

SIMULATION OF ELECTRON DIFFRACTION PATTERNS IN THE CuAu L1<sub>0</sub> PHASE

by

Nathaniel Levi Ralston

A senior thesis submitted to the faculty of

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Bachelor of Science

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BRIGHAM YOUNG UNIVERSITY

DEPARTMENT APPROVAL

of a senior thesis submitted by

Nathaniel Levi Ralston

This thesis has been reviewed by the research advisor, research coordinator,  
and department chair and has been found to be satisfactory.

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Date

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Richard Vanfleet, Advisor

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Date

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Eric Hintz, Research Coordinator

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Date

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Spencer Ross, Chair

## ABSTRACT

### SIMULATION OF ELECTRON DIFFRACTION PATTERNS IN THE CuAu L1<sub>0</sub> PHASE

Nathaniel Levi Ralston

Department of Physics and Astronomy

Bachelor of Science

Many intermetallic systems are characterized by chemical ordering, and when in the ordered phase display many scientifically interesting and technology useful properties. The materials system investigated in this document is CuAu, which can chemically order in the L1<sub>0</sub> phase, which is a layer by layer stacking sequence of Cu and Au atoms on an FCC lattice. Multislice simulations are used to study the electron scattering intensity of chemically ordered CuAu. A chemical order parameter ( $S$ ) is used to quantify the degree of ordering in the material. This chemical order parameter is determined by the ratio of the intensity of the (110) peak to that of the (220) peak. The relation between peak intensities and the chemical order parameter is found for fifteen individual thicknesses ranging from  $\sim 6$  Å to  $\sim 100$  Å. The (110) peak to (220) peak intensity ratio increases for increasing thickness and increasing order parameter. The calculated intensity ratios can now be compared to experimental

electron scattering results to extract the sample order parameter.

## ACKNOWLEDGMENTS

I thank Dr. Richard Vanfleet for his guidance in my research. I also give a heartfelt thanks to my wife and children for their patience and support.

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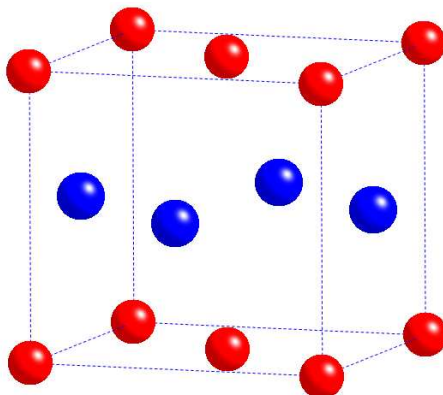


# Chapter 1

## Introduction

Ordered intermetallic materials systems include some of the most scientifically interesting and technologically important materials known. For example, the aluminides are used for their high temperature mechanical properties, while the state-of-the-art in magnetic materials are the ordered phases of transition metals with either rare earth or noble metals. There is a strong relationship between ordering and many materials properties; for example, the ordered phases of the ferromagnetic CoPt, FePt, and others are excellent hard magnetics but the disordered phases are poor magnets.

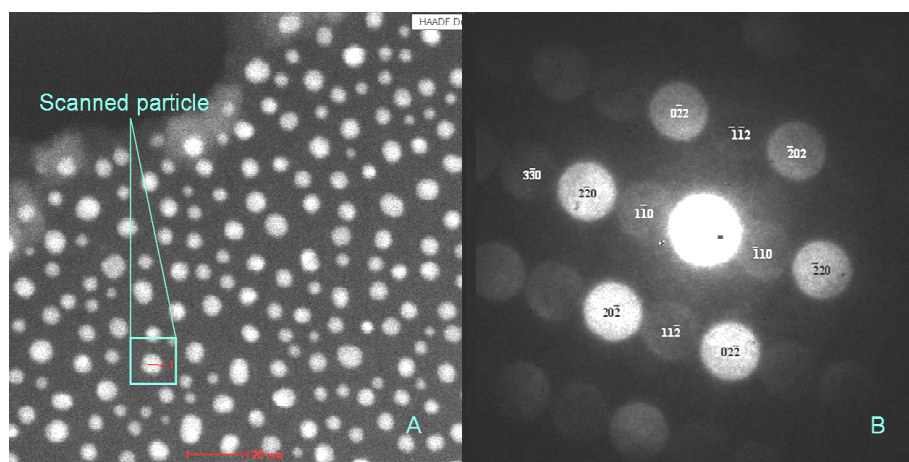
Previous experiments with FePt have brought to light limitations in our understanding of intermetallic magnetic nanoparticles. One of the motivations for this research was to form nanoparticles of FePt, allowing for high density data storage. Experimental and theoretical work has shown that as the particle size decreased the system failed to order itself, denying the desired magnetic properties. This has led the BYU research group of Richard Vanfleet and his collaborator Kevin Coffey at the University of Central Florida to question the physical reasons for these limitations.



