needs to be significant agreement to characterize the samples. For this to be fulfilled theoretical representations must be developed and utilized in combination with concise experimental data. The reflectance data for the above mentioned FTIR measurements can be rendered using effective medium theory approximations.

In this thesis we will present the necessary background and utilize effective medium approximations to match experimental data. This work will also include several other theoretical tools to model reflectance data which include and is not limited to: interface roughness corrections, surface roughness corrections and sample thickness consideration.
ACKNOWLEDGMENTS

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CHAPTER I

INTRODUCTION

1-1 Historical Introduction of Semiconductors

Since the early foundations of human history our species has had the intellectual capacity to utilize the material resources contained within our environment. This trait is the catalyst that caused our species to form societies and develop new and better suited technologies and innovations. Over the course of time we have further utilized material constructs to gain more of an advantage for our race and society. With this ongoing evolution of innovation we have begun to construct tailored materials with specific properties one such material development is that of the field of semiconductors.

The characterization of elements according to their chemical properties created the pathway to the development of grouping different elements according to their common observed properties. This element grouping lead Chemist Dmitri Mendeleev to develop the periodic table which provided a useful piece of information, though not fully understood at that time, the atomic number. With the further development of the understanding of protons and electrons the periodic table became a useful tool distinguishing elements according to the number of electrons in the outmost electron shell. The growing classifications of materials gave rise to two predominant material classifications conductors and insulators.

The first material type that possessed the property to conductor both heat and electricity with ease and was justly named conductor. These metallic substances when in bulk lose their outer shell of electrons causing a cloud or sea of flowing electrons which leads to the aforementioned ability of high heat and electrical conductivity. With
properties that differ greatly from metals, nonmetals conduct heat and electricity very poorly and are often referred to as insulators. With the material distinctions well known the materials innate ability to oppose the flow of an electron, or resistivity, was tabulated for the two groupings of elements. Metallic substances have low resistivity whereas nonmetallic substances generally having high values, it became apparent that there existed a group of materials that had an intermediate value of resistivity being between the low values for metals and the high values for nonmetals. This new material also exhibited the property of resistivity going down with an increase in temperature opposing the general trend found with metallic substances. With this unique property these substances were termed semiconductors. Though this dated definition gives little insight into the chemical nature of semiconductors it provided this material type its own distinct footing in the scientific world.10,11

1-2 Band State Definition of Semiconductors

Wolfgang Pauli’s exclusion principle explained among other things that two fermions, particles with half integer spin, such as electrons cannon occupy the same quantum state at the same time. This gave rise to the understanding of the electric shells in atoms and bonding between two atoms sharing electrons. Having paramount importance to the field of semiconductor physics this principle dictates the interaction between the electrons within the same atom, which gives rise to the discrete allowed energy states. The combination of these available energy states leads to the formation of energy bands within a solid material consisting of many atoms. The first energy band is the valance band which is the highest electron energy range that is normally present at
absolute zero. The electrons that occupy the valance band are considered bound to individual atoms. The next energy band of which electrons may occupy is called the conduction band which is the range of energies where the election is free of any individual atom and possesses the ability to freely move within the atomic lattice.\footnote{11}

The conditions laid by the Pauli Exclusion Principle dictate that there is a region where no electron states can exist called the band gap. The transition of the band gap is physically equivalent to an electron moving from the outermost electron shell to be a free charge carrier. This mobile charge caring election is free to move about the solid material greatly contributing to the thermal and electrical conductivity of the material. The band gap theory of solid materials gives clear insight of the difference between conductors, semiconductors and nonconductors. The materials can be understood by the energetic size of the gap between the valance and conduction bands. In metallic materials there is an overlap between the two bands giving rise to a large number of mobile carriers at room temperature leading to the conducting nature. For nonmetal materials there is a large band gap at room temperature requiring a large temperature increase for these materials to possess electrons within the conduction band giving rise to the insulating nature. For semiconductor materials there exists a very small band gap in the order of magnitude for thermal excitations caused by small temperature increases to be significant. The band gaps of these three material types are illustrated in Figure 1-1 below.\footnote{10}
Figure 1-1. Three possible band structures for a solid. The first structure is a conductor because the allowed bands overlap. The Insulator structure has a forbidden band with a large energy gap between the filled band and the next allowed band. The Semiconductor band structure has an energy gap that is very small, so that electrons may be excited to the conduction band at normal temperature.

The development of band theory and subsequent understanding of the implications of a material with a small band gap paved the way for the birth of semiconductor physics.

1-3 Semiconductor Classifications

Within the field of semiconductor physics there is several ways that semiconductors may be classified. One such classification is by the nature of the current carriers. The first type of this classification is ionic semiconductors where the conduction takes place through the movement of ions by mass transport. The second subtype is electronic where the current is carried by electrons and no mass transport is necessary.
For the focus of this study the following way of classification is of greater importance which is by the relationship of the elements that comprise the semiconductors. One subtype is Elemental having the composition of atoms consist of one element type such as bulk Silicon. The other being compound semiconductors whereby the semiconductor is comprised of two or more different element types. An additional way of classifying semiconductors is by their structure. There are several subdivisions within the structure classification such as the following: amorphous, polycrystalline, or single crystal. The areas of semiconductor classification are quite robust and are covered in detail in other works and additionally do not provide enough insight into this study to warrant a detailed divulging into this subject.

Development of new hardy microelectronic mechanical systems utilizable in a wide variety of applications has been an area of great interest to physicists researching in the field of semiconductor physics. One material that possesses the ability to maintain high operating temperature as well as chemical inertness is silicon carbide.

Silicon carbide is a non-oxide ceramic with numerous industrial applications. The desirable material properties that silicon carbide possesses are: high strength and hardness, thermal and chemical stability, high melting point, oxidations resistance, high erosion resistance and various other properties. The previously mentioned properties make SiC useful for high power, high temperature electronic device. Silicon carbide has over 200 different polytypes, different possible stacking arrangements. One of the most useful forms of Silicon carbide is 3C-SiC, or β–SiC, being the only silicon carbide polytype having the diamond-like Zinc-blend Structure.
With the advancements in the field and success of deposition methods of 3C-SiC accurate cheap nondestructive characterization techniques of these samples becomes necessary. One such method of nondestructive material characterization is by the use of Infrared reflectivity spectroscopy.\textsuperscript{11}

\textbf{1-4 Fourier Transform Spectroscopy}

Through the utilization of a system consisting of a Michelson Interferometer and then applying Fourier optical techniques to the resulting data the reflection and transmission data of a film sample can be obtained. The basics of a Michelson Interferometer in the use of a Fourier Transform Infrared Spectrometer are shown in Figure 1-2 and explained below.

Light from an external source is collimated and directed to a beam splitter represented by the teal path. The beam splitter divides the wave into two optical paths by reflecting half of the incident light and transmitting the remaining light shown by the red paths. The transmitted path travels toward a fixed mirror and is subsequently reflected (Green path) back to the beam splitter where it undergoes additional splitting and is noted by the blue path. The reflected beam goes through the sample and on to the detector, while the transmitted path goes back toward the source.
Figure 1-2. Schematic of a Michelson Interferometer with beam interactions (transmission or reflection) denoted by a color change.

In the other side of the interferometer the initially reflected beam is reflected by a mirror with an adjustable optical path length. The light green light beam that is reflected by the moveable mirror is returned to the beam splitter and undergoes additional splitting. The transmitted component of this split beam propagates through the sample and goes to the detector. It should be noted that the light of the source may be incoherent, when split
into two components by the beam splitter the component parts of the beam are coherent and can produce an interference pattern when combined.\(^6\)

The light intensity that reaches the detector is the sum of the two beams. When the optical paths are equal the beams are in phase. With the adjustment of the location of the moveable mirror which changes the optical path length of that side the optical path length difference \(L_i\) is induced. When the adjustable mirror is moved a distance \(L_{am}\) the optical path distance \(L_i\) becomes \(2*L_{am}\) due to the light beam having to travel an additional path length to the mirror and the same distance to reach the beam splitter. The series of maxima and minima makes up the interferogram. The optical response of the sample is the piece of information that is useful using this technique and can be obtained by taking a Fourier transform of the interferogram.

1-5 Raman Spectroscopy

Raman spectroscopy is based upon the Raman scattering. When a light beam is scattered from the surface of a sample most of the scattered light is scattered elastically where it retains the same wavelength. A small distribution of the scattered light is scattered in-elastically due to interactions with the matter. The interaction of the incident light with acoustical phonons results in what is called Brillouin scattering and the interaction with optical phonons is termed Raman Scattering. If the incident photon gives part of its energy to the lattice in the form of a phonon it emerges as a lower energy photon. The lower energy shifted photon process is called stokes scattering. When the photon receives energy from the lattice the process is called anti-stokes scattering. For Raman spectroscopy measurements a laser beam is used to produce the incident light on
the sample. The scattered light is then passed through a double monochromator and the
shifted wavelengths are detected by a photo-detector. With the use of lasers with different
wavelengths and absorption depths the sample can be probed to some depth.

