On the LEEM Spectra of Graphite and Graphene on Bulk Hexagonal Boron Nitride

THESIS

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On the LEEM Spectra of Graphite and Graphene on Bulk Hexagonal Boron Nitride

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Abstract

To better understand the LEEM spectra of 2D materials we explored using transfer matrices to model them. We applied transfer matrices to find an analytical expression for the LEEM spectra of graphite. We found that it results in an approximate solution that correctly predicts the position of the minima and general shape of the curve in the 0-25 eV range. We also applied transfer matrices to model the spectrum of few-layer graphene on bulk hexagonal boron nitride. The modeling of graphene on hBN was done in a coherent, incoherent and a modified coherent case. We found that the model manages to show the 8 eV minima in the coherent case. But the general shape we found is less accurate than for graphite. The other cases did not model the 8 eV dip of the spectra.

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Chapter 1

Introduction

We are interested in looking at the effects a substrate has on the spectra of a 2D material obtained using a low energy electron microscope, LEEM. A LEEM operates using electrons at an energy scale of several eV as opposed to the energy scale of keV that a conventional electron microscope uses.

We use an ESCHER LEEM [1]. It decelerates electrons from 15 keV to low energies, typically 0-50 eV, just before they hit the sample, after being reflected the electrons are accelerated back up to 15 keV. After this they are deflected into an electron mirror for aberration correction after which an image is formed. Spectroscopic information is obtained by scanning the sample voltage and recording images, such that the reflectivity of a sample area as a function of electron energy can be extracted. A schematic overview is given in figure 1.1.

A 2D material is what the name suggests, a material that only exists in a single plane. Materials like this are graphene and single-layer hexagonal boron nitride. These types of materials have many reasons to be interesting, from them having potential to be used as molecular lego blocks [2] to being used as semi-conductors to build transistors and other semi-conductor devices from.[3] [2] We will mostly discuss graphene, whose spectra has been measured by Hibino et al. [4], and graphene on bulk hBN whose spectra has been measured by Jobst et al. [5]

The spectra of graphene will be explored using a transfer matrix method which was previously done by Geelen et al.[6] This method will be applied to the spectra of graphite and graphene on hBN. This will be compared to experimental data. For graphene on bulk hBN we use the data from Jobst et al. [5]. We also use their data on hBN to model the spectra of graphene on bulk hBN. The ESCHER LEEM setup[1] was used to make a bright field measurement of the reflectivity of graphite with a contrast aperture

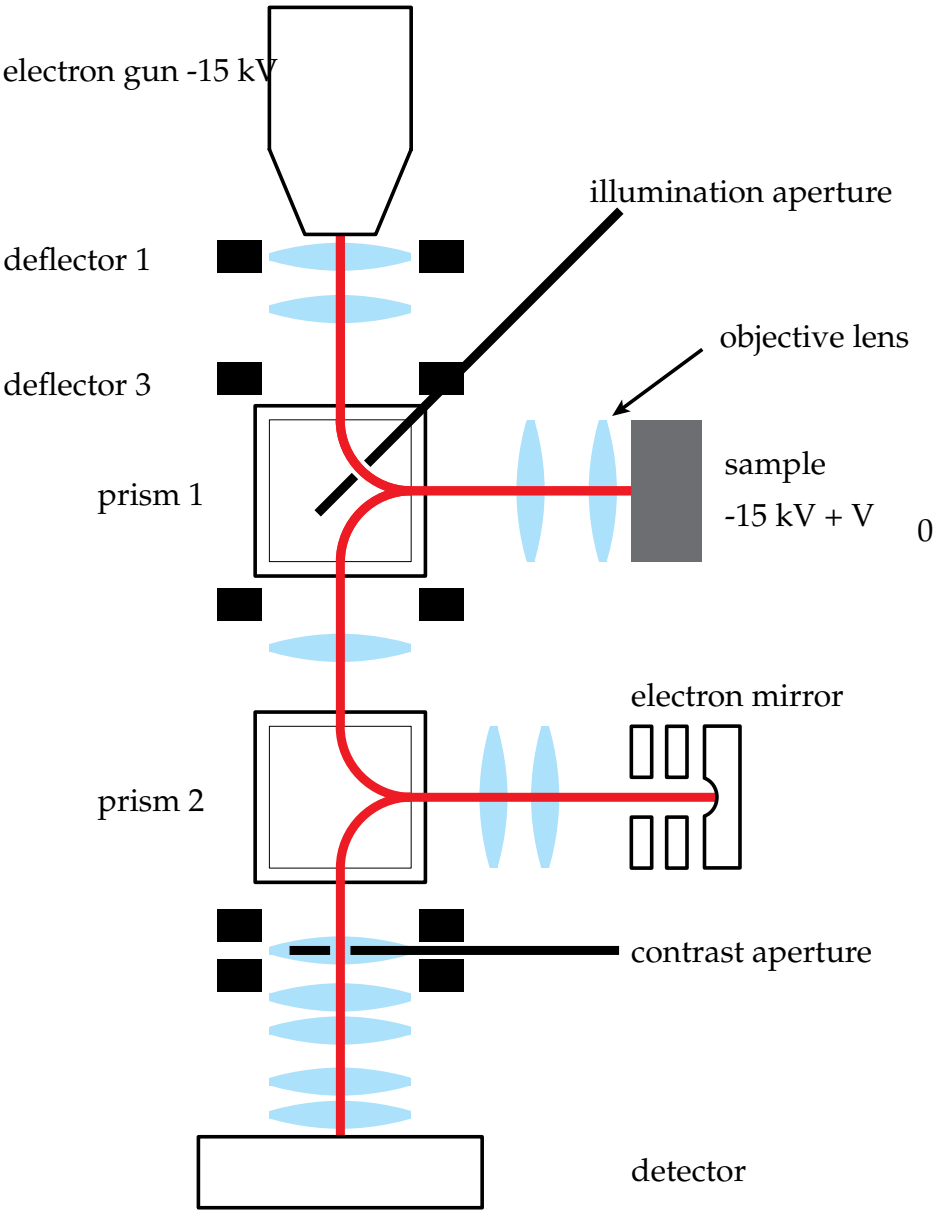

Figure 1.1: *Schematic of the ESCHER LEEM[1] setup*

around the central spot in the diffraction plane, meaning that only elastically, specularly backscattered electrons contribute to the measured intensity.