**Figure 1.1** Unit cell of the  $L1_0$  phase of CuAu, with Cu and Au stacking in alternating layers.

Particular interest lies in the role of processing (kinetics) vs. particle size (thermodynamics) on the factors like the chemical order parameter and the order-disorder temperature. To determine which of these (kinetics or thermodynamics) dominates within the  $L1_0$  ordering of intermetallic nanoparticles, we are combining computational modeling and experimental Transmission Electron Microscopy (TEM) measurements to study the ordering and disordering process. The materials systems of choice in this study are CuAu and FeNiPt. The high temperature phase of these materials is disordered (A1 structure) with a random atom at each lattice site. In the low temperature phase ( $L1_0$  structure) atoms of the same element stack in alternating layers with a compression of the lattice constant in the stacking direction. The  $L1_0$  phase is shown in Fig. 1.1. The order parameter ( $S$ ) quantifies the degree of ordering related to the number of atoms of each type in the correct ordered layer. A fully ordered system has an order parameter of 1 and a disordered system has an order parameter of 0.

This document focusses on the computational simulation of electron scattering from CuAu in the (111) orientation with the goal of obtaining a way to determine the chemical order parameter of CuAu from the experimental TEM measurements.



**Figure 1.2** Experimental TEM photo of FePt in (111) orientation [6].

Traditionally, X-ray scattering is used to obtain diffraction patterns as the X-rays interact with the atoms in the crystal, revealing crystal structure of the material. Electron scattering may be preferable for thin films or nanoparticles since the electrons interact more strongly than X-rays and thereby allow sufficient signal to study small volumes. The diffraction pattern obtained from this method displays an order dependent peak (110) which, when compared to the peak next to it (220), quantifies the degree of ordering (see Fig. 1.2). The data from this work will be used in conjunction with experimentally observed diffraction patterns to extract the order parameter of CuAu particles.

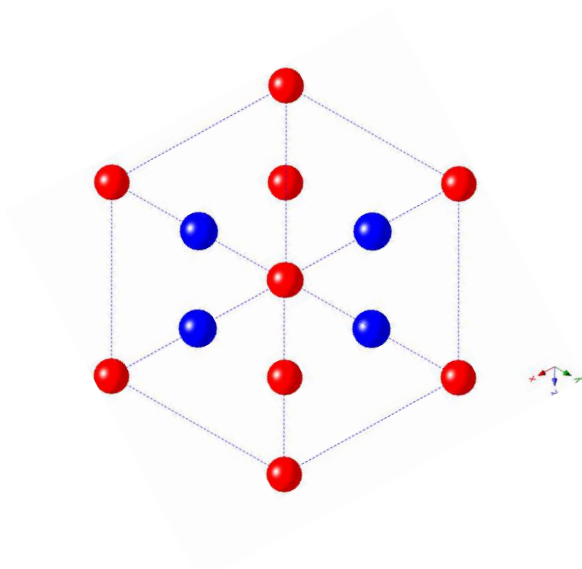
# Chapter 2

## Methods

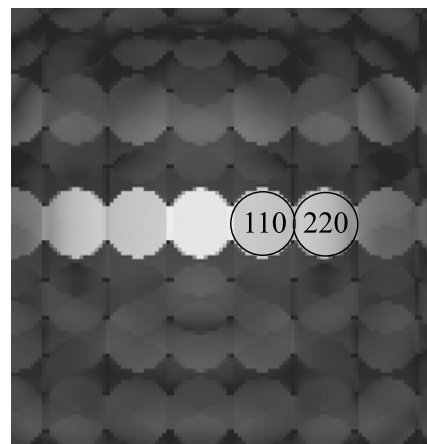
The computational aspect of the investigation on the  $L1_0$  ordering of CuAu depends upon single particle characterization (imaging, diffraction, and composition analysis). This will take into account  $S$ , thermal effects, and output diffraction patterns, which can then be analyzed and quantitatively compared to experimentally derived patterns. These diffraction patterns are created using a simulated electron beam of 200 keV at normal incidence and a cell orientation of (111) (see Fig. 2.1 and 2.3).

The diffraction in this orientation of the cell provides the (110) and (220) peaks needed for analysis (see Fig. 1.2). The intensity of (110) peak is order dependent—present for well-ordered structures while absent for disordered structures (see Fig. 2.3, 2.2, 2.1, and 2.4). The ratio of the intensity of the (110) peak to that of the (220) peak for a given sample thickness should give a unique value which determines  $S$ . The end goal is to use this order parameter dependency to obtain graphs that display the peak intensity ratio versus chemical order parameter for different thicknesses in CuAu for comparison to experimental results.