In semiconductor materials the phonon modes that are involved in the scattering
process are referred as Raman active modes. For crystals that possess inversion symmetry
such as diamond structured materials infrared active modes are not Raman active. For
crystals lacking inversion symmetry transverse optical (TO) modes may be both Raman
and IR active thus being observable in both the scattering process and infrared
absorption. 3C-SiC having zinc-blend structure does not have inversion symmetry due to
different bond lengths for the two interpenetrated Face centered cubic (FCC) lattices.
With sufficiently high resolution the acoustic modes may be also be observable. This
allows Raman spectroscopy to probe information not obtainable by Fourier transform
infrared spectroscopy measurements. Therefore this technique can give information about
the TO, TA, LO, LA modes at the center of the Brillouin zone. Unlike the use of FTIR
Spectroscopy which is limited by dipole effects Raman spectroscopy effects have basis in
polarization effects and can see features inherit of nonlinear dielectric materials.6
CHAPTER II

BASIC THEORETICAL BACKGROUND

2-1 Dielectric Function Theoretical basis

For understanding the reflectance experimental data presented and theoretically modeled in the results of this thesis the following basic principles and derivation of the complex dielectric function or relative permittivity will be presented.

For nonmetallic substances the presence of an electric field will have an interaction on both the positive and negative charges held in each atom. This interaction has an impact on the charge distribution of the atoms. To give a simple example we may consider two diatomic-ally bound charge neutral atoms placed into a uniform electric field. With the contemporary model of the atom it is known that there will be a positively charged nucleus region as well as a negatively charged electron distribution cloud. The force applied by the field upon the charges acts as,

\[ \vec{F} = q \vec{E} \] (2.1)

The force will therefore push the nucleus in the direction of the field and shift the electron distribution cloud opposite of the direction of the applied field as illustrated in Figure 2-1.
Figure 2-1. Force on electron distribution cloud and nucleus of an atom in an electric field

With the Coulomb attraction between the two charges still effective the total system will soon reach equilibrium as long as the field strength is not so great as to overpower this attractive force and cause the atom to ionize. The net effect will be that the atom is polarized with the charges being lightly shifted in opposite directions leaving the atom with a dipole moment. The dipole moment will have a direct proportionality with the electromagnetic wave passing through the medium. The dipole is given in the following form \(^3\),

\[ \vec{\rho} = \alpha \vec{E} \]  

(2.2)

The proportionally term \( \alpha \) is the atomic polarizability which depends upon the atomic structure. For molecular systems with strong degrees of asymmetries the polarization is more complicated due to the likely hood that there will be a preferential direction of polarization. If the field is applied at some angle to the axis the dipole moment can be broken down into perpendicular and parallel components in the following form,
\[ P = \alpha_s \vec{E}_s + \alpha_p \vec{E}_p \]  \hspace{1cm} (2.3)

For molecules lacking symmetry simplifications the polarizability becomes a tensor of rank two with nine components.

For a large number of materials considered the polarization of the material is linearly proportional to the electromagnetic field passing through the material. Such materials are called linear dielectrics and the equation for Polarization of these materials takes the following form,

\[ \vec{P} = \varepsilon_0 \chi_e \vec{E} \]  \hspace{1cm} (2.4)

It should be noted that for this linear dielectric equation that the electric field is the total field which may encompass contributions from free charges and the polarization itself. The factor, \( \chi_e \), in equation 2.4 is the electric susceptibility which depends upon the microscopic structure of the material. To correctly consider this system the electric displacement, \( \mathbf{D} \), needs to be introduced.

The effect of polarization produces accumulations of bound charges in the form of the following equation,

\[ -\nabla \cdot \vec{P} = \rho_b \]  \hspace{1cm} (2.5)

In the above equation the density of bound charges, \( \rho_b \), is equal to the negative change of the polarization in space. That is to say that the change in polarization throughout a material gives rise to an accumulation of bound charges. Utilizing Maxwell’s first equation which is the relationship between the distribution of total charge and the change of the field as follows,

\[ \nabla \cdot \vec{E} = \frac{1}{\varepsilon_0} \ast \rho_t \]  \hspace{1cm} (2.6)
For the above equation the total charge is defined as the sum of the free and bound charges and is expressed as follows,

\[ \rho_t = \rho_f + \rho_b \]  

(2.7)

When the above is combined with equation 2.5 the expression becomes,

\[ \rho_f + \rho_b = -\nabla \cdot P + \rho_f \]  

(2.8)

By replacing the total charge in Maxwell’s equation by the above the following equation is obtained,

\[ \varepsilon \nabla \cdot E + \nabla \cdot P = \rho_f \]  

(2.9)

By combining the two divergence terms the following expression is obtained,

\[ \nabla (\varepsilon \hat{E} + \hat{P}) = \rho_f \]  

(2.10)

The term inside the divergence is the electric displacement which is a vector that represents the part of an electric field associated with the presence of separated free electric charges. The electric displacement vector is given in the following form,

\[ \vec{D} = \varepsilon \hat{E} + \hat{P} \]  

(2.11)

Using the definition of polarization as noted above combined into the expression for the electric displacement yields the following expression relating the electric displacement directly to the electric field.

\[ \vec{D} = \varepsilon \hat{E} + \hat{P} = \varepsilon \hat{E} + \varepsilon \chi \hat{E} \]  

(2.12)

Taking the permittivity of free space and the electric field common the above expression reduces to,

\[ \vec{D} = \varepsilon (1 + \chi) \hat{E} \]  

(2.13)

With the quantity of proportionality between the displacement and the electric field being the permittivity of the material, \( \varepsilon \), removing the permittivity of free space
from the permittivity expression yields the dielectric, or relative permittivity which has the tremendous advantage of being a dimensionless quantity. The dielectric and relative dielectric are expressed as follows,

\[ \varepsilon = \varepsilon_0 (1 + \chi) \]  

(2.14)

\[ \varepsilon_r = (1 + \chi) \]  

(2.15)

In a medium the propagation of an electromagnetic wave is dictated by three properties of the material: the permittivity, the permeability, and the conductivity. These parameters each have dependency upon the frequency of the propagating waves being considered. To gain better insight into the behavior of these properties a simple example of a wave propagating through a medium is considered.

With the consideration of an incident periodic wave in a dispersive medium each frequency will correspond to a separate speed within the medium. If a point is imagined associated with a particular frequency moving along the wave the velocity at which this point moves is given in the following form,

\[ u = \lambda f \]  

(2.16)

Given the definition of wavenumber as the number of waves existing in a given region of space the following equation can be written in terms of the wavelength,

\[ k = \frac{2\pi}{\lambda} \]  

(2.17)

With a minor adjustment the wavelength can be written terms of the wavenumber for convenience as follows,

\[ \lambda = \frac{2\pi}{k} \]  

(2.18)

While using the angular frequency given as,
\[ \omega = 2\pi f \] 

Equations 2.18 and 2.19 can be taken into the velocity equation 2.16 for the wave creating the following result for the phase velocity,

\[ v = \frac{\omega}{k} \] 

The above velocity equation is the velocity at which the crests and trough of the wave move and is termed the phase velocity.\(^3\)

For non-conducting materials the electrons are effectively bound to specific molecules. To understand and consider this system a model with the binding forces between the electrons and nucleus can be approximated as a simple spring with a force constant of \( k \) in this case the angular frequency is given by the following equation,

\[ \omega = \sqrt{\frac{k}{m}} \] 

The general force for a spring is given by the displacement from equilibrium multiplied by the spring rigidity factor. Taking the spring constant and rearranging in terms of the angular frequency leaves the binding force as follows,

\[ F_b = -m\omega^2x \] 

Where \( x \) is the displacement the spring stretches from its equilibrium position. As the electron moves toward or away from the nucleus, it will be pushed or pulled toward its equilibrium position.

To show that most chosen forces of binding can be approximated in this away as long as the displacement from equilibrium is sufficiently small the following mathematical illustration will be conducted. Taking the potential energy for the spring as
\[ U = U(x) \]  

(2.23)

By taking the Taylor expansion of the potential about the equilibrium position where the displacement is equal to zero yields the following form,

\[ U(x) \cong U(0) + xU'(0) + \frac{1}{2}x^2U''(0) + \ldots \]  

(2.24)

Since the potential energy is a relative quantity the first term in the above expression can be chosen to be zero resulting in elimination. The second term yields the force from that the first derivative of the potential is equal to the negative force, and given that the force on an object at equilibrium is zero, this term vanishes. That leads to the above equation having just the third and higher terms left looking as follows,

\[ U(x) \cong \frac{1}{2}x^2U''(0) + \frac{1}{6}x^3U'''(0) \]  

(2.25)

The third term can be recognized as the potential energy of a spring with force constant equal to the second derivative of the potential at the equilibrium point. When displacements from equilibrium are sufficiently small the higher order terms will vanish. Most binding forces can be approximated as springs for small displacements about the equilibrium position.3

The following calculations can be conducted with or without a damping force but the damping term plays a significant role in theatrical modeling of dielectric functions affording them due consideration. The damping force on the electrons will be chosen to be proportional to the velocity but also opposes the electrons motion and therefore has the following form,

\[ F_{damp} = -m\gamma \frac{dx}{dt} \]  

(2.26)

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An incident electromagnetic wave interacting through the medium with frequency \( \omega \) oriented along the x direction will create a driving force upon the electrons according to the Lorenz force law. The equation of the incident wave and the resultant driving force are as follows,

\[
E = E_0 e^{-i\omega t} \tag{2.27}
\]

\[
F = q \left[ \vec{E} + (\vec{V} \times \vec{B}) \right] \tag{2.28}
\]

The second term in the Lorentz force law equation will go to zero for the considerations of this calculation due to then relative minor contribution of the magnetic field. The combination of equation 2.17 with equation 2.28 gives the following driving force on the electrons,

\[
F_{drive} = qE_0 e^{-i\omega t} \tag{2.29}
\]