Chapter 2

Methods

In this section we give an overview of the methods we use to model graphite and graphene on bulk hexagonal boron nitride. Further we also explain what we used to analyze the data.

2.1 Modeling Graphite

We try to model the LEEM spectra of graphite using a method which uses transfer matrices that were used to model few-layer graphene by Geelen et al. [6] We do this by modeling graphite as infinitely many graphene layers stacked on top of each other. In a thick sample, more than 10 layers, areas of different layer count are not distinguishable by LEEM spectra, so we expect that these can be modeled by taking the limit of infinite layers. By diagonalizing the transfer matrix and taking the amount of graphene layers to infinity we also try to find an analytical expression for what this model predicts the spectrum of graphite to be. We then compare this to measurements of the LEEM spectra of graphite.

2.2 Graphene on Bulk hBN

We try to model graphene on bulk hBN in 3 different ways using the method of transfer matrices. First we assume incoherence of the electron wave function after it passes through the graphene, i.e the electrons do not maintain their phase information. Then we look at the system if the electron wave function is not incoherent after it passes through the graphene. In this case we can take two different approaches to the reflectivity for bulk hBN.Firstly, we take the measured data as our reflectivity, which causes a

loss of the phase information of the electrons that get reflected off the hBN because our measurements are only on the magnitude of the reflectivity. We also try to substitute the loss of phase information by using the phase information we found for the calculations of graphite, with the crude assumption that graphite and bulk hBN will have similar phase information.

2.3 Data Analysis

The data analysis is done using python. On all data sets we applied the drift correction algorithm from de Jong et al. [7]

Chapter 3

Transfer Matrix Models

We will now elaborate on the model we will use to model graphite and graphene on hexagonal boron nitride. We will also explore what we know about the LEEM spectra of graphene and hBN.

3.1 Transfer Matrix

In this section we explain a model used by Geelen et al. [6] Using this method they were able to capture the characteristics of the LEEM spectra of graphene. This model and results will then in later chapters be used to give an analytical expression for the LEEM spectra of graphite and to make an attempt at modelling van der Waals heterostructures.

3.1.1 What is a Transfer Matrix?

First consider a system with a single boundary between two regions and a wave traveling between these two regions across this boundary. When the wave crosses this boundary it will be partially reflected and transmitted. For example, imagine you look out of the window at night, what do you see? You see your own reflection. However, someone that is looking from outside would of course still be able to see you. Thus windows partially reflect and transmit light waves. This is the same for the type of systems that we are looking at, but instead of light we will be using electrons and instead of a window we will be using materials like graphene or hexagonal boron nitride.

The amplitude with which a wave gets reflected we call r and the amplitude with which it gets transmitted we call t and we also define $R = |r|^2$

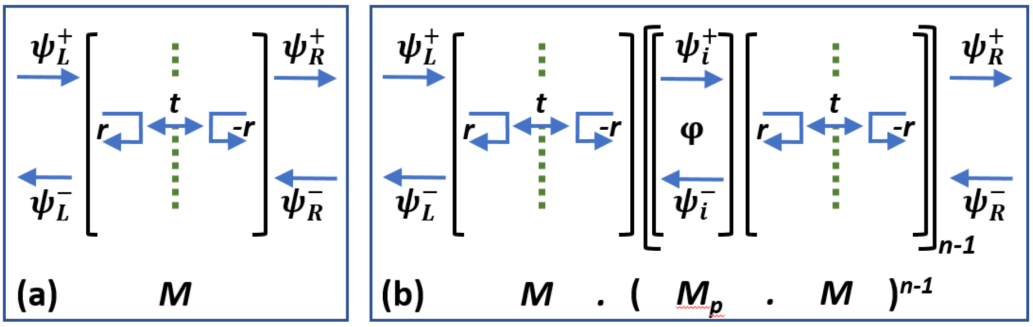

Figure 3.1: *a. a single boundary, the green dashed line, which has in going and out going waves and their reflections. The reflection and tranmission amplitudes are given by r and t respectively. b. An n-boundary system, here waves gain a phase ϕ when traveling between the first and second boundary. The equations under the figure are explained in the main text. Figure taken from Geelen et al. [6]*

and $T = |t|^2$ because R and T are the intensities you observe when doing a measurement. Note that r and t can be complex valued. To describe the waves in a single region there are two options, an outgoing wave and an in going wave. Thus if we have two regions with a boundary in between we have 4 waves to consider, a wave going into the left region, a wave going out of the left region, a wave going into the right region and a wave going out of the right region. The waves traveling to the left will be denoted as Ψ^-, the waves traveling right as Ψ^+, the waves in the left region as Ψ_L and the waves in the right region as Ψ_R as seen in figure 3.1a. To abide by the boundary conditions of the system we have that the reflection amplitude for Ψ_R and Ψ_L differ by a sign, thus $r_R = -r_L$. More on this can be read about in Optics 4th edition chapter 4.10 by Hecht [8].

When applying these conditions we get the set of equations 3.1

$$\begin{cases} \Psi_R^+ = t\Psi_L^+ - r\Psi_R^- \\ \Psi_L^- = r\Psi_L^+ - t\Psi_R^- \end{cases} \tag{3.1}$$

This system of equations can then be rewritten in terms of matrix multiplication.

$$\begin{pmatrix} \Psi_R^+ \\ \Psi_R^- \end{pmatrix} = M \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix} = \begin{pmatrix} \frac{1}{t}(r^2+t^2) & -\frac{r}{t} \\ -\frac{r}{t} & \frac{1}{t} \end{pmatrix} \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix} \tag{3.2}$$

Where M is the transfer matrix for a single boundary like sketched in figure 3.1a.

When we want to go to a multi-layer system the behavior between layers needs to be considered. We will assume that the wave acquires some phase when traveling between two boundaries which we can model using a rotation matrix M_p which adds a phase ϕ to the wave function.

$$M_p = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix} \tag{3.3}$$

An N-layer system like the two-layer system in figure 3.1b is described using equation 3.4

$$\begin{pmatrix} \Psi_R^+ \\ \Psi_R^- \end{pmatrix} = M(M_P M)^{N-1} \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix} = \begin{pmatrix} \frac{1}{t}(r_N^2 + t_N^2) & -\frac{r_N}{t_N} \\ -\frac{r_N}{t_N} & \frac{1}{t_N} \end{pmatrix} \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix} \tag{3.4}$$

Where r_N is the total reflectivity of the n-layer system.