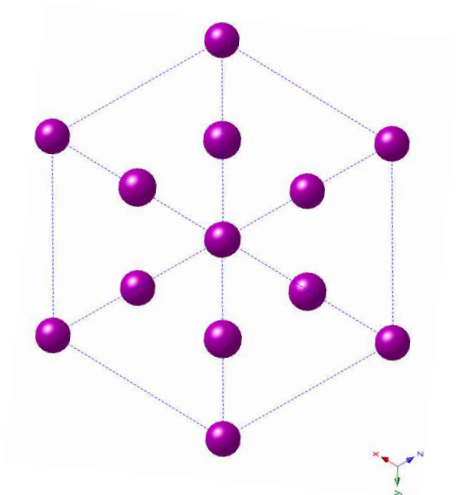
A file containing atom positions of a CuAu structure is needed to begin the simu-



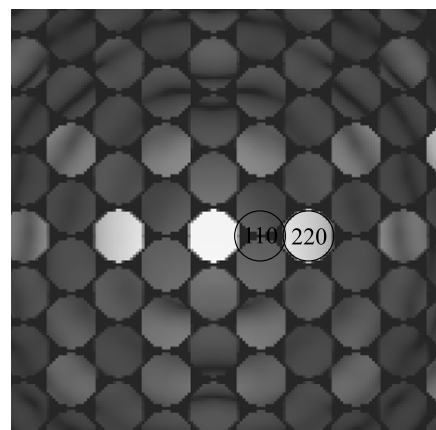
**Figure 2.1** Figure of the  $L1_0$  structure in the  $(111)$  orientation. The red represents one element, e.g. Cu, while the blue represents the other, Au.



**Figure 2.2** Simulated diffraction pattern of a CuAu atoms in the ordered  $L1_0$  phase in the  $(111)$  orientation. Scaling is logarithmic.



**Figure 2.3** Figure of the  $A1$  structure in the  $(111)$  orientation. The lack of different colors represents the absence of any discernible order in the structure.



**Figure 2.4** Simulated diffraction pattern of a CuAu atoms in the disordered  $A1$  phase in the  $(111)$  orientation. Scaling is logarithmic.

lation. This structure becomes the input for a multislice routine. A multislice routine is a program that takes a file of atomic positions and simulates the interaction of an incident beam of a specified energy with the given structure. The program used in this study is the Kirkland Multislice routine.

## 2.1 .xyz Files and Kirkland Multislice Routine

### 2.1.1 Creation of .xyz files

The .xyz files accepted by the Kirkland Multislice Routines were created through Matlab and simulate atom positions in a three dimensional binary structure. The L1<sub>0</sub> structure possesses an fcc-like arrangement with a compression of the lattice constant in the ordering direction. Lattice constants of  $a = 0.3962$  nm and  $c = 0.3670$  nm were used [4]. To simulate the thermal vibrations of the structure the atomic random thermal root-mean-square (RMS) displacements are needed in the input. This is referred to as the wobble factor ( $\sigma$ ), which was calculated to be between 0.96–0.12 nm using the relation

$$2M = \frac{12h^2T}{mK\Theta_D^2} \left[ \Phi(x) + \frac{x}{4} \right] \frac{\sin^2 \theta}{\lambda^2}, \quad (2.1)$$

where

$$\Phi(x) = \frac{1}{x} \int_0^x \frac{\epsilon d\epsilon}{e^\epsilon - 1}, \quad (2.2)$$

and  $x = \frac{\Theta_D}{T}$  with the Debye temperature ( $\Theta_D$ ) given as a range between 203.8–241.1 K [5] [1]. The Debye-Waller factor was calculated using the formula

$$2M = 16\pi^2 \sigma^2 \frac{\sin^2 \theta}{\lambda^2} = B \frac{\sin^2 \theta}{\lambda^2}. \quad (2.3)$$

I chose  $\sigma = 0.105$  nm after taking an average of my calculations and comparing with the value for  $\sigma$  from Barmak et al. [2] With the structure sized and the proper value

for  $\sigma$ , the *.xyz* file is divided into a number of smaller, equally spaced segments. These segments are used as the input for the Kirkland Multislice routine. Once the total thickness of the structure is defined, the number of segments into which it can be divided are limited to segments with integer numbers of atomic layer. For example, if the structure is 100.229544645 Å thick, then it cannot be divided into forty segments. The reason for this is that the program creates an A1 structure (fcc), which consists of three layers of atoms (the ordered phase is an L1<sub>0</sub> structure), and this structure is then stacked in the z direction, or the dimension of the thickness. If the cell structure is divided into too many segments, then many of those segments will contain no information and the spacings between layers that do have information will be incorrect. For this simulation, I divided the 100.229544645 Å structure into fifteen segments of thickness 6.681969643 Å.