By using newton’s second law the individual forces can now be summed yielding the following expression,

\[
F_{total} = F_{drive} + F_{binding} + F_{damp} \tag{2.30}
\]

\[
m \frac{d^2 x}{dt^2} = qE_0 e^{-i\omega t} - m\omega^2 x - my \frac{dx}{dt} \tag{2.31}
\]

The steady state solution determined by the driving force take the following form.

\[
\ddot{x}(t) = \ddot{x}_0 e^{-i\omega t} \tag{2.32}
\]

With the appropriate derivatives plugged into the equation of motion the expression for the displacement becomes,

\[
\ddot{x}_0 = \frac{q}{m} \frac{E_0}{\omega_0^2 - \omega^2 - i\gamma \omega} \tag{2.33}
\]

With the dipole moment as the product of magnitude of charge and the displacement of separation between the charges the following relation can be expressed,
\[ \tilde{\rho} = q \tilde{x}(t) = q \tilde{x}_0 e^{-i \omega t} = \frac{q^2}{m} E_0 e^{-i \omega t} \omega_0^2 - \omega^2 - i \gamma \omega \]  

(2.34)

As the number of molecules increase the sum of all the dipole moments becomes the polarization. With the total number of molecules per unit volume as \( N \) and with \( f_j \) as the total electrons the complex polarization becomes,

\[ \tilde{P} = N \frac{q^2}{m} \left( \sum_j \frac{f_j}{\omega_j^2 - \omega^2 - i \gamma_j \omega} \right) E \]  

(2.35)

By using the complex susceptibility as the proportionally between the Polarization and the Electromagnetic field and the previous equation 2.15 for the relative dielectric constant we arrive at the following expression for the complex dielectric constant,

\[ \varepsilon_r = 1 + N \frac{q^2}{m \varepsilon_0} \left( \sum_j \frac{f_j}{\omega_j^2 - \omega^2 - i \gamma_j \omega} \right) \]  

(2.36)

Though it may be disregarded in some materials the imagery component of the polarization equation is of great importance in the optical modeling of semiconductor films and will be treated appropriately.3, 4

For dispersive mediums the wave equation for a given frequency is given as follows

\[ \nabla^2 \tilde{E} = \varepsilon_\mu_0 \frac{\partial^2 \tilde{E}}{\partial t^2} \]  

(2.37)

With plane wave solutions of the following form,

\[ \tilde{E}(y, t) = \tilde{E}_0 e^{i (k y - \omega t)} \]  

(2.38)

And the complex wave number as,

\[ k = \sqrt{\varepsilon_\mu \omega} \]  

(2.39)
The complex wavenumber can be expressed as the summation of its real and imaginary components,
\[ \tilde{k} = k + ik \] (2.40)

Equation 2.38 becomes
\[ \tilde{E}(y, t) = \tilde{E}_0 e^{-ky} e^{i(ky - \omega t)} \] (2.41)

From the preceding equation it is apparent that the wave is damped. This damping absorbs energy as the wave travels through the medium leading the intensity of the incident light to be of importance. The relation between intensity and the field is given by the poynting vector and is proportional to the field squared. By squaring the magnitude of both sides of equation 2.41 the following expression in terms of intensity forms,
\[ I = I_0 e^{-\alpha y} \] (2.42)

The amount of energy absorbed by the medium as the light wave propagates through will result from the exponent term of exponential expression giving the absorption coefficient equal to 2k.
\[ \alpha = 2k \] (2.43)

With the wave velocity of the incident wave as the phase velocity found in equation 2.20 being equal to the speed of light over the refractive index the equation rearranges to,
\[ n = \frac{ck}{\omega} \] (2.44)

Rearranging equation 2.39 in terms of k gives the following form after using a binomial expansion in the form of,
\[ \sqrt{1 + x} \cong 1 + \frac{x}{2} \] (2.45)
\[ \vec{k} \approx \frac{\omega}{c} \left[ 1 + N \frac{q^2}{2m \varepsilon_0} \left( \sum_j \frac{f_j}{\omega_j^2 - \omega^2 - i\gamma_j\omega} \right) \right] \]  

(2.46)

Finally with the relations for the index of refraction and absorption coefficient coupled with what is found for \( k \) gives the following expressions,

\[ n \approx 1 + N \frac{q^2}{2m \varepsilon_0} \left( \sum_j \frac{f_j(\omega_j^2 - \omega^2)}{\left(\omega_j^2 - \omega^2\right)^2 + (\gamma_j\omega)^2} \right) \]  

(2.47)

\[ \alpha \approx N \frac{q^2 \omega^2}{m \varepsilon_0 c} \left( \sum_j \frac{f_j \gamma_j}{\left(\omega_j^2 - \omega^2\right)^2 + (\gamma_j\omega)^2} \right) \]  

(2.48)

Alternatively from equation 2.34 with considering \( N \) as contributing electrons per units volume the polarization becomes,

\[ \vec{P} \approx \frac{Nq^2}{m} \left( \frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega} \right) \]  

(2.49)

The electric susceptibility can be written as the difference between the permittivity\(^1\) of a material and the vacuum permittivity or,

\[ \vec{P} = (\varepsilon - \varepsilon_0)\vec{E} \]  

(2.50)

Rearranging equation 2.50 the permittivity can be expressed as,

\[ \varepsilon = \varepsilon_0 + \frac{\vec{P}}{\vec{E}} \]  

(2.51)

\[ \varepsilon = \varepsilon_0 + \frac{Nq^2}{m} \left( \frac{1}{\omega_j^2 - \omega^2 - i\gamma\omega} \right) \]  

(2.52)

The application of Maxwell’s relation the following dispersion equation comes about,

\[ n^2(\omega) = 1 + \frac{Nq^2}{\varepsilon_0 m} \left( \frac{1}{\omega_j^2 - \omega^2 - i\gamma\omega} \right) \]  

(2.53)
For the limits of long wavenumber and negligible bound electron contribution, $\gamma$, equation 2.53 reduces to,

$$n^2(\omega) = 1 - \frac{Nq^2/\varepsilon_0 m}{1 - \left(\frac{1}{\omega^2}\right)}$$

(2.54)

The numerator expression in equation 2.54 has the same dimensions as the square of the angular frequency and represents the Plasmon frequency.\(^4\,5\) The Plasmon frequency is the collective oscillations of the electron density of the electron cloud. The Plasmon frequency due to free carries within semiconductor is often expressed as,

$$\omega_p^2 = \frac{4\pi Nq^2}{\varepsilon_\infty m^*}$$

(2.55)

The free-carrier damping constant is expressed as $\gamma$ and is related to the carrier mobility.

### 2-2 Dispersion Relation

Much like the plasmons being a result of the oscillations of the electron gas density there are quantum oscillations associated with the ionic oscillations. As a consequence of the much greater mass of the protons, the ionic movement is restricted to small oscillations about an equilibrium position. These collective excitations of the lattice are termed phonons. The phonons within the lattice play the predominate role in the determination of thermal properties of materials.\(^3\,5\)

To build the necessary theoretical framework to fully understand the reflectivity theoretical models and formulate a connection to observed experimental data a derivation of the phonon complex dielectric function will be conducted with the necessary connection to the dispersion relation. The dispersion curves yield the guiding material specific features of the optical-phonon branch and acoustical-phonon dispersion.
A one dimensional arrangement of two atoms types with intermittent masses of $M_1$ and $M_2$. The atoms are indexed starting from the center atom in the figure denoted as the $j^{th}$ atom and extends in both directions indefinitely. The masses are bound by massless connecting springs obeying hooks law. For this model only nearest neighbor interactions will be considered. The separation between two adjacent atoms, $a$, is the interatomic distance. For this case as an illustrating derivation the motion of the atomic masses will behave as harmonic motion neglecting any anharmonic terms that may indeed exist in any real system. Consequence of the harmonic condition the system will oscillate with constant angular frequency and amplitude.\textsuperscript{5}

For the separation the force will be positive for the atom when it is further away than the interatomic separation as the system will tend to reestablish equilibrium and likewise negative for when the distance between the atom and its established equilibrium position is less this separation. The force on the ion will always be pushing it toward its equilibrium position. Utilizing that the potential is equal to the negative integral of the force following equations for the force and potential are obtained,

\[
F = -kx \quad \quad (2.56)
\]

\[
V = -\int -kx \, dx = \frac{1}{2}kx^2 \quad \quad (2.57)
\]

The value for the separation for atoms from their equilibrium position as $x_j$ and placing this into equation 2.57 will yield the following general expression for the potential energy for a given $j^{th}$ and $(j+1)^{th}$ atom pair as,

\[
V = \frac{1}{2}k(x_j - x_{j-1})^2 \quad \quad (2.58)
\]
To find the potential for a system of N atoms the preceding equation 2.49 is summed over j atoms.

\[ V = \frac{1}{2} k \sum_{j=1}^{N} (x_j - x_{j-1})^2 \]  

(2.59)

And the total kinetic energy of the system will be expressed as follows,

\[ T = \frac{1}{2} \sum_{j=1}^{N} \frac{p_j^2}{2M_j} \]  

(2.60)

The Lagrangian of the system is as follows:

\[ L = T - V = \frac{1}{2} k \sum_{j=1}^{N} (x_j - x_{j-1})^2 - \frac{1}{2} \sum_{i=1}^{N} \frac{p_i^2}{2M_i} \]  