3.1.2 The Reflectivity of a Basic System

Using this model we can now calculate the reflectivity for different layer counts. We calculated this with a single layer having $R = 0.5$ and $T = 0.5$, the results from this are plotted in figure 3.2. From this we note a splitting of the minima around $\phi = n * \pi + \frac{1}{2}\pi$ with the number of minima between 0 and π being $N - 1$.

3.2 Application to Few-Layer Graphene

Now we will be considering graphene and how we need to model this using transfer matrices.

The phase ϕ of a wave advances by $\phi = q * d$ where q is the wave vector and d is the distance traveled, thus in this case the distance between two graphene layers which is $3.35 * 10^{-10}$ m [9]. Upon entering the material from vacuum the electron gains energy equal to the workfunction ϕ_w of graphene which equals 4.6 eV. Thus we get that ϕ is given by equation 3.5 with E_0 the energy of the incoming electron in vacuum and m_e the free electron mass. We use m_e because the effective electron mass for the interlayer state is close to 1 m_e[10].

$$\phi = \sqrt{\frac{2m_e}{\hbar^2}(E_0 + \phi_w)} \tag{3.5}$$

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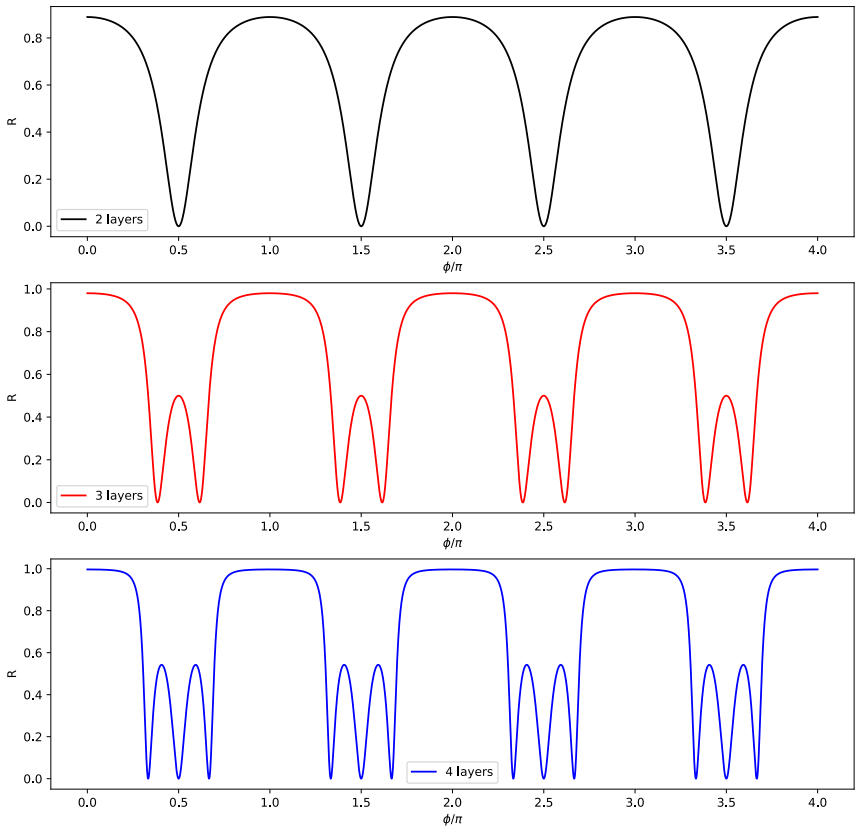

Figure 3.2: *Plots of the reflectivity the model predicts for two, three and four layers that each have $R = 0.5$ and $T = 0.5$. The minimum at $\phi = n * \pi + \frac{1}{2}\pi$ split into $N - 1$ minima*

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To account for absorption at higher energies we have that R and T of a single layer depends on energy and are given by equations 3.6 and 3.7 and that $r = \sqrt{R}$ and $t = \sqrt{T}$

$$T = \begin{cases} 0.6 \text{ for } E_0 < 6\text{eV} \\ 0.6 * e^{\frac{E_0 - 6}{9}} \text{ for } E_0 > 6 \text{ eV and } T > 0.2 \\ 0.2 \text{ for all other values of } E_0 \end{cases} \tag{3.6}$$

$$R = \begin{cases} 0.1 \text{ for } E_0 < 6\text{eV} \\ 0.1 * e^{\frac{E_0 - 6}{9}} \text{ for } E_0 > 6 \text{ eV and } R > 0.033 \\ 0.033 \text{ for all other values of } E_0 \end{cases} \tag{3.7}$$

The chose for this is explained by Geelen et al.[6]

The results from this are plotted in figure 3.4. We note that this model captures the characteristics of the measured data from Hibino et al [4] which is also plotted in figure 3.3.

It models the minima correctly where in the 0-6 eV range there are $N - 1$ minima for N-layer graphene. It also models the peak at 25 eV.

3.3 Spectra of hBN

The spectra of hBN are very similar to those of graphene. Both exhibit the same pattern where the amount of local minima in the 0-5 eV range depends on the layer count. Both also have a local maximum at 25 eV. However they differentiate themselves in that hBN has a local minimum at 8 eV that graphene does not.