### 2.1.2 Kirkland Multislice Routine

The Kirkland Multislice routine is a program developed by Earl Kirkland [3] that receives atomic positioning data in an *.xyz* format and simulates electron beam scattering through a chosen orientation of the lattice. The first part of the routine is to simulate the incoming wave as either a plane wave or a focussed beam. For this simulation I used a focussed electron beam. The pixel size of the output image was chosen to be 1024x1024 and 2048x2048. The comparison between the two pixel sizes will determine if the smaller size is sufficient to give a good solution. A more detailed description of the program inputs can be found in Appendix C. The program simulates and records the interactions of the electron beam and outputs the electron beam data through a particular segment, or slice, of the structure. This output becomes the input for the next slice. This pattern propagates all the way through the structure, outputting beam data for various thicknesses. This data can be used

to calculate diffraction patterns, which can either be viewed as a .tif file or converted to a format recognized by another program, such as Matlab.

I ran ten sets of simulations for eleven chemical order parameters, five sets with pixel dimensions of 1024x1024 and five sets of 2048x2048, with each set containing fifteen series, each series being averaged over ten thermally simulated runs. The order parameters used were 1, 0.9, 0.8, 0.7, ..., 0. The total thickness of the fifteen series used for each chemical order parameter was 100.229544645 Å, with each series having an individual thickness of 6.681969643 Å.

## 2.2 Data Processing

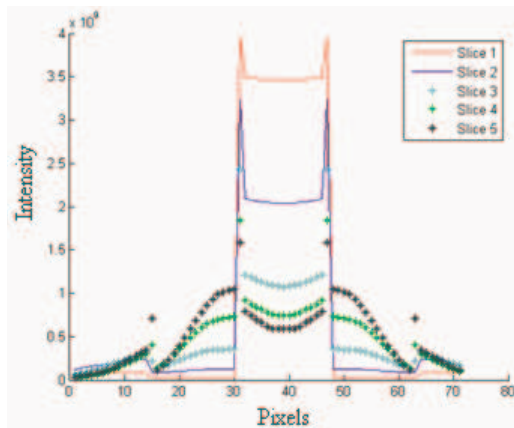
After a diffraction pattern has been simulated using the Kirkland routines and converted to a format that Matlab can recognize (such as a .dat or .chn file), the file can be loaded into Matlab. The diffraction pattern can be viewed using an image-scaled (syntax - `imagesc()`), which allows for comparison of the intensity ratio of the (110) and (220) peaks. The Matlab programs I created, named `loader` and `loader2048` (see Appendix A and Appendix B), load the data created by the Kirkland routine and analyze the relationships between intensity, thickness, and the chemical order parameter from the ratio of the intensity of the (110) peak to that of the (220) peak.



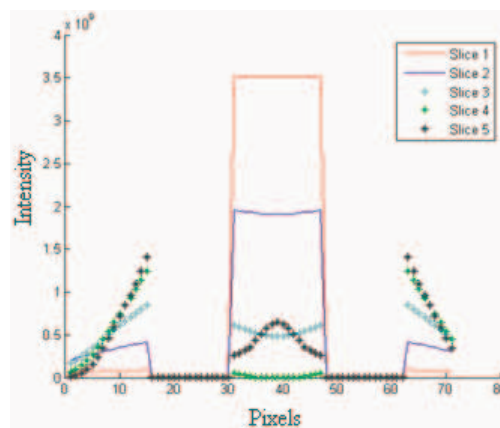
# Chapter 3

## Data

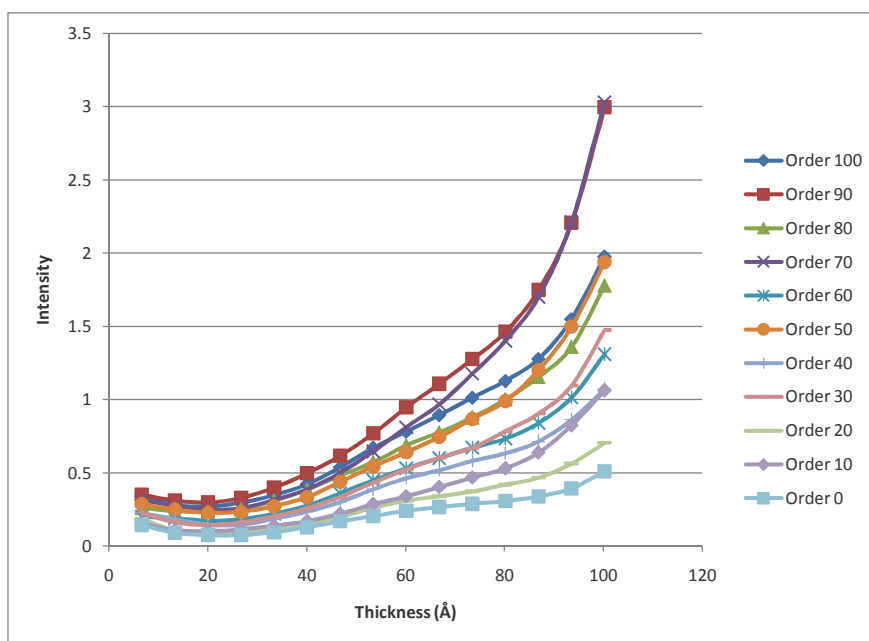
An output of the Multislice routine comes in the form of a .tif file. These files are then converted into .chn files, which are then loaded into Matlab. After determining which pixels contain the (110) and (220) peaks, the intensities of each are saved and then averaged (Fig. 3.1-3.2). The ratio of the intensity of the (110) peak to that of the (220) peak is calculated for every order and thickness. These ratios are plotted versus thickness (Fig. 3.3).