(2.61)

Using the Euler-Lagrangian relation the equation of motion can be determined in the following way. First the expression is greatly simplified if the condition of nearest neighbor interactions is applied here. Since the atom at lattice position j has two interaction one from the atoms on each side resulting in the Lagrangian for the jth atom taking on the following form.

\[ L_j = T - V = \frac{1}{2} k (x_j - x_{j-1})^2 + k (x_{j+1} - x_j)^2 - \frac{p_j^2}{2M_j} \]  

(2.62)

With the Euler-Lagrangian equation taking the form as follows a few relations will also need to be noted,

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_j} \right) - \frac{\partial L}{\partial x_j} = 0 \]  

(2.63)

The momentum is equal to the mass times the velocity or the mass times the change in displacement over time yields the following expression for kinetic energy.
\[ T = \frac{(M_j \dot{x}_j)^2}{2M_j} \]  

(2.64)

With the separation from equilibrium being noted as \( x \) the Lagrangian takes on the following form,

\[ L_i = T - V = \frac{1}{2} k(x)^2 + k(x)^2 - \frac{(M_j \dot{x}_j)^2}{2M_j} \]  

(2.65)

Since the derivative is with respect to \( x_j \) the second term undergoes a sign change when applying the chain rule giving,

\[ \frac{dL}{dx_j} = k(x_j - x_{j-1}) - k(x_{j+1} - x_j) \]  

(2.66)

Since the only term that possess dependency on the change in displacement with respect to time is the kinetic energy, \( V \), the first term in equation 2.65 for the equation of motion become as follows,

\[ \frac{\partial L}{\partial \dot{x}_j} = M_j \dot{x}_j \]  

(2.67)

Now taking the derivative with respect to time the expression becomes

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_j} \right) = M_j \ddot{x} \]  

(2.68)

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_j} \right) = M_j \left( \frac{\partial^2 x_j}{\partial^2 T} \right) \]  

(2.69)

\[-M_j \ddot{x} + k(x_j - x_{j-1}) - k(x_{j+1} - x_j) = 0 \]  

(2.70)

\[ M_j \ddot{x} = -k(x_j - x_{j-1}) + k(x_{j+1} - x_j) \]  

(2.71)

And the resultant equation of motion for the \( j^{th} \) atom takes on the following form.

\[ M_j \ddot{x}_j = -k(2x_j - x_{j-1} - x_{j+1}) \]  

(2.72)

Likewise the \((j+1)^{th}\) atom takes the same similar form as
\[ M_{j+1} \ddot{x}_{j+1} = -k(2x_{j+1} - x_j - x_{j+2}) \]  

(2.73)

The general solution to this differential equation will be in Pfaffian form. In this case in particular the derivative and second derivative will produce the necessary constant terms in front of the original function. For this task the exponential function can be chosen and the equations for \( x_i \) and \( x_{i+1} \) are as follows,

\[
    x_j = Ae^{i(\omega t - kna)}
\]

(2.74)

\[
    x_{j+1} = Be^{i(\omega t - k(n+1)a)}
\]

(2.75)

By rearranging the exponential terms for \( x_{j+1} \) and applying the product of powers property of exponents the equation becomes.

\[
    X_{j+1} = Be^{i(\omega t - kna - ka)} = Be^{i(\omega t - kna)}e^{-ika}
\]

(2.76)

In the same fashion the above equation was determined \( x_{j-1} \) and \( x_{j+2} \) are also found and listed below.

\[
    X_{j-1} = Be^{i(\omega t - kna + ka)} = Be^{i(\omega t - kna)}e^{ika}
\]

(2.77)

\[
    X_{j+2} = Be^{i(\omega t - kna + 2ka)} = Be^{i(\omega t - kna)}e^{-2ika}
\]

(2.78)

Substituting the above equations for \( x_{j-1}, x_j, x_{j+1}, \) and \( x_{j+2} \) into the equations of motion for the \( M_2 \) and \( M_2 \) atoms generates the following expressions for the equations of motion,

\[
    -M_1 \omega^2 A = k(Be^{-ika} + Be^{ika} - 2A)
\]

(2.79)

\[
    -M_2 \omega^2 Be^{-ika} = k(Ae^{-2ika} - 2Be^{-ika} + A)
\]

(2.80)

For equation 2.70 by rearranging terms with like amplitudes and utilizing that the definition of cosine in the form of exponentials as

\[
    \frac{e^{-ika} + e^{ika}}{2} = \cos ka,
\]

(2.81)

The first expression becomes,
Likewise if the equation for the second mass is multiplied by a factor of $e^{ika}$ a similar rearrangement can be made by using the alternate cosine form.

$$2k\cos(ka)A + (2k - M_2\omega^2)B = 0$$

This system of equations can be solved through direct substitution or by using linear algebra either case yields the following equation,

$$M_1M_2\omega^4 - 2kM_1\omega^2 - 2kM_2\omega^2 + 4k^2 - 4k^2\sin^2(ka) = 0$$

The equation further reduces with some minor rearrangements to yield the following equation,

$$\omega^4 - \frac{2k(M_1 + M_2)\omega^2}{M_1M_2} + \frac{4k^2\sin^2(ka)}{M_1M_2} = 0$$

Applying the quadratic equation to the above expression and solving for $\omega^2$ gives the following two expressions,

$$\omega^2(k) = \frac{k(M_1 + M_2)}{M_1M_2} \left[ 1 \pm \sqrt{1 - \frac{M_1M_2\sin^2(ka)}{(M_1 + M_2)^2}} \right]$$

The above equation is the phonon dispersion relation. The upper band as the wavenumber approaches zero is the optical-phonon branch, while the lower branch is the acoustic-phonon branch. 

2-3 Superlattices and Phonon Folding

A superlattice (SL) is a large one-dimensional periodicity imposed on a monocrystalline semiconductor from periodically varying the doping concentration. The basic principle behind superlattices comes from the viewpoint of the total composite structure as a single crystal lattice with a large unit cell. For systems with composite materials with
close lattice constants the topological crystal structure is unaffected by the compositional alteration of layers. For 3C-SiC the crystal structure is zinc blend which consists of two interpenetrating face centered cubic lattices. For the ability of the superlattice to behave like a single crystal the period needs to be comparable to the length scale of the phenomenon under consideration. One predominate effect of superlattice layering is the folding of the bulk phonon dispersion curve into a new Brillouin mini-zone. Superlattices have properties that differ from traditional layered materials interlayer, (between layers); forces are stronger and roughly equal to intralayer, (within the layer), forces. This different nature creates different vibrational effects than typical layered materials.

For a Supelattice that is comprised of two layers of materials one with lattice constant $A_1$ and the other with lattice constant $A_2$ the period will be the sum of the two lattice constants $A_1 + A_2$ as illustrated in Figure 2.2 below.

![Figure 2-2](image)

**Figure 2-2.** Illustration of a superlattice comprised of two different materials with lattice constants $A_1$ and $A_2$.

The reciprocal space lattice vectors are given as,
\[ A_1 = 2\pi \frac{A_2 \times A_3}{A_1 \cdot A_2 \times A_3} \tag{2.87} \]

The Brillouin zones are defined as a wigner-seitz primitive cell in the reciprocal lattice. Therefore the first Brillouin zone edge of the superlattice is given by \(2\pi/(A_1 + A_2)\). A larger unit cell leads to a smaller or reduced Brillouin Zone. This corresponds to the Brillouin zones of superlattice materials to be folded into a smaller zone resulting into many mini-bands being formed. This folding of Brillouin zones is called the zone folding effect. The interesting feature of Brillouin zone folding is that phonon features found in outer regions can be found within the first Brillouin zone. Coupled with Raman spectroscopy experimental data mathematical methods can be applied to the reduced Brillouin zone to obtain additional information about the dispersion relation of the material unobtainable by other techniques giving great strength to this technique for the characterization of semiconductor materials.

The Following section follows Colvard’s work for a dielectric continuum model and helps to give more basic understanding to the Berreman effect discussed later in this work. Though ignoring mechanical dispersion and by approximating the superlattice as a layered dielectric continuum the effects of the electric field due to long-wave LO modes can be illuminated a bit. The dielectric constant can be represented in binary layers

\[ \varepsilon (\omega) \varepsilon_\infty \left( 1 + \frac{\omega_L^2 - \omega_T^2}{\omega_T^2 - \omega^2 - i\Gamma(\omega)} \right) \tag{2.88} \]

Applying the condition that damping is ignored the above equation becomes,

\[ \varepsilon (\omega) = \varepsilon_\infty \frac{\omega_L^2 - \omega^2}{\omega_T^2 - \omega^2} \tag{2.89} \]

The factored form can be used for the alloy,
\[ \varepsilon(\omega) = \varepsilon_\infty \left( \frac{\omega_{L1}^2 - \omega^2}{\omega_{L1}^2 - \omega^2} \right) \left( \frac{\omega_{T2}^2 - \omega^2}{\omega_{T2}^2 - \omega^2} \right) \]  

(2.90)

The parameters \( \omega_L, \omega_T \) represent the long wavelength longitudinal and transverse phonon frequencies respectively where the subscripts denote the compositional dependent behavior of the alloy. Maxwell’s equations can be used for the polarization waves propagating parallel or perpendicular to the layers for the wave-vector \( (q \to 0) \) approaches zero limit. The basic principles behind the results can be understood by reiterating that for long waves the superlattices behaves like a homogenous anisotropic crystal. The average dielectric constants are as follows,

\[
\bar{\varepsilon}_x(\omega) = \bar{\varepsilon}_y(\omega) = \frac{\bar{\varepsilon}_1(\omega)A_1 + \bar{\varepsilon}_2(\omega)A_2}{A} 
\]