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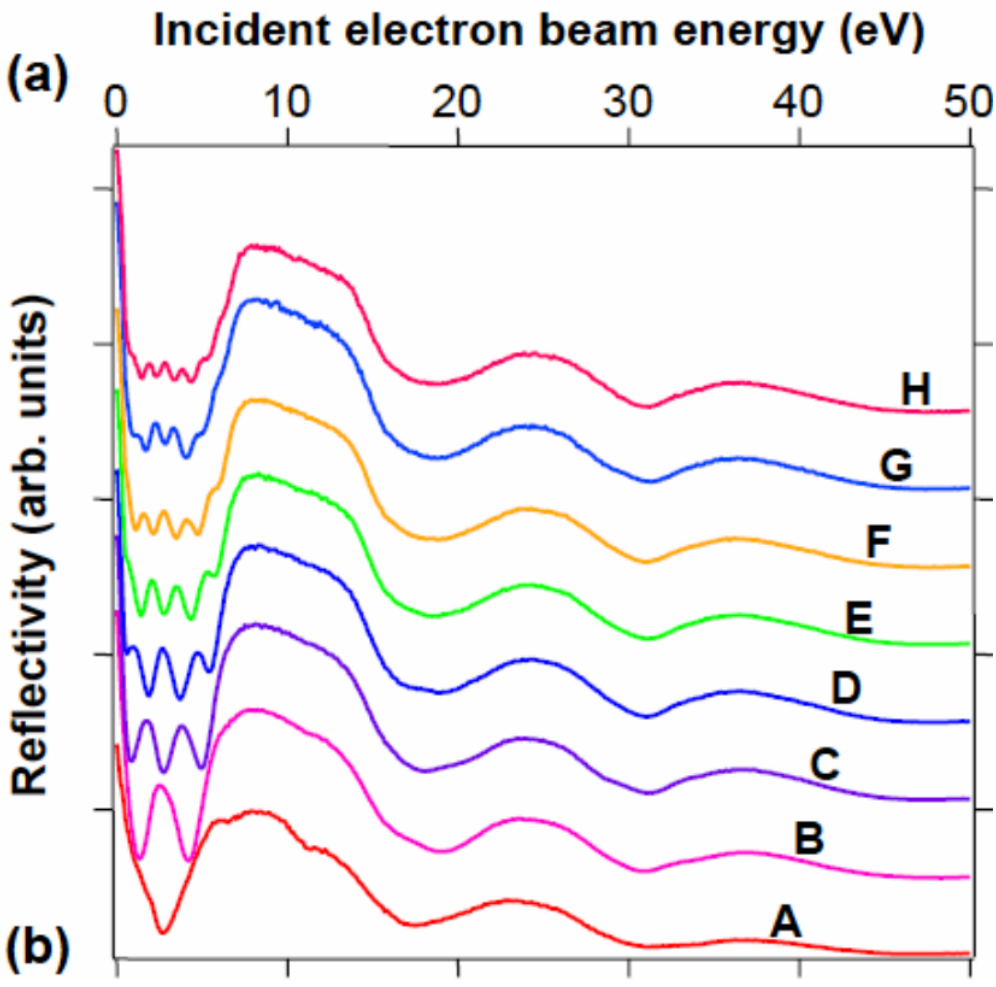

Figure 3.3: *The graphene spectra as measured by Hibino et al. [4], the figure is from the same paper. A = 2 layers of graphen, B = 3, C = 4 etc. We note that the n-layer graphene has $n - 1$ minima in the 0-5 eV range.*

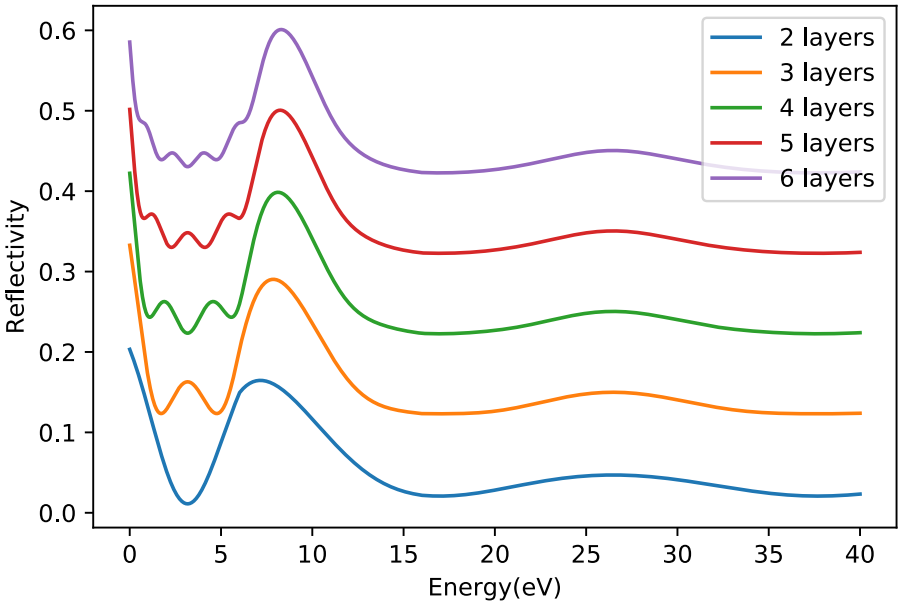

Figure 3.4: *The spectrum of graphene that equation 3.4 predicts with the R and T from equations 3.7 and 3.6 with an offset of $(\text{number of graphene layers} - 2) * 0.1$ for clarity*

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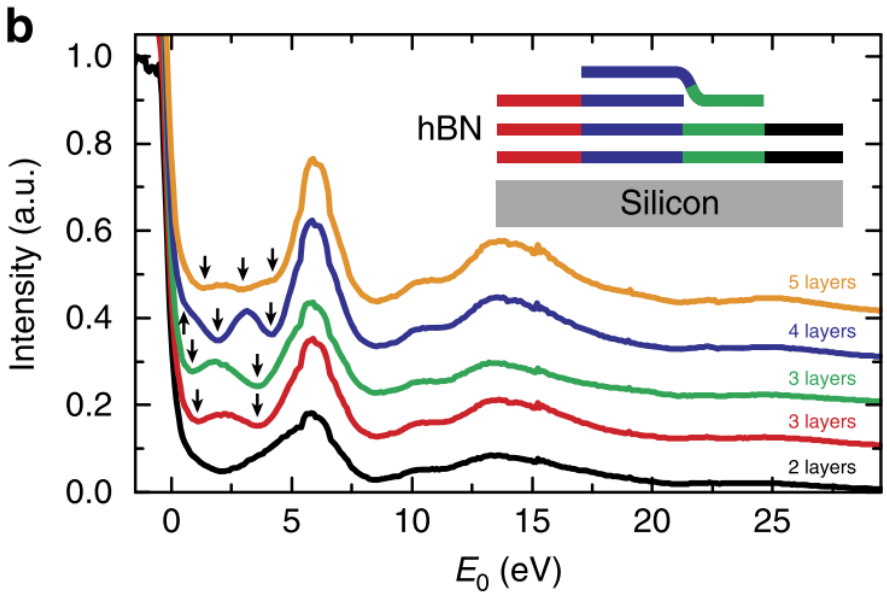

Figure 3.5: *Reflectivity of hBN as measured by Jobst et al. [5] we note that the hBN shows the same local minima in the 0-5 eV range as graphene. It also has a minimum at 8 eV that the graphene does not.*

Chapter 4

Results

We will be applying the model from section 3.1 to find an analytical expression for the spectra of graphene.

