Characterising Quasicrystal Surfaces using STM

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BSc Project

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Abstract

In this project a program called WsXm was used to analyse step heights on the surfaces of a twofold and a threefold icosahedral Silver–Indium-Ytterbium (i-Ag-In-Yb) quasicrystal. The values for step heights found were then compared to those in the theoretical model. Fast Fourier transforms of high resolution STM images are used to check for long range order in sample structure. High resolution images are then compared to the theoretical model to check for similarities. For both twofold and threefold samples the experimental data was found to be in good agreement with theoretical data. Values for step heights for both samples were found to be consistent. Fast Fourier transforms showed some long range order on the sample surface and some similarities could be seen in surface structure.

Contents

1. Introduction

Quasicrystals are a solid material made up of two or more elements with specific chemical composition. They display long range order but lack periodicity. Quasicrystals can display rotational symmetries which the classical theory of crystals does not allow such as fivefold and tenfold. They manage to display these other symmetries because; unlike normal crystals they do not have a simple unit cell that is repeated in all directions to fill up space. They are instead made up of two or more building blocks that fit together to fill all space like a Penrose tiling.

Quasicrystals were discovered in 1982 by Dan Shechtman when he observed unusual electron diffraction patterns from a rapidly cooled Al-Manganese alloy. He first published his results on 5th November 1984 in a Physical Review Letter entitled "Metallic Phase with Long-Range Orientational Order and No Translational Symmetry". This announcement came as a surprise for most physicists in the field (1).

Since their discovery, hundreds of quasicrystals have been discovered. Over 80% of those discovered contain Aluminium along with a simple metal or transition metal. The other 20% are either rare earth based elements or solely transition metals. 82% of the quasicrystals discovered have an icosahedral structure, 16% decagonal structure and the remaining 2% either orthorhombic or dodecahedral structure (2).

Extensive research has gone into preparing samples of quasicrystals and so quality has improved and it is now possible for single grain samples to be grown up to 10 mm in length. Most quasicrystals are grown by rapid cooling of a liquid with cooling rates of $10^5 – 10^9$ Ks^{-1} employed (3). A large size of sample and well ordered good quality surface are important to enable surface science techniques. Only a few of the hundred quasicrystals discovered are usable for studies in ultra high vacuum (UHV) conditions. This is due to the requirement for low-vapour-pressure elements that don't evaporate when heat treatments are used in a vacuum. Scanning in UHV is important to avoid contamination of the quasicrystal surface via oxidisation and other unwanted molecules. UHV also eliminates the interference of gas molecules with the probe during experiments.

The main aim of surface science techniques is to try and confirm the aperiodic arrangements of atoms on the surface of quasicrystals and then use these surfaces as templates to grow single element film with an aperiodic arrangement. This will enable physicists to gain greater understanding into the growth of aperiodic systems and their physical properties.

In this project a program called WsXm is used to analyse STM images taken from a twofold and a threefold surface of icosahedral Silver–Indium-Ytterbium (i-Ag-In-Yb) quasicrystal sample. This program allowed step heights of terraces on the surface of the quasicrystal to be calculated. The results calculated are then compared with the theoretical model for the quasicrystal. STM images of high resolution are also used to relate arrangement of atoms on the surface to the theoretical model.

1.1 Periodic and Aperiodic Order

Quasicrystals display aperiodic order in their structure. In this section the basic theory of aperiodic structure will be explained along with the basic theory of periodic structures that can be used as a comparison. In practice the atomic arrangement of such systems are never perfect, but for theory these imperfections are ignored.

Periodic Structures

In crystallography crystals are described by a reference to perfect infinite arrays of geometrical points called lattices. Every point in a lattice is surrounded by an identical set up of other points. This means crystals show perfect translational symmetry. Crystal lattices can be described relative to a chosen origin by the following equation (3),

$$\boldsymbol{r} = n_1\boldsymbol{x} + n_2\boldsymbol{y} + n_3\boldsymbol{z}$$

where the numbers n_i are integers and **x**, **y** and **z** are unit vectors describing distance and direction between points in the lattice.