**Figure 3.1** Graph of intensity along the center row of pixels. The intensities farthest from the center represent the (220) peaks and those closest to the center represent the (110) peaks. The presence of the (110) peaks demonstrates an ordered structure.



**Figure 3.2** Graph of intensity along the center row of pixels. The intensities farthest from the center represent the (220) peaks and the lack of intensities near the center demonstrate a disordered structure.



**Figure 3.3** Graph of Intensity vs. Thickness for each Order Parameter (S).

# Chapter 4

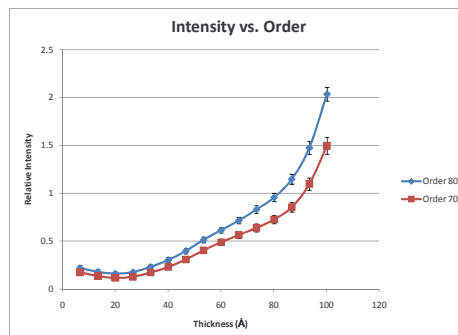
## Results and Conclusion

Each of the five sets (pixel dimensions 1024x1024 and 2048x2048) was averaged. The results are presented as graphs of the average relative intensity ratio vs. thickness (see Fig. 4.1) for varying order parameter and average relative intensity ratio vs. the chemical order parameter (see Fig. 4.2) for varying thickness. The error is calculated as standard deviation from average.

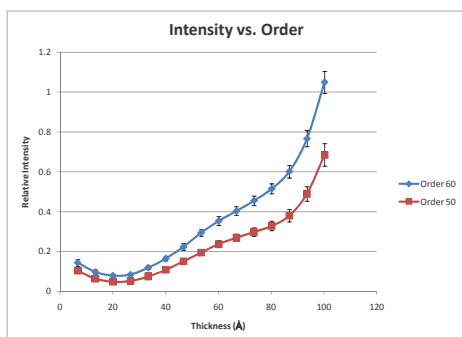
The relative intensity increases for increasing thickness, but as the chemical order parameter decreases, so does the relative intensity (see Fig. 4.1). The data for the three smallest thicknesses may be unreliable since the smallest thickness has a greater relative intensity than the two thicknesses above it (Fig. 4.2(f)). For data points after this thickness, a usable relationship between the relative intensity and the chemical ordering parameter is demonstrated.