Followed by this we will examine the spectra of graphene on hexagonal boron nitride, hBN, found by Jobst et al. [5] and try to explain this using the same model. We explore this problem from two different angles, one is the incoherent case, where after the electrons have travelled through the hBN they have lost all phase information. The other case we will look at is the coherent case, where we treat the layers of hBN the same was as we would treat additional layers of graphene but with different R and T associated to those layers compared to the layers in the bulk graphite.

4.1 Finding an Analytical Expression for Graphite

Using the method of transfer matrices we want to start by finding an analytical expression for the spectra of graphite. We do this by treating graphite as an infinitely large stack of graphene layers. To do this we will exploit the properties of the eigenvalues of this matrix, allowing us to take this model to the limit of an infinite amount of layers. In this whole process we can limit ourselves to the matrices of the form in equation 4.1.

$$(M_p M)^N = \begin{pmatrix} \frac{1}{t}(r^2+t^2)e^{i\phi} & -\frac{r}{t}e^{i\phi} \\ -\frac{r}{t}e^{-i\phi} & \frac{1}{t}e^{-i\phi} \end{pmatrix}^N \tag{4.1}$$

Because, as the amount of graphene layers go to infinity the transmittivity goes to 0. The reason for that is that for graphene $r^2 + t^2 < 1$ there has to be a loss of electrons when they interact with a layer of graphene. However, as the electrons pass through each layer of graphene there will

be less and less of them because some got reflected. This means that if we have a large amount of layers the electrons that interact with the last layer are few, and this last layer will have minimal effect on the resulting spectra.

Then we shall consider equation 4.1 to be a transfer matrix. If we calculate $M_2 = MM'$ with M and M' arbitrary transfer matrices. We find the results from equation 4.2.

$$r_2 = \frac{r(r'^2 + t'^2) + r'}{rr' + 1} \tag{4.2}$$

If we then apply the condition that $t' = 0$ we find that $r_2 = r'$. Thus we can limit ourselves to investigating equation 4.1 instead of equation 3.4. This is what one would expect. M' is the first system through which the wave passes. Thus if the transmittivity of the first system is 0 you would not expect for the reflection to be affected by whatever is behind it.

4.1.1 Diagonalization of the Transfer Matrix

We want to be able to diagonilize equation 4.1 to use equation 4.3 such that we can easily calculate M^N.

$$M^N = DQ^N D^{-1} \tag{4.3}$$

With D the matrix with the eigenvectors and Q a diagonal matrix with the eigenvalues on the diagonal. Using SymPy[11] we find that the eigenvalues $\lambda_\pm$ are given by equation 4.4.

$$\lambda_\pm = \frac{((r^2 + t^2)e^{2i\phi} + 1 \pm p)e^{-i\phi}}{2t} \tag{4.4}$$

With p being given in equation 4.5

$$p = \sqrt{((r^2 + t^2)e^{2i\phi} - 2te^{i\phi} + 1)((r^2 + t^2)e^{2i\phi} + 2te^{i\phi} + 1)} \tag{4.5}$$

With corresponding eigenvectors given in equation 4.6

$$v_\pm = \begin{pmatrix} v_{\pm,0} \\ v_{\pm,0} \end{pmatrix} = \begin{pmatrix} \frac{2r}{\lambda_\mp t - 1} e^{2i\phi} \\ 1 \end{pmatrix} \tag{4.6}$$

Next we note that D^{-1} is given by equation 4.7

$$\frac{1}{\det(D)} \begin{pmatrix} v_{-,1} & -v_{-,0} \\ -v_{+,1} & v_{+,0} \end{pmatrix} \tag{4.7}$$

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combining equations 4.3, 4.4, 4.5, 4.6 and 4.7 we find the t_N and r_N are given by equations 4.8 and 4.9

$$t_N = \frac{1}{\lambda_-^N v_{+,0} v_{-,0} - \lambda_+^N v_{+,1} v_{-,0}} \tag{4.8}$$

$$r_N = -\frac{\lambda_+^N v_{-,1} v_{+,1} - \lambda_-^N v_{+,1} v_{-,0}}{\lambda_-^N v_{+,0} v_{-,0} - \lambda_+^N v_{+,1} v_{-,0}} \tag{4.9}$$

4.1.2 Eigenvalue Analysis

We will start by analyzing the eigenvalues if $r^2 + t^2 = 1$ and $r, t \in \mathbb{R}$. In that case the eigenvalues can be simplified to equation 4.10.

$$\lambda_\pm = \frac{2\cos\phi \pm e^{-i\phi}\sqrt{e^{2i\phi}(2(1-2t^2) + 2\cos 2\phi)}}{2t} \tag{4.10}$$

We note that $e^{-i\phi}\sqrt{e^{2i\phi}} = e^{-i\phi} * \pm e^{i\phi} = \pm 1$. With $+1$ if $-\frac{1}{2}\pi + n * 2\pi \leq \phi \leq \frac{1}{2}\pi + n * 2\pi$ and -1 if $-\frac{3}{2}\pi + n * 2\pi \leq \phi \leq \frac{1}{2}\pi + n * 2\pi$.

This leads to us being able to say that

$$\lambda_- = \frac{|2\cos\phi| - \sqrt{2(1-2t^2) + 2\cos 2\phi}}{2t} = \frac{|\cos\phi| - \sqrt{\cos\phi^2 - t^2}}{t}$$

We will now show that $|\lambda_-|_{max} \leq 1$ for certain ϕ where $\sqrt{\cos\phi^2 - t^2}$ is real we note that if $t = 1$ we see that $|\lambda_-|_{max} = 1$ for $\phi = n * \pi$, and less than $|\lambda_-|_{max} < 1$ for other ϕ. Then for $t = 0$ we get the following limit which can be solved using L'Hôpital's rule.

$$\lim_{t\to 0} \frac{|\cos\phi| - \sqrt{\cos\phi^2 - t^2}}{t} = 0$$

Then we note that $|\lambda_-|_{max}$ increases monotonically for $0 \leq t \leq 1$, thus $0 \leq |\lambda_-|_{max} \leq 1$.