(2.91)

and

\[
\bar{\varepsilon}_z(\omega) = \frac{A(\bar{\varepsilon}_1(\omega) + \bar{\varepsilon}_2(\omega))}{A_1\bar{\varepsilon}_2(\omega) + A_2\bar{\varepsilon}_1(\omega)} 
\]

(2.92)

The poles and zeroes of these dielectrics constants occur at the longitudinal and transverse frequencies of the layered structure corresponding to the average displacement \( \mathbf{D} \) or electric field \( \mathbf{E} \) vanishing. For polarization that is in the plane of the layers and the wave-vector along the \( z \)-direction, the poles of equation 2.91 give TO modes of \( E \)-symmetry (From Raman selection rules/ molecular symmetry) at the bulk TO frequencies. For polarization parallel to the supelattice axis the zeros of equation give LO modes of \( A_1 \) or \( B_2 \) symmetry at the bulk LO frequencies. For both instances the electric field and polarization, they exist only in the layer at whose normal frequency the vibration occurs. For consideration of the phonon dispersion, these modes are the quantized phonons due to zone folding.
2-3 Optical excitation of Phonons

Much like the section for the derivation of the index of refraction and extinction coefficients this section follows the same form as equation 2.31 with condition of being a two atom lattice system. As a starting point a two atom ionic crystal will be considered. A time dependent electromagnetic wave propagates through the crystal. The equation of the time dependent light field is in the following form,

$$E = E_0 e^{-i\omega t}. \quad (2.93)$$

The positive and negative ions will experience a forced vibration caused by the Lorentz force law as discussed earlier. As this same principle was discussed in a preceding section and will be covered with sufficiently less detail here with more emphasis on the significance of the end result in connection with the basic principles of semiconductor optics. The system will have the following equation to describe its motion,

$$M_1 \ddot{x} + M_1 \gamma \dot{x} - k(-2x_k + x_{k-1} + x_{k+1}) = -eE_0 e^{-i\omega t} \quad (2.94)$$

$$M_2 \ddot{x} + M_2 \gamma \dot{x} - k(-2x_{k+1} + x_k + x_{k+2}) = eE_0 e^{-i\omega t} \quad (2.95)$$

The main differences between these two equations are the masses and the direction of the driving force. For the same reasons as the preceding sections an exponential function is chosen for both the $k^{th}$ and $(k+1)^{th}$ ion behavior,

$$x_k = A_- e^{-i\omega t} \quad (2.96)$$

$$x_{k+1} = A_+ e^{-i\omega t} \quad (2.97)$$

Placing the above equations into the equation of motion and performing the same steps as the dispersion section gives the following two equations,

$$[2k - M_1(\omega^2 + i\gamma\omega)]A_- - 2kA_+ = -eE_0 \quad (2.98)$$

$$[2k - M_2(\omega^2 + i\gamma\omega)]A_+ - 2kA_- = +eE_0 \quad (2.99)$$
Noticing that these equations bear a similarity to equation of motion from the general
dielectric derivation section and by applying the relation for the high limit wavenumber
from the dispersion section the following equations arise for the displacements of the
positive and negative ions,

\[ A_- = \frac{-eE_0}{M_1} \frac{1}{\omega^2_0 - (\omega^2 + i\gamma\omega)} \]  \hspace{1cm} (2.100)

\[ A_+ = \frac{eE_0}{M_2} \frac{1}{\omega^2_0 - (\omega^2 + i\gamma\omega)} \]  \hspace{1cm} (2.101)

By separating the polarization into the ionic and bound contributions the following
equation results,

\[ \vec{P} = \vec{P}_i + \vec{P}_b \]  \hspace{1cm} (2.102)

The ionic contribution will be the ionic moment between two ions summed over N, the
number of ions pairs. With equation the two preceding equations being the displacements
for the negative and positivity ion respectively they can be used to find the ionic
contribution to the polarization as follows,

\[ \vec{P}_i = 4\pi Ne(A_+ - A_-) \]  \hspace{1cm} (2.103)

The dielectric function with all the above relations takes on the following form,

\[ \varepsilon(\omega) = 1 + \frac{M_1M_24\pi Ne^2}{(M_1 + M_2)\omega^2_0} \frac{1}{1 - \frac{(\omega^2 + i\gamma\omega)}{\omega^2_0}} \]  \hspace{1cm} (2.104)

Equation 2.98 can be used to find the dielectric constant for high and low frequencies
which are summed in the following equations:

\[ \varepsilon_0 = 1 + \frac{4\pi P_b}{E} + \frac{M_1M_24\pi Ne^2}{(M_1 + M_2)\omega^2_0} \]  \hspace{1cm} (2.105)
Applying the difference between the low and high dialectic constants to the dielectric function yields the following equation for the dielectric function,

$$\varepsilon_0 - \varepsilon_\infty = \frac{M_1 M_2 4\pi N e}{(M_1 + M_2) \omega_0^2}$$

(2.107)

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 - \frac{\omega(\omega + i\gamma)}{\omega_0^2}}$$

(2.108)

The above equation is the basic starting dielectric before more complicated damping terms are considered such as Plasmon damping. This result shows the dispersion relation’s deep connection to the dielectric function for the semiconductor films as well as illuminating the principles behind understanding light matter interactions.

The equation used for the dielectric constant for plotting the reflectivity in this work is generally given by the following standard form unless otherwise stated in that particular section. The standard form used is as follows,

$$\varepsilon(\omega) = \varepsilon_\infty \left( 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} + \frac{\omega_L^2 - \omega_T^2}{\omega_T^2 - \omega^2 - i\Gamma\omega} \right)$$

(2.109)

The last two terms in the right-hand side of equation 2.109 are the contributions to the dielectric function from the Drude and Lorentz (polar lattice) oscillators. The reflectivity equation coming about from the dielectric function combined with manipulation of the Fresnel equations takes on the following general form,²

$$R = \frac{(n - 1)^2 + k^2}{(n + 1)^2 + k^2}$$

(2.110)
CHAPTER III
EFFECTIVE MEDIUM THEORY

3-1 Roughness Modeling

For many thin films the simplistic models such as equation 2.110 fail to accurately predict features of the reflectivity function that is found by experimental observation. One feature of particular interest is the damping effect of the reflectance for values of large wavenumber. One method of correcting the reflectance model is through the modeling of roughness in the air-film interface and accommodating for film thickness. Following the work by Holm et al. the reflectance accounting for film thickness in terms of the film refractive index, $n_f$, the surface extinction coefficient, $k_f$, the substrate refractive index, $n_s$, and the substrate extinction coefficient, $k_s$, takes on the following form$^{18}$,

$$R = \frac{A_1 - 2\chi B_1 \cos \phi + 4k_f C_1 \sin \phi + D_1 \chi^2}{A_2 - 2\chi B_2 \cos \phi + 4k_f C_2 \sin \phi + D_2 \chi^2}$$ (3.1)

$$\chi = e^{-4\pi\omega k_f}$$ (3.2)

$$\phi = 4\pi\omega n_f$$ (3.3)

$$A_1 = \left[ (1 - n_f)^2 + k_f^2 \right] \left[ (n_f + n_s)^2 + k_f^2 \right]$$ (3.4)

$$B_1 = (n_f^2 + k_f^2 - 1)(n_f^2 + k_f^2 - n_s^2) + 4n_s k_f^2$$ (3.5)

$$C_1 = n_s (n_f^2 + k_f^2 - 1) - (n_f^2 + k_f^2 - n_s^2)$$ (3.6)

$$D_1 = \left[ (n_f - n_s)^2 + k_f^2 \right] \left[ (1 + n_f)^2 + k_f^2 \right]$$ (3.7)

$$A_2 = \left[ (1 + n_f)^2 + k_f^2 \right] \left[ (n_f + n_s)^2 + k_f^2 \right]$$ (3.8)

$$B_2 = (n_f^2 + k_f^2 - 1)(n_f^2 + k_f^2 - n_s^2) + 4n_s k_f^2$$ (3.9)
\[ C_2 = n_s (n_f^2 + k_f^2 - 1) + (n_f^2 + k_f^2 - n_s^2) \]  
\[ D_2 = \left[ (n_f - n_s)^2 + k_f^2 \right] \left[ (1 - n_f)^2 + k_f^2 \right] \]  

With the reflectance given in equation 3.6 as \( R_0 \) the reflectance with an air film interface roughness correction takes on the following form\(^{16} \),

\[ R = R_0 \exp[-8(\delta \omega)^2] \]  

The roughness region thickness, \( \delta \), is in micrometers and the values were found to typically vary from nonexistent to nearly one tenth of the total film thickness. For multiple interface films that may have more than one layer of roughness another model accounting for interface roughness needs to be implemented.

Treating the reflectance of a thin film grown on a substrate we adopt a three medium “air-film-substrate” system. Roughness was considered between both the Air-Film layer and between the total film thickness is denoted by \( D \). The air film surface roughness thickness is denoted by \( d_1 \). The film substrate interface roughness is given by \( d_2 \). An illustration of a film with Air-Film roughness and Film-Substrate roughness is shown in Figure 3-1 below.