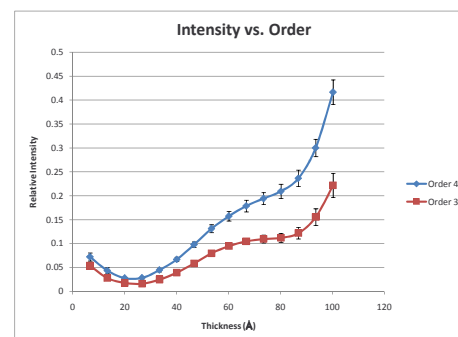
(a) Order parameter=1,0.9



(b) Order parameter=0.8,0.7



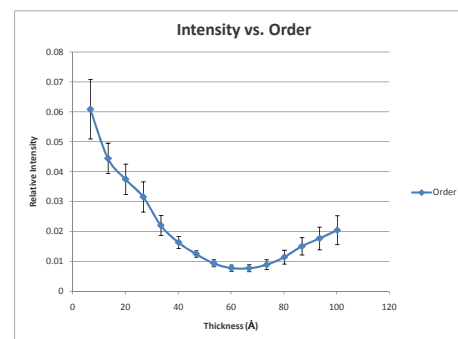
(c) Order parameter=0.6,0.5



(d) Order parameter=0.4,0.3

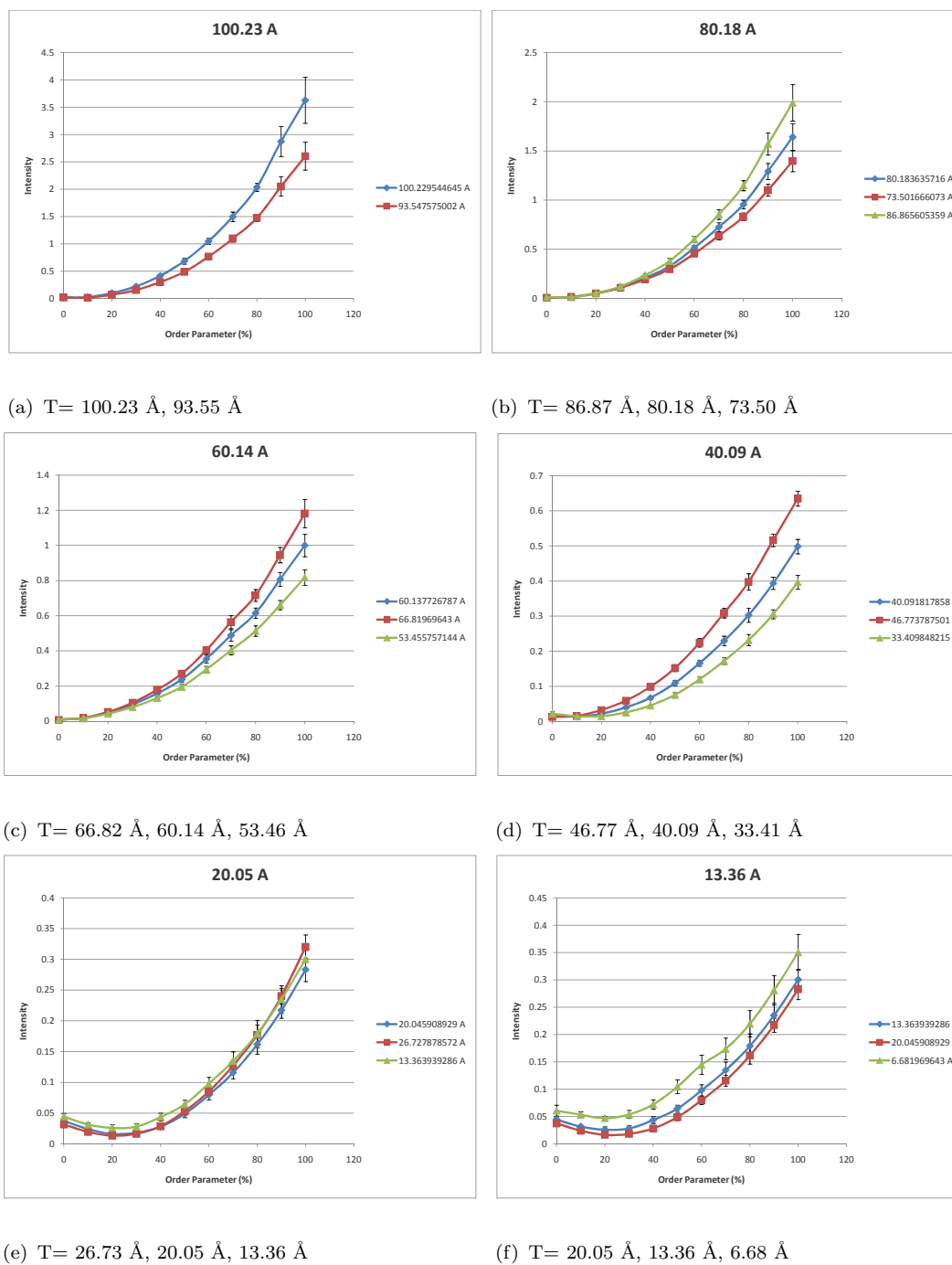


(e) Order parameter=0.2,0.1



(f) Order parameter=0

**Figure 4.1** Graphs of Relative Intensity vs. Thickness



**Figure 4.2** Graphs of Relative Intensity vs. Order Parameter for varying Thickness (T) in Å

# Appendix A

## A.1 Matlab code: loader

```
% This program loads data in the form of .chn files. It is designed to
% load in diffraction patterns of size 1024x1024 and then plot the relative intens
% 110/220 peaks with respect to either the order parameter for different
% thicknesses of the sample or the thickness of each order parameter (which
% must be the same for all orders).
```

```
close all;
```

```
global ordparnumbers
```

```
% This variable allows the user to change the order parameters to be loaded
% into the program, e.g., 100:-10:0 will load into the program order
% parameters of 100, 90, 80, 70, ... 10, 0.
```

```
ordparnumbers=0;
```

```
question='y';
```

```
while (question=='y' | question=='Y')
```

```
    question=input('Do you want to load data, y or n?', 's')
```

---

```

if (question=='y' | question=='Y')
    name=input('Enter the file name :','s')
    ordpar=input('Enter the order parameter:')
    num=input(['Enter number of individual .chn files' ...
              '(each new file must have same number of .chn files):'])

% The format for a variable that will hold data is name, then number.
% This can be changed if needed within this eval function. E.g.,
% if the filename is CuAu100sig105_1024_1.chn, the input needed is
% CuAu for name, then 100 for order parameter. The last number of
% the filename designates its position within the data to be
% loaded. If there are 15 files to load, then 15 should be entered
% for num.
for i=1:num
    filename1= [name,num2str(ordpar)];
    eval(['diffpatt' num2str(ordpar) num2str(i) '= load(''...'
          filename1 'sig105_1024_' num2str(i) '.chn'');' ])
end
end
end

% Calculate the total intensity of each datum
for ordpar=ordparnumbers
    for i=1:num