Next we will consider the ϕ such that $\sqrt{\cos\phi^2 - t^2}$ is imaginary, we find that

$$\lambda_- = \frac{|2\cos\phi| - \sqrt{-\cos\phi^2 + t^2}i}{2t}$$

and thus that

$$|\lambda_-| = \sqrt{\frac{4\cos\phi^2 - 2 + 4t^2 - 4\cos\phi^2 + 2}{4t^2}} = 1$$

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if the square root is imaginary for $r^2 + t^2 = 1$

Thus we have proven that

$$|\lambda_-|_{max} \leq 1$$

if $r^2 + t^2 = 1$ and $r, t \in \mathbb{R}$.

Using this we can show by a simple argument that $|\lambda_-|_{max} < 1$ if $r^2 + t^2 < 1$. Let us take a fixed $t < 1$ and let $r = 0$. And we note that equation 4.5 is now minimized with respect to our chose of t. and that it increases monotonically as r increases and so does the $r^2 + t^2$ term of equation 4.4. Thus $|\lambda_-|$ has to increase monotonically as well when r increases.Together with the upper bound of 1 for r2+t2=1 derived above, we find:

$$0 \leq |\lambda_-|_{max} < 1$$

If $r^2 + t^2 < 1$ and $r, t \in \mathbb{R}$.

4.1.3 The Limit of Taking the Number of Layers to Infinity

Now we will consider the limit of an infinite amount of layers. We have shown that if $r^2 + t^2 < 1$, then $|\lambda_-| < 1$. This gives us the result from equation 4.11.

$$\lim_{N\to\infty} |\lambda_-|^N = 0 \tag{4.11}$$

Using this we can take find the r_N for an N-layer system as N goes to infinity. This gives us the results from equations 4.12-4.15 and we plot this expression in figure 4.1. These expressions come from the fact that for a transfer matrix with elements a_{ij} with the index i representing the row number and index j the column number $r = -\frac{a_{21}}{a_{22}}$ and that $a_{21} = a_{12}$. And then writing a_{ij} out in terms of eigenvalues and elements from the eigenvectors of the transfer matrix.

$$r_\infty = \lim_{N\to\infty} r_N = \lim_{N\to\infty} -\frac{\lambda_+^N v_{-,1} v_{+,1} - \lambda_-^N v_{+,1} v_{-,0}}{\lambda_-^N v_{+,0} v_{-,0} - \lambda_+^N v_{+,1} v_{-,0}} = \frac{v_{-,1}}{v_{-,0}} \tag{4.12}$$

$$= \lim_{N\to\infty} -\frac{\lambda_+^N v_{-,0} v_{+,0} - \lambda_-^N v_{+,0} v_{-,0}}{\lambda_-^N v_{+,0} v_{-,0} - \lambda_+^N v_{+,1} v_{-,0}} = \frac{v_{+,0}}{v_{+,1}} \tag{4.13}$$

$$= \frac{\lambda_- t - 1}{2r} e^{-2i\phi} = \frac{((r^2 + t^2)e^{2i\phi} + 1 - p)e^{-i\phi} - 2}{4r} e^{-2i\phi} \tag{4.14}$$

$$= \frac{2r}{\lambda_+ t - 1} e^{2i\phi} = \frac{4r}{((r^2 + t^2)e^{2i\phi} + 1 + p)e^{-i\phi} - 2} e^{2i\phi} \tag{4.15}$$

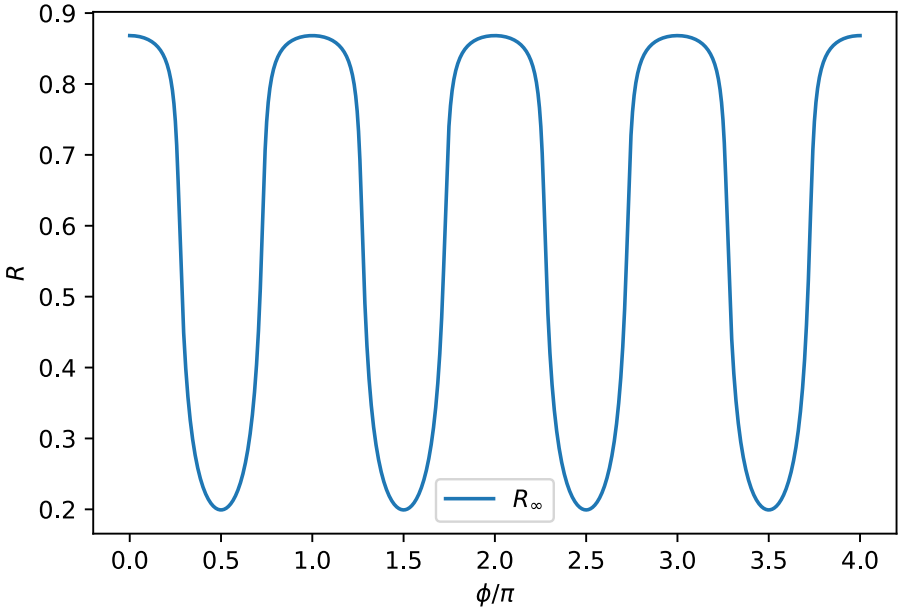

Figure 4.1: *Plot of the expression we found for R_∞ in equations 4.12-4.15 with that for a single layer $R = 0.5$ and $T = 0.4$ for a single layer*

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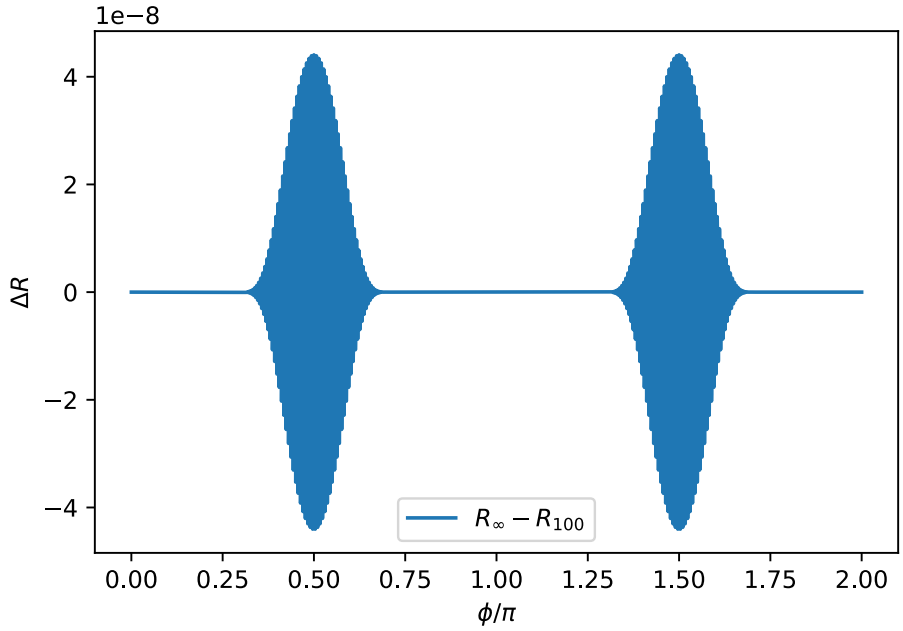

Figure 4.2: *Plot of the difference between the analytical expression for R_∞ and the numerical expression for 100 layers with $R = 0.5$ and $T = 0.4$*

We plot the difference between the analytical expression and the numerical calculation in figure 4.2. We also note that as we increase the amount of simulated layers the difference between the two expressions decreases.