Following previous published works and applying the above discussed roughness regions to the “air-film-substrate”, the reflection coefficient takes the following form\(^{13} \),

\[ R = \left( \frac{\rho_1 r_{12} + \rho_2 r_{23} \exp[i\beta]}{1 + \rho_1 \rho_2 r_{12} r_{23} \exp[i\beta]} \right)^2 \]  

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**Figure 3-1.** Illustration of Air-Film interface roughness ($d_1$) and Film-Substrate interface roughness ($d_2$).

\[
\begin{align*}
r_{12} &= \frac{\sqrt{n_1} - \sqrt{n_2}}{\sqrt{n_1} + \sqrt{n_2}} \\
r_{23} &= \frac{\sqrt{n_2} - \sqrt{n_3}}{\sqrt{n_2} + \sqrt{n_3}} \\
\rho_1 &= \text{Exp}\left[-8(\omega d_1 \cos \theta)^2\right] \\
\rho_2 &= \text{Exp}\left[-8(\omega d_2 \cos \theta)^2\right] \\
\beta &= 2 \pi \sqrt{\varepsilon} D \omega
\end{align*}
\]

The effects of Air-Film roughness is shown in Figure 3-2 below. Four different values for roughness are considered $d_1 = 0, 100, 250, 500$ nm. The effect of Air-Film roughness has the effect to damp the entire range of wavelengths of the infrared spectrum.
Figure 3-2. Plot showing the effect of Air-Film interface roughness

The effects of Film-Substrate roughness is shown in Figure 3-3 below. Four different values for Film-Substrate roughness are considered \(d1= 0 , 100, 250, 500\) nm. The effect of Film-Substrate roughness has the effect to damp the range of wavelengths beyond the reststrahlen region of the infrared spectrum. The interesting feature shown for Film-Substrate roughness is that the observed stretching feature of the interference fringes given becomes such a dominating factor that the fringes disappear. Unlike for Air-Film roughness the fringe stretching caused by Film-Substrate does not significantly damp the reflectance.
The main differences between Air-Film roughness and Film-Substrate roughness are that the Film-Substrate only effects beyond the reststrahlen region and that the effect of the Air-Film roughness has a stronger contribution per thickness. The additional effect to “stretch” the long wavelength reflectance oscillations is observed by both types of roughness modeled.

3-2 Theoretical Basis for Effective Medium Approximations

The microscopic structure of a material dictates the permittivity. For homogenous materials it is generally the atomic structure alone that play the predominante role at determining the permittivity. But for composite materials there are additional polarization effects resulting from the inhomogeneities of the material as well as the usual structure polarization effects. For the study and analysis of these materials an effective permittivity
can be defined to adequately represent the dielectric function of these materials.
Illustrated in Figure 3-4 the spheres of material permittivity A (green) are immersed in a
background of material with permittivity B (light blue), the resulting effective
permittivity is represented by a combination of both materials (blue).\textsuperscript{18}

\textbf{Figure 3-4.} Illustration of how an incident wave treats a two phase composite

For modeling these materials as long as the size of the inhomogeneities is smaller
than the wavelength of the electromagnetic wave propagating through the medium the
representation of the permittivity for the whole system holds true. The effective
permittivity is a function of the dielectric function of each composite material, the
volume fraction, and geometry of the material structure.

A way that the dielectric function can be modeled is by representing the system as
a mixture of spheres of one of the materials within a background of a different dielectric
material. In the case when the distance between spheres is large in comparison to their
radii an accurate depiction of the effective permittivity can be approximated.
3-3 Maxwell-Garnet Mixing Theory

For the Maxwell garnet mixing equation the spherical incursions are replaced with equivalent dipole moments using the general form of equation 2.2. By tabulating the combined effects of all these dipoles together the effective permittivity can be calculated. The electric field becomes the localized electric field on the sphere and in place of the atomic polarizability a more complicated polarizablity comes about. The polarizablity of each sphere is \( \alpha \), is given in the following form,

\[
\alpha = V_s (\varepsilon_i - \varepsilon_e) \frac{3\varepsilon_e}{\varepsilon_i + 2\varepsilon_e}
\]  
(3.18)

For equation 3.1 the permittivity around the sphere is given as \( \varepsilon_e \). Accordingly \( \varepsilon_i \) acts as the internal permittivity of the sphere. The parameter in equation 3.18 \( V_s \) is the spherical incursion’s volume. This equation is justified for the assumptions of a homogenous field with a wavelength that is much greater than the radius of the spherical incursions. Following from the work of jylha[18] the effective permittivity of a mixture of spheres can be represented as

\[
\bar{D}_{avg} = \varepsilon_{eff} \bar{E}_{avg} = \varepsilon_e \bar{E}_{avg} + \bar{P}_{avg}
\]  
(3.19)

Where \( \bar{E}_{avg} \) is the overall average electric field, \( \bar{D}_{avg} \) is the overall average electric flux density, and \( \bar{P}_{avg} \) is the average electric polarization density:

\[
\bar{P}_{avg} = n \bar{p}
\]  
(3.20)

The term \( n \) in equation 3.2 is the number density of spheres.

The local electric field acting on each sphere is given as follows,

\[
\bar{E}_{local} = \bar{E}_{avg} + \frac{1}{3\varepsilon_e} \bar{P}_{avg}
\]  
(3.21)
The factor of one third in equation 3.21 arises from the depolarization factor for a sphere and may be adjusted accordingly to model effects of ellipsoidal incursions. When the spheres are separated sufficiently the effects of other dipoles can be taken into account by just the summation of far field effects. The Maxwell-Garnet approximation works best for low volume fractions of spheres and underestimates the effective permittivity of random mixtures.\textsuperscript{18}

For the Maxwell garnet approximation used in this study the cavity Maxwell garnet mixing equation is used. With having the same basic theoretical basis as described above the cavity Maxwell-Garnett equation is as follows\textsuperscript{18,17},

\[\varepsilon_{\text{eff}}(\omega) = \varepsilon_1(\omega) \left\{ \frac{1 + \frac{2f_2(\varepsilon_2 - \varepsilon_1)}{\varepsilon_2 + 2\varepsilon_1}}{1 - \frac{f_2(\varepsilon_2 - \varepsilon_1)}{\varepsilon_2 + 2\varepsilon_1}} \right\} \]

The subscript two in the above equation denotes the second material that is surrounded by the first material. Due to the straightforward layout of this form of the Maxwell-Garnet effective medium approximation most multiple medium models constructed throughout this thesis had their parameters adjusted with this model as the starting template.

3-4 Bruggeman Symmetric Mixing Model

The Bruggeman approximation derivation is very similar to the Maxwell-Garnet with the addition of an assumed symmetry between the incursion and environment phases. Arising from this assumption the Bruggeman model obeys the self-consistency condition which states: the net polarization of the medium is zero and the effective electric field is the same as the average electric field in every region. The general form of the Bruggeman effective medium model is as follows\textsuperscript{16,18},
\[
\sum_{i}^{N} \frac{f_i[\varepsilon_i(\omega) - \varepsilon(\omega)]}{\varepsilon_i(\omega) + 2\varepsilon(\omega)} = 0
\]  

(3.23)

The first term in the summation corresponds to the polarizability of a sphere with permittivity \( \varepsilon_i \) weighted with the volume fraction of that same material. The Bruggeman approximation reduces to the following for two component mixtures,

\[
\frac{f_1[\varepsilon_1(\omega) - \varepsilon(\omega)]}{\varepsilon_1(\omega) + 2\varepsilon(\omega)} + \frac{f_2[\varepsilon_2(\omega) - \varepsilon(\omega)]}{\varepsilon_2(\omega) + 2\varepsilon(\omega)} = 0
\]  

(3.24)

Equation can be solved giving the effective permittivity for the composite system in the form of two solutions. Based upon the requirement of the self-consistency condition the Bruggemen Model offers superiority when modeling materials with fractional compositions not completely dominated by one material.
CHAPTER IV

THEROETICAL REFLECTANCE MODELING

4-1 Basics of Theoretical Reflectance Modeling

The primary focus of this study has been the optical treatment of semiconductors specifically 3C-SiC/Si focusing on mid infrared reflectivity measurement models. Through many previous works the optical constants of numerous semiconductor composites have been tabulated. Due to the very large number of fitting parameters used throughout this thesis all models expressed as figures will have a corresponding tabular data section in the appendix A section.

<table>
<thead>
<tr>
<th>Substance</th>
<th>$\varepsilon_\infty$</th>
<th>$\omega_{TO}$</th>
<th>$\omega_{LO}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystalline SiC</td>
<td>6.7</td>
<td>794</td>
<td>973</td>
</tr>
<tr>
<td>Intergranular SiC</td>
<td>6.0</td>
<td>940</td>
<td>980</td>
</tr>
<tr>
<td>6H-SiC</td>
<td>6.7</td>
<td>969</td>
<td>793</td>
</tr>
</tbody>
</table>

Given the tabulated data values theoretical models for reflectivity can be represented by plotting the reflectivity function versus wavelength. Using equation 2.109 without Plasmon frequency and equation 2.110 a simple theoretical model for 6H C-SiC is illustrated in Figure 4-1. Observable from Figure 4-1 the simplistic model lacks a great deal of information about the substance.
4-2 Oblique incidence effects

Under normal incident conditions from the transverse characteristics of electromagnetic radiation only the zone center TO phonons will be observable for polar materials. However in the case of thin films the interaction of the electromagnetic field with the film can be enhanced by incurring an oblique incidence. With the use of Infrared spectroscopy at an oblique incident Berreman predicted theoretically and subsequently demonstrated experimentally the observation of TO and LO phonons in Lithium fluoride (LiF), thin films grown on a collodion (flash paper) film. The parallel polarized light the longitudinal optical structure is generated by the surface charges from the normal component of the electric field. In recent studies the detection of the p-polarization minimum attributed to the TO phonon and high –frequency LO Phonon-Plasmon-
Coupled modes has made oblique incident FIR a tool for estimating free charge carrier density in semiconductor films. Within the constructs of multilayer optics and by utilizing the effective medium dielectric tensor we can simulate the reflection and transmission spectra at oblique incident for epilayers, and superlattices. Polar semiconductors exhibit distinct response to FIR radiation between s- and p-polarization when light is incident at an oblique angle to the surface of the material. Shown in Figure 4-2 below the p and s notation imply to the directions of the linear polarization that are parallel and perpendicular to the plane of incidence.