```

```
        eval(['totalI' num2str(ordpar) num2str(i) '=sum(sum(diffpatt'...
              num2str(ordpar) num2str(i) '));'])
    end
end$

% Calculate the intensity of the superlattice. This is specific to a
% diffraction pattern of size 1024x1024.
for ordpar=ordparnumbers
    for i=1:num
        eval(['superI' num2str(ordpar) num2str(i) '=sum(sum(diffpatt'...
              num2str(ordpar) num2str(i) '(504:520,493:501));'])
    end
end

% Calculate the intensity of the fundamental. This is specific to a
% diffraction pattern of size 1024x1024.
for ordpar=ordparnumbers
    for i=1:num
        eval(['fundI' num2str(ordpar) num2str(i) '=sum(sum(diffpatt'...
              num2str(ordpar) num2str(i) '(504:520,477:485));'])
    end
end

% Calculate the averaged values of the fundamental and superlattice by
% dividing by the area used to obtain superI and fundI.
```



```
for ordpar=ordparnumbers
    for i=1:num
        eval(['avsuperI' num2str(ordpar) num2str(i) '=1/128*superI'...
            num2str(ordpar) num2str(i) ';''])
        eval(['avfundI' num2str(ordpar) num2str(i) '=1/128*fundI'...
            num2str(ordpar) num2str(i) ';''])
    end
end

% Calculate the value of averaged super/fundamental
for ordpar=ordparnumbers
    for i=1:num
        eval(['ratioI' num2str(ordpar) num2str(i) '=avsuperI'...
            num2str(ordpar) num2str(i) './avfundI' num2str(ordpar)...
            num2str(i) ';''])
    end
end

% The variable plotratio__ contains the relative intensity ratio
% information needed to produce the desired graphs.
for ordpar=ordparnumbers
    for i=1:num
        eval(['plotratio' num2str(ordpar) '(' num2str(i) ')=ratioI'...
            num2str(ordpar) num2str(i) ';''])
    end
end
```

```
% Create the plot of Intensity vs. Order Parameter
askplot=input('Would you like to make plots of this data, y or n?', 's')
if (askplot=='y' | askplot=='Y')

    xaxis=input('What do you want on the x axis: order (o) or thickness (t)?', 's')
    if(xaxis=='o')
        for i=1:num
            figure
            hold on
            for ordpar=ordparnumbers
                eval(['plot(' num2str(ordpar) ',plotratio' num2str(ordpar)...
                    '(' num2str(i) '),','b.',','MarkerSize',10)']);
                xlim([0 101])
                ylim([0 max(ratioI10015)])
                title(['Slice' int2str(i)])
                xlabel('Order Parameter (in %)')
                ylabel('Relative Intensity (I)')
            end
            hold off
        end
    end
end
if(xaxis=='t')
    xmax=input('Enter the thickness of the sample:')
    step=input('Enter the step size of the sample:')
    for ordpar=ordparnumbers
```

```
figure
hold on
for i=1:num
    eval(['plot(step*i,ratioI' num2str(ordpar) num2str(i)...
            ','r.'','MarkerSize',10)']);
    xlim([0 xmax+1])
    ylim([0 max(ratioI10015)])
    title(['Order Parameter' num2str(ordpar)])
    xlabel('Thickness (A)')
    ylabel('Relative Intensity (I)')
end
hold off
end
end
end
```

# Appendix B

## B.1 Matlab code: loader2048

```
% This program loads data in the form of .chn files. It is designed to
% load in diffraction patterns of size 2048x2048 and then plot the relative intens
% 110/220 peaks with respect to either the order parameter for different
% thicknesses of the sample or the thickness of each order parameter (which
% must be the same for all orders).
```

```
close all;
```

```
global ordparnumbers
```

```
% This variable allows the user to change the order parameters to be loaded
% into the program, e.g., 100:-10:0 will load into the program order
% parameters of 100, 90, 80, 70, ... 10, 0.
```

```
ordparnumbers=0;
```

```
question='y';
```

```
while (question=='y' | question=='Y')
```

```
    question=input('Do you want to load data, y or n?', 's')
```