4.1.4 Graphite

We will now apply this to model the spectra of graphite. We will again use the same R, T and ϕ as we did to model the few-layer graphene and model graphite as infinite-layer graphene using equation 4.15. We plot this with the experimental results gotten from the measurements on graphite in figure 4.3.

We now note that the analytical model for graphite captures the essential characteristics of the low energy spectra, the 8-10 eV peak and the peak at 25 eV. We also see that this model breaks down after this. If this could be fixed by changing the input parameters is something to be explored.

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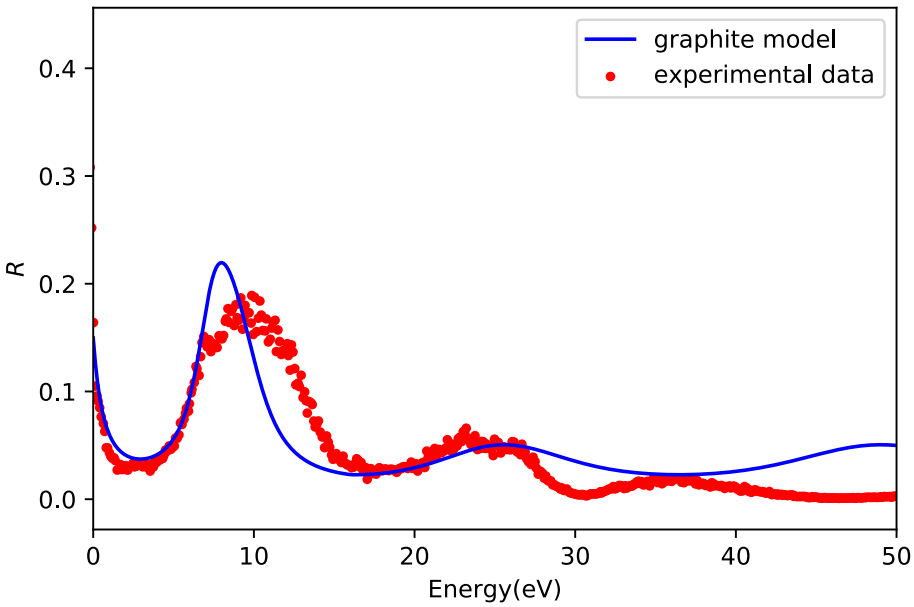

Figure 4.3: *The analytical results of the reflectivity of the spectra of graphite modeled as an infinite amount of layers of graphene stacked on top of one another plotted with the measurements of the spectra. See equations 4.12-4.15 using our assumptions for graphene from section 3.2*

4.2 Graphene on Hexagonal Boron Nitride

Next we will apply the model on system of graphene on hBN. We will look at it in three different cases, one where after the electrons pass through the graphene the system is incoherent, this means that we discard all phase information and redefine $r = R$ and $t = T$ for graphene. In the second approach we treat the bulk hBN as we would treat adding extra layers of graphene to the system but using the transfer matrix that represents bulk hBN instead. This has as complication that we only know R but not r for bulk hBN, and thus do not have any information on the phase of electrons that reflect from hBN. We try solving this issue by substituting this with the phase that our model predicts for graphite. Lastly we approach this problem as a mix of the previous two where we do not add the add the phase information of graphite to that of bulk hBN and we call this case the modified coherent case. The data we use for the bulk hBN and graphene on hBN is from Jobst et al. [5]

Incoherent

In the incoherent case we will substitute for the reflection and transmission amplitudes r and t for the measurements of R and T. Thus that our reflection and transmission amplitudes are the measurements, and not their root. Because R and T are real valued we can use equation 4.2 with $r' = R_{graphene}$, $r = R_{hBN}$, $t' = T_{graphene}$. The results of this are plotted in figure 4.4c. We note that the incoherent model doesn't show a clear minimum at 8 eV, a defining feature of the hBN spectra], that you see in the spectra in figure 4.4d.

Coherent

For the coherent model we treat the bulk hBN like we would treat another layer of graphene but using a transfer matrix that would represent bulk hBN. To do this we will reconstruct the r for bulk hBN from the measurements on R_{hBN} and substituting the phase of r with the phase of bulk graphite.Using this we can reconstruct the transfer matrix for bulk hBN because we know that the transmittivity of it is near 0 like with graphite. Because we do not have measurements on the phase of r_{hBN} we substitute this with the phase information from graphite that we found with our model. Thus we write $r = \sqrt{R}e^{i\phi_{graphite}}$ with $\phi_{graphite}$ being the phase of the electron wave function after it has been reflected of graphite. This means we implicitly assume that the minima at 8 eV for hBN is not caused by

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resonance phenomena but by something else. For the distance between the graphene and hBN we take the same distance as between two layers of graphene. We do this because the distance between layers of hBN is very similar to that of graphene [12]. And we do not know of the distance between two layers of graphene and hBN. But we think it is a reasonable enough assumption to take a distance that is similar to the distance between two layers of graphene or the distance between two layers of hBN. For the workfunction between graphene and hBN we use $4.4eV$ as found by Ogawa et al.[13] The results from this model for graphene on top of hBN is plotted in figure 4.4a. And like the measurements in figure 4.4d the model approaches the spectra of graphene in 3.4 as the number of graphene layers increases.