**Figure 4-2.** Polar semiconductor thin film grown on a thick substrate. The directions of p (parallel) and s (perpendicular) components of the FIR radiation incident are at an oblique angle to the surface of a thin film (perpendicular to the phonon wave-vector $\mathbf{q}$) of thickness much smaller than the wavelength of incident radiation grown on a thick substrate.$^{23}$

Berreman’s argument consisted of a demonstration that for thin films when the wavelength of Electromagnetic radiation is much greater than the thickness the long-wavelength phonons have the wave-vector $\mathbf{q}$ perpendicular to the film surface in a way that the normal incident radiation can only interact with the Transverse Optical modes. The p-polarized component of the oblique incident radiation has components parallel and
perpendicular to the films surface that can excite TO and LO phonons. Following piro the
analytical expression for reflectance at an arbitrary angle of incidence can be derived for
an isotropic thickness of A grown on a thick isotropic substrate\textsuperscript{23}. The dielectric tensor of
the superlattice consisting of two optically active layers $A_1, A_2$ grown alternatively on a
substrate has the form of a uniaxial crystal with $D_{2d}$ point group symmetry:

$$\tilde{\varepsilon}_{SL} = \begin{bmatrix} \tilde{\varepsilon}_s & 0 & 0 \\ 0 & \tilde{\varepsilon}_s & 0 \\ 0 & 0 & \tilde{\varepsilon}_p \end{bmatrix}$$  \hspace{1cm} (4.1)

The Z-axis is set along the optical axis perpendicular to the plane of the Superlattice.
When polarized along the x or y axis the dielectric function is the same but when the
incident radiation is polarized into the plane the dielectric function will be different. It
should be noted that these equations will match equations 2.91 and 2.92 from section 2-3
for the dielectric continuum mode. If the wavelength of the radiation is much greater than
the period of the superlattice, the electromagnetic boundary conditions give $\tilde{\varepsilon}_s$ values of
$\tilde{\varepsilon}_s$ and $\tilde{\varepsilon}_p$:

$$\tilde{\varepsilon}_s(\omega) = \frac{\tilde{\varepsilon}_{A_1}(\omega)A_1 + \tilde{\varepsilon}_{A_2}(\omega)A_2}{A_1 + A_2}$$  \hspace{1cm} (4.2)

and

$$\tilde{\varepsilon}_p(\omega) = \frac{(A_1 + A_2)\tilde{\varepsilon}_{A_1}(\omega)\tilde{\varepsilon}_{A_2}(\omega)}{A_1\tilde{\varepsilon}_{A_2}(\omega) + A_2\tilde{\varepsilon}_{A_1}(\omega)}$$  \hspace{1cm} (4.3)

For a superlattice grown on a thick substrate the amplitude reflectance can be obtained
using

$$R = |\tilde{r}_{3(p)}|^2 = \frac{(1 - \alpha_1)\cos \alpha_2 - i(\alpha_3 - \alpha_4)\sin \alpha_2}{(1 + \alpha_1)\cos \alpha_2 - i(\alpha_3 + \alpha_4)\sin \alpha_2}$$  \hspace{1cm} (4.4)
For s polarization

\[ \alpha_1 = \frac{\sqrt{\varepsilon_{sub} - \sin^2 \theta_i}}{\cos \theta_i} \]  

\[ \alpha_2 = 2\pi h \omega \sqrt{\varepsilon_s - \sin^2 \theta_i} \]  

\[ \alpha_3 = \frac{\left(\frac{\varepsilon_{sub} - \sin^2 \theta_i}{\varepsilon_s - \sin^2 \theta_i}\right)}{\sqrt{\frac{\varepsilon_s - \sin^2 \theta_i}{\sqrt{\varepsilon_{sub}}}}} \]  

\[ \alpha_4 = \frac{\sqrt{\varepsilon_s - \sin^2 \theta_i}}{\cos \theta_i} \]

For p polarization

\[ \alpha_1 = \frac{\sqrt{\varepsilon_{sub} - \sin^2 \theta_i}}{\varepsilon_{sub} \cos \theta_i} \]  

\[ \alpha_2 = 2\pi A \omega \sqrt{\frac{\varepsilon_p - \sin^2 \theta_i}{\varepsilon_p}} \]  

\[ \alpha_3 = \frac{\varepsilon_s \varepsilon_p (\varepsilon_{sub} - \sin^2 \theta_i)}{\sqrt{\varepsilon_{sub}^2 (\varepsilon_s - \sin^2 \theta_i)}} \]  

\[ \alpha_4 = \frac{\varepsilon_p - \sin^2 \theta_i}{\sqrt{\varepsilon_s \varepsilon_p \cos^2 \theta_i}} \]

As expected the s-polarization coefficients have no dependency upon the dielectric function along the parallel direction.\textsuperscript{23,24}

In the above equations \( \varepsilon_{sub} \) represents the dielectric function of the substrate, the incident angle is given as \( \theta_i \) and the total thickness of the superlattice is given as \( A \).
4-3 Bruggeman EMA Modeling of Reflectance

The second effective medium approximation used in this study is the Bruggeman symmetric. As discussed in the effective medium theory section the Bruggeman symmetric has the advantage of obeying the self-consistency condition affording more accurate results for volume fractions where both composites have significant fractional compositions.

Applying the condition that the sum of the fractional components is equal to one and solving for the dielectric function in equation 3.5 yields the following solutions,

$$\varepsilon = \frac{1}{4} \left( -\varepsilon_1 + 3f\varepsilon_1 + 2\varepsilon_2 - 3f\varepsilon_2 \pm \sqrt{8\varepsilon_1\varepsilon_2 + (-\varepsilon_1 + 3f\varepsilon_1 + 2\varepsilon_2 - 3f\varepsilon_2)^2} \right)$$

(4.13)

For many studies the imaginary root of the dielectric function is altered to yield the physically feasible dielectric function solution, however in this thesis the reflectance is considered instead. By plotting the reflectance solutions together as shown in Figure 4-3 it becomes apparent that the minimum of these two functions is the physical solution.
Figure 4-3. Illustration of the two Reflectance’s minimum as the correct Bruggeman model. It should be noted that the plot is only shown slightly above one as values above one correspond to over one hundred percent reflection which is unphysical.

In this work while using Mathematica the Bruggeman method can be easily solve for the reflectance with built in functionality. But for this work it was chosen to overview the method of solving reflectance for the Bruggeman method for general study, allowing this solving method to be extended to numerous other computer programs. For each of the solutions of the dielectric function obtained by solving the Bruggeman equation there will exist one unique reflectance. But the unique solution may or may not be physical, there will exist at least one physically feasible solution comprised of some combination of all the root solutions. By separately solving the dielectric solutions and applying some equation for reflectance such as equation 3.1 as done in this study, two reflectance functions are found in the case of the two component mixture. The minimum of the two reflectance measurements is plotted yielding the physically significant reflectance. Figure
Figure 4-4 shows the Minimum of the reflectance roots giving the correct Bruggeman Symmetric model.

**Figure 4-4.** Plotting of Bruggeman symmetric model using the minimum reflectance obtained by solved solutions
5-1 3C-SiC/Si Growth and Characterization

The exact experimental details are given in but a brief overview is necessary. 3C-SiC films considered in this study were grown on (100) Si Substrate under normal atmospheric pressure by using chemical vapor deposition method in vertical reactor configuration. The samples prepared were characterized by conventional x-ray diffraction, Raman Spectroscopy, Rutherford backscattering and Ion channeling methods. Surface examination of the films by secondary mass spectrometry and x-ray photoemission spectroscopy (XPS) was also performed. The films were found to be n-type with residual doping density ranging from $10^{16}$ to $10^{17}$ cm$^{-3}$ by the capacitance-voltage (CV) method. The spectral measurements were conducted at room temperature with normal incidence by using a nitrogen purged Perkin Elmer 2000 spectrometer with a $\sim 2\text{cm}^{-1}$ resolution. These spectral measurements were carried out in the infrared range (200 to 6500 cm$^{-1}$). The beam splitter used was potassium bromide (KBr) along with a deuterated (deuterium in place of hydrogen) triglycine sulfate detector. The mirrors used were gold and aluminum whose absolute reflectance are measured directly and used for references in the reflection spectra. Multiple scans were taken for each sample to ensure repeatability of the Infrared spectra. 22
5-2 EMA Modeling Results

The first model used in this study is the Cavity Maxwell-Garnet as given in equation 3.22. The second modeling method used is the Bruggeman symmetric as detailed section 4.4. Both models use consideration of Air-Film (surface) roughness, Film-Substrate (conducting layer or interface) roughness, as detailed by equation 3.13 in section 3.1.