---

```

if (question=='y' | question=='Y')
    name=input('Enter the file name :','s')
    ordpar=input('Enter the order parameter:')
    num=input(['Enter number of individual .chn files' ...
              '(each new file must have same number of .chn files):'])

% The format for a variable that will hold data is name, then number.
% This can be changed if needed within this eval function. E.g.,
% if the filename is CuAu100sig105_2048_1.chn, the input needed is
% CuAu for name, then 100 for order parameter. The last number of
% the filename designates its position within the data to be
% loaded. If there are 15 files to load, then 15 should be entered
% for num.
for i=1:num
    filename1= [name,num2str(ordpar)];
    eval(['diffpatt' num2str(ordpar) num2str(i) '= load(''...'...
          filename1 'sig105_2048_' num2str(i) '.chn''');' ])
end
end
end

% Calculate the total intensity of each datum
for ordpar=ordparnumbers
    for i=1:num

```

```
        eval(['totalI' num2str(ordpar) num2str(i) '=sum(sum(diffpatt'...
              num2str(ordpar) num2str(i) '));'])

    end

end

% Calculate the intensity of the superlattice. This is specific to a
% diffraction pattern of size 2048x2048.
for ordpar=ordparnumbers
    for i=1:num
        eval(['superI' num2str(ordpar) num2str(i) '=sum(sum(diffpatt'...
              num2str(ordpar) num2str(i) '(1016:1032,1005:1013)));'])

    end

end

% Calculate the intensity of the fundamental. This is specific to a
% diffraction pattern of size 2048x2048.
for ordpar=ordparnumbers
    for i=1:num
        eval(['fundI' num2str(ordpar) num2str(i) '=sum(sum(diffpatt'...
              num2str(ordpar) num2str(i) '(1016:1032,989:997)));'])

    end

end
```

```
% Calculate the averaged values of the fundamental and superlattice by
% dividing by the area used to obtain superI and fundI.
for ordpar=ordparnumbers
    for i=1:num
        eval(['avsuperI' num2str(ordpar) num2str(i) '=1/128*superI'...
              num2str(ordpar) num2str(i) ';''])
        eval(['avfundI' num2str(ordpar) num2str(i) '=1/128*fundI'...
              num2str(ordpar) num2str(i) ';''])

    end
end

% Calculate the value of averaged super/fundamental
for ordpar=ordparnumbers
    for i=1:num
        eval(['ratioI' num2str(ordpar) num2str(i) '=avsuperI'...
              num2str(ordpar) num2str(i) './avfundI' num2str(ordpar)...
              num2str(i) ';''])

    end
end

% The variable plotratio__ contains the relative intensity ratio
% information needed to produce the desired graphs.
for ordpar=ordparnumbers
```

```
        for i=1:num
            eval(['plotratio' num2str(ordpar) '(' num2str(i) ')=ratioI'...
                num2str(ordpar) num2str(i) ';''])
        end
    end

end

% Create the plot of Intensity vs. Order Parameter
askplot=input('Would you like to make plots of this data, y or n?', 's')
if (askplot=='y' | askplot=='Y')
    xaxis=input('What do you want on the x axis: order (o) or thickness(t)?', 's')
    if(xaxis=='o')
        for i=1:num
            figure
            hold on
            for ordpar=ordparnumbers
                eval(['plot(' num2str(ordpar) ',plotratio' num2str(ordpar)...
                    '(' num2str(i) '),','b.',','MarkerSize',10)']);
                xlim([0 101])
                ylim([0 0.2])
                title(['Slice' int2str(i)])
                xlabel('Order Parameter (in %)')
                ylabel('Relative Intensity (I)')
            end
            hold off
        end
    end
end
```



```
if(xaxis=='t')
    xmax=input('Enter the thickness of the sample:')
    step=input('Enter the step size of the sample:')
    for ordpar=ordparnumbers
        figure
        hold on
        for i=1:num
            eval(['plot(step*i, ratioI' num2str(ordpar) num2str(i)...
                ', 'r.', 'MarkerSize', 10)']);
            xlim([0 xmax+1])
            ylim([0 max(ratioI8015)])
            title(['Order Parameter' num2str(ordpar)])
            xlabel('Thickness (A)')
            ylabel('Relative Intensity (I)')
        end
        hold off
    end
end

end

end
```

# Appendix C

## C.1 Kirkland Multislice Parameters

The Kirkland Multislice routine requires many input parameters. The more important parameters are as follows: incident beam energy, probe position, output pixel dimensions, output image dimensions, spherical aberration, defocus, aperture size, cell orientation, crystal tilt, slice thickness, temperature for thermal vibrations. The input parameters were chosen to best match the electron microscope that will be used for the experimental work. These parameters are as follows: incident beam energy — 200 keV, spherical aberration — .5mm, defocus — 200 Å, aperture — 5 mrad.

To insure that slight changes in these values would not adversely affect the simulation, I ran simulations using a change of  $\pm 0.1$  mm in spherical aberration,  $\pm 200$  Å in defocus, and  $\pm 0.5$  mrad in aperture size. I also verified that the probe position would not adversely affect the results of the simulation by placing the probe on a random column of atoms as well as off the atomic columns. The results can be seen in figure (show figure).

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