Modified Coherent

We also modeled the system where for graphene we kept the phase information intact but for hBN used that $r = \sqrt{R}$ from our measurements on R and thus assume that r is real valued. We call this case the modified coherent case. It gave results that were very similar to the incoherent case. But to have the 0-5 eV range agree with measurements we had to set the distance between the graphene and hBN to 0, otherwise the amount of minima did not match up with those found in the measurements and you would have one too many minima. The results of this are plotted in figure 4.4b

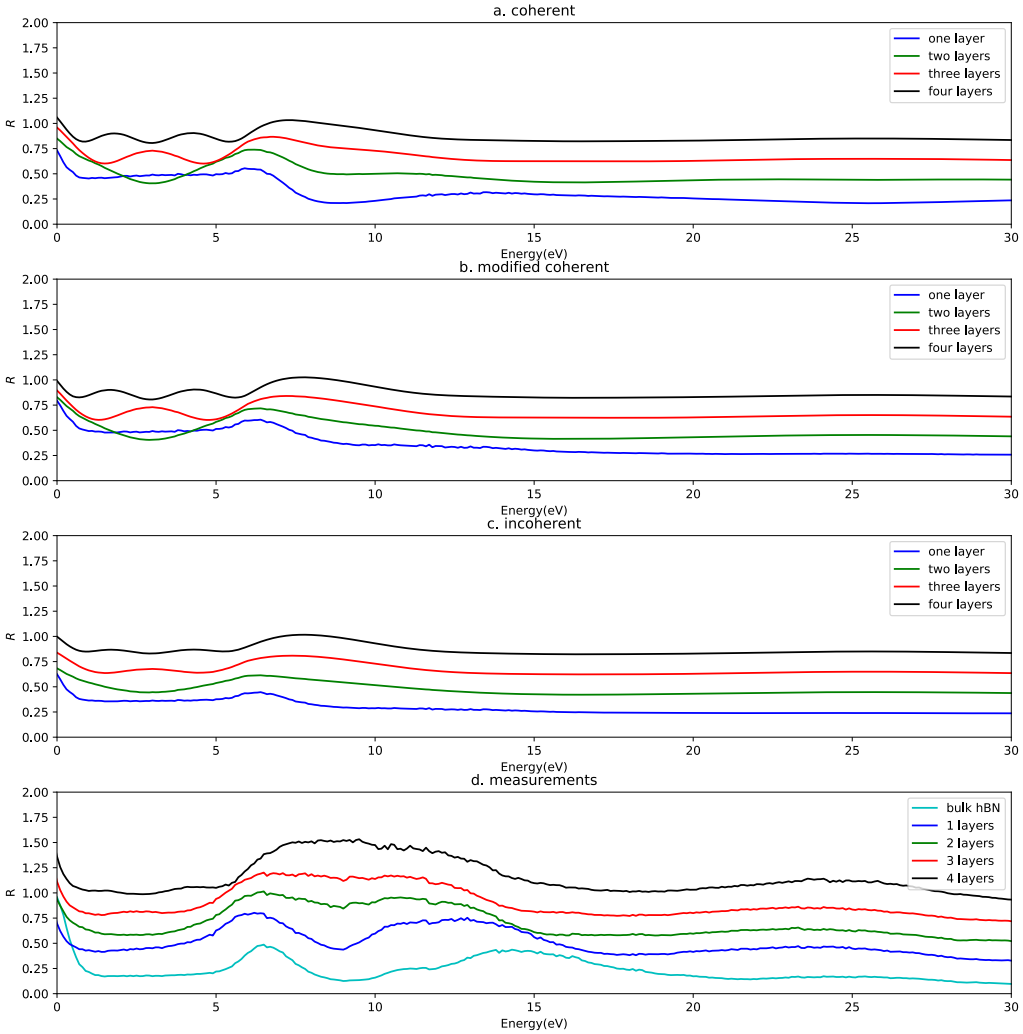

Figure 4.4: *in plots a,b and c we plot the reflectivity our models predict for graphene on hBN, we plot one, two, three and four layers of graphene on top of bulk hBN. In plot d we plot Measurements on the reflectivity of graphene on bulk hBN. using data from Jobst et al [5] All graphs are offset with an offset of number of graphene layers* $*$ 0.2 *for clarity*

Chapter 5

Discussion

We found an analytical expression for the reflectivity of graphite at low energies using our method of transfer matrices that captures the essential features of the graphite spectra. However, it doesn't fit perfectly. The maxima do not overlap exactly and there is a difference in their periodicity.

For graphene on hBN we found that the coherent model explains the data on graphene on bulk hBN from Jobst et al.[5] best. However we still find issues in the magnitude of the maxima. In the measurements it is found that the maximum at 6 eV and the maximum at 14 eV have approximately the same magnitude, while our model predicts a lower maximum at 14 eV. This could have two root causes. The issue could lie in how we model the system as a whole and that treating bulk hBN akin to another layer of graphene still misses interactions vital to explaining the spectra. The other, more likely, possibility is that we need to modify the assumptions we made for graphene to make the data of graphene fit better to that of the measurements by Hibino et al. [4]. This is based on that the biggest issue our model has is the width of the 8 eV maximum. While the measured data has a wider maximum at 8 eV. It is possible that this is obscuring the effects that the hBN has on the spectra. A possible way to check this hypothesis, without having to modify the assumptions we made for graphene, is to apply the same procedure to the measurements of few-layer graphene as we did to bulk hBN in the coherent case. Take the measurements of R for few-layer graphene, and reconstruct r using the phase our model predicts. Because we are talking about few-layer graphene the same procedure needs to be applied to the transmittivity T. This method would not be fully correct because it is a likely possibility that our phase is not wholly correct either. However, it should give insights into whether this is the correct approach to take, or if there might be

graphene-hBN interactions that we are missing.

Chapter 6

Conclusion

We used transfer matrices to find an analytical solution to the LEEM spectra of graphite. The expression we found from this method captures the essential features of the graphite spectra just like it captures the essential features of the few-layer graphene spectra measured by Hibino et al.[4] The analytical expression we found for graphite exhibits the same problem as the spectra our model predicts for few-layered graphene. With details like the width of the 8 eV peak in the spectra not agreeing with experiment.

The same method was also applied to graphene on hexagonal boron nitride. We applied the model in three different ways, coherent, incoherent and a modified coherent way. The coherent case, where we assume that the phase of the reflectivity of bulk hBN and graphite are the same, seems to agree the best with the measurements that were previously done on the reflectivity of graphene on hBN by Jobst et al.[5] We do not know if the differences between the model and measured data is because of how we modeled the combination of graphene and hBN or if it is because of how we modeled the graphene spectra.

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