The modeling of experimental data from Dr. Z done with the Bruggeman Symmetric models can be shown in Figures 5-1, 5-2, 5-3, and 5-4 below. All three modeled sample fits have reasonably thick Substrate-film layers (360nm-530nm) the long wavenumber range as shown by Figure 5-2 dictates the Substrate-film thickness contribution. Due to high free carrier contribution the region immediately outside the reststrhalen band becomes shifted as shown in Figure 5-3 dictating that the Substrate-film and air-film thickness needs to be determined before carrier concentration effects. The charge carrier information obtained by applying Berreman effect gives great insight into the order of parameter adjustment to correctly model the IR data in a manner consistent with a sound theoretical understanding of the system. As expected the degree of carrier effects in the sample without a dip in the reststrhalen band is significantly smaller than the samples where there was a significant dip within that region.
Figure 5-1. 3C-SiC sample #414 modeled with accuracy in both the reststrahlen and longer range regions.

Figure 5-2. 3C-SiC sample #113 showing the long range wavenumber feature modeled accurately by applying a thick Film-Substrate interfacial region.
Figure 5-3. 3C-SiC sample #113 showing dipped feature in the reststrahlen region modeled and the shifting effect of the free charge carriers.

Figure 5-4. Modeling of 3C-SiC experimental sample without dip in the reststrahlen region.
With the combination of The Maxwell-Garnet and Bruggeman Symmetric Mixing approximations a much more accurate modeling method is utilized for 3C-SiC. The significance of applying both modeling techniques comes from the proper adjustment of modeling parameters such as the free carrier concentration (modeled via Plasmon resonance contributions) and the fractional composition of intergranular SiC. Without sufficient agreement between the theoretical models used the choice of material specific adjustable parameters would be arbitrary and meaningless.

The tremendous modeling strength of considering not only the interface roughness but roughness between deposited layers. The modeling of additional roughness at layer interfaces provides potential increased long wavenumber damping modeling at the cost of increased unknown parameter complexity.

5-3 Phonon Folding Effects and Coupled Modes

In Figure 5-6 below we have displayed the calculated results of the transmission spectra for a 1 µm thick 3C-SiC/Si film both at normal ($\theta_i = 0^\circ$) and oblique ($\theta_i = 45^\circ$) incidence. In Figure 5-5 the comparison with existing experimental data of Dean Sciacca et al has offered a strong corroboration to the Berreman’s effect by showing a sharp minima at for both normal and oblique transmission with an additional dip appearing at for $\theta_i = 45^\circ$ in p-polarization.
Figure 5-5. Experimental transmission spectra of the 3C-SiC/Si(100) 1 μm thick film for two configurations. $\theta_i = 0^\circ$, $\theta_i = 45^\circ$ by Dean Sciacca et al.\textsuperscript{22}
Figure 5-6. Theoretical transmission spectra of the 3C-SiC/Si(100) 1 µm thick film for two configurations. $\theta_i = 0^\circ$, $\theta_i = 45^\circ$. \textsuperscript{22}

The real and imaginary part of the phonon wave vector for bulk 3C-SiC and Si are plotted below in Figure 5-5. The imaginary component of the phonon wave vector indicates the rate of attenuation of a vibration at a particular frequency. The plot indicates that the non-split (Coupled LO-TO) mode frequencies and vibrations of Si extend several monolayers into the 3C-SiC. Figures 5-6 and 5-7 show the zone folding effects for 3C-SiC and Si respectively. In the absence of experimental Raman data the phonon zone folding effects can give information about the coupled modes that will arise from substrate interfacing effects.\textsuperscript{22}
**Figure 5-7.** Real and imaginary part of phonon wave-vector $q$ for 3C-SiC and Si.
Figure 5-8. Linear chain model calculations of phonon dispersion for 3C-SiC. Dashed lines: transverse modes. Solid Lines: Longitudinal modes.
Figure 5-9. Linear chain model calculations of phonon dispersion for Si. Dashed lines: transverse modes. Solid Lines: Longitudinal modes.
Calculated Raman intensity for 3C-SiC Zinc-Blend Superlattice is shown in figure 5.3 for four values of interface width $\delta$. The interfusion effects of Silicon into the 3C-SiC Structure can clearly be observed. The increasing contribution of Silicon can be seen at 750 cm$^{-1}$ for when $\delta = 1$. The peak continues to shift toward the region corresponding to the dipped reststrahlen feature observed in obtained experimental samples of 3C-SiC/Si. There is a gain in the intensity with increasing $\delta$ for some of the 3C-SiC modes. The gain occurs in steps of one monolayer for modes at the 760-950 cm$^{-1}$ (modes 30-38) region (corresponding to modes starting at the arrow onward). These
effects can be understood by examining the atomic displacements and the effect of
interfacing upon them. The atomic displacements of selected modes are given in Figures
5-11-5-16, for all four values of width among the five values considered in this study.
Modes 30, and 32 transform from a 3C-SiC pseudo-confined mode to pseudo-localized at
the 3C-SiC interface giving agreement with the Raman intensity enhancement in steps of
one monolayer. Modes 34, 36, and 38 evolve continually from a 3C-SiC pseudo-confined
mode to a pseudo-localized mode with atomic displacements at the 3C-SiC/Si interface
type with increasing interface thickness, δ.

Figure 5-11. Interfacial transition region effects on the Raman scattering from optical
modes of (3C-SiC)_{10-δ} / (3C-SiC_{0.5}Si_{0.5})_{δ} / (Si)_{10-δ} / (3C-SiC_{0.5}Si_{0.5})_{δ} superlattices. The
interface thickness δ (in units of monolayers) considered in this calculation is shown on
the left-hand side of each spectrum.

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Figure 5-12. Atomic displacements of optical mode 30 for a (3C-SiC)_{10-\delta} / (3C-SiC_{0.5}Si_{0.5})_{\delta} / (Si)_{10-\delta} / (3C-SiC_{0.5}Si_{0.5})_{\delta} superlattice for \(\delta = 0, 1, 2, 3\). Green and red circles stand for Si and C respectively.
Figure 5-13. Atomic displacements of optical mode 32 for a (3C-SiC)_{10-\delta} / (3C-SiC_{0.5}Si_{0.5})_\delta / (Si)_{10-\delta} / (3C-SiC_{0.5}Si_{0.5})_\delta superlattice for \( \delta = 0,1,2,3 \). Green and red circles stand for Si and C respectively.

Figure 5-14. Atomic displacements of optical mode 34 for a (3C-SiC)_{10-\delta} / (3C-SiC_{0.5}Si_{0.5})_\delta / (Si)_{10-\delta} / (3C-SiC_{0.5}Si_{0.5})_\delta superlattice for \( \delta = 0,1,2,3 \). Green and red circles stand for Si and C respectively.
Figure 5-15. Atomic displacements of optical mode 36 for a (3C-SiC)\textsubscript{10-\(\delta\)}/(3C-SiC\textsubscript{0.5}Si\textsubscript{0.5})\textsubscript{\(\delta\)}/(Si)\textsubscript{10-\(\delta\)}/(3C-SiC\textsubscript{0.5}Si\textsubscript{0.5})\textsubscript{\(\delta\)} superlattice for \(\delta=0,1,2,3\). Green and red circles stand for Si and C respectively.
Figure 5-16. Atomic displacements of optical mode 38 for a (3C-SiC)$_{10-\delta}$ / (3C-SiC$_{0.5}$Si$_{0.5}$)$_{\delta}$ / (Si)$_{10-\delta}$ / (3C-SiC$_{0.5}$Si$_{0.5}$)$_{\delta}$ superlattice for $\delta=0,1,2,3$. Green and red circles stand for Si and C respectively.
CHAPTER VI
CONCLUSIONS

The progression of the basic representation of physical principles is a necessity in the development of theoretical models of thin film systems. As shown by the results section the different model representations of a film with the same system parameters effects such as Plasmon resonance and interface thickness have complex often competing independencies effecting the optical interaction of the material. The effective medium approximations with both roughness effects modeling approach is shown to be successful for the theoretical of 3C-SiC Experimental samples given by the Dr. Z.C. Feng research group. The features of interface roughness and the silicon substrate interfacing into the 3-SiC lattice are supported by theoretical modeling of the Raman intensity produced by considering up to several monolayers of Si interfaced.

The development and study of the effective medium models lead to the discovery of an alternative procedure for the numerical solving of reflectance for a several component material using the Bruggemen symmetric effective medium approximation. The modeling approach to use both the Cavity Maxwell-Garnet and Bruggeman symmetric in tandem for both the adjustment of parameters and verification of well-matched fits was shown to be successful.
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### Table A.1: Optical Parameters for Figures

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<th>f1</th>
<th>f2</th>
<th>$\Gamma_1$ (cm$^{-1}$)</th>
<th>$\Gamma_2$ (cm$^{-1}$)</th>
<th>$\omega_p^2$ (cm)</th>
<th>$\gamma_1$ (cm$^{-1}$)</th>
<th>$\gamma_2$ (cm$^{-1}$)</th>
<th>d x10$^{-4}$ (cm)</th>
<th>$\delta$ x10$^{-7}$ (cm)</th>
<th>$\delta_i$ x10$^{-7}$ (cm)</th>
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