Classical theory of crystals only allows 2, 3, 4 and 6 fold symmetries of crystals. A good way of showing how symmetries of 5 fold or 10 fold were forbidden is to look at two dimensional space tilings.

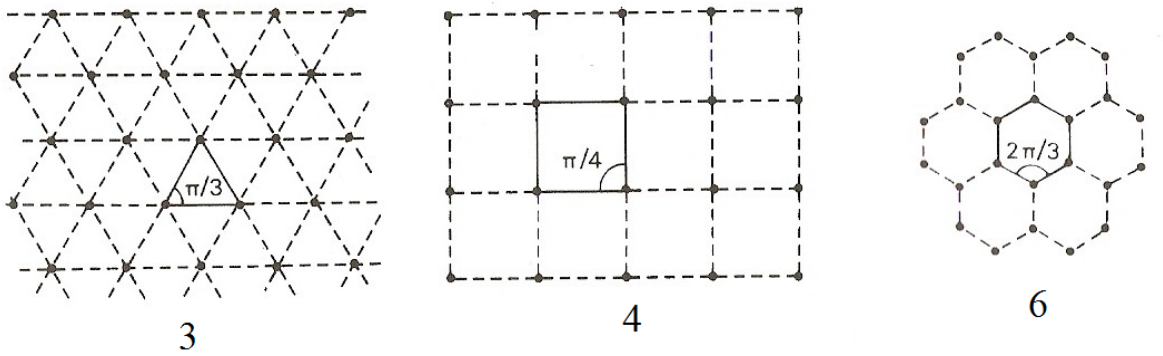

Figure 1- Allowed symmetries (3)

As can be seen in Fig. 1 the triangle, square and hexagon can tile a plane to fill up all space. This shows that 3, 4 and 6 fold rotations can tile a plane.

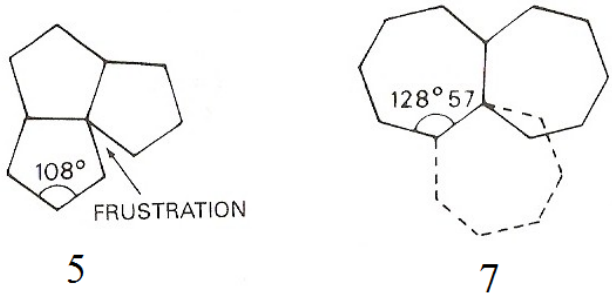

Figure 2 - Disallowed Symmetries (3)

Fig. 2 shows how 5 fold rotations and also rotations over 6 fold are forbidden by periodic space tiling. This is due to the fact that the vertex angles do not divide into 360° to give an integer. For the pentagon its vertex angle is 108°. This divides into 360° 3.3333... times meaning only 3 pentagons plus a gap with the angle 36° meaning the pentagon alone cannot tile a plane (3).

Aperiodic Structures

Quasicrystals fit into the aperiodic structure category. They show long range order without the periodicity that was shown in the previous section. Because they lack this periodicity it becomes harder to sum them up with a generalised equation as in crystals.

The idea of quasiperiodicy can however be described in a much simpler way in 1D using the Fibonacci chain. This chain works by starting with two different lengths, one small (S) and one large (L). As the sequence progresses a rule that S →L and L→LS must be applied to extend the chain. This sequence contains long range order due to the fact that at any point in the chain will have been decided depending on the starting sequence. The sequence looks as below:

L

LS

LSL

LSLLS

LSLLSLSL

LSLLSLSLLSLLS

etc.

If L/S = τ is equal to an irrational number then the sequence has no repetition distance and shows aperiodic order. The simplest form of the Fibonacci sequence corresponds to a τ = 1.618038... A number which is known as the golden mean. This number is holds very interesting properties in context of aperiodicity (3).

Although quasicrystals were discovered in 1982 a 2D model exhibiting an aperodic order just like quasicrystals was discovered by a British mathematician named Roger Penrose almost a decade before in 1974. He used two tiles, both rhombi with equal side length but with different opening angles to tile a plane. This tiling is known as rhombic Penrose tiling and is shown below in Fig. 3. The tiling shows a 5 fold symmetry due to the opening angles of 36° (360°/10) and 72° (360°/5) (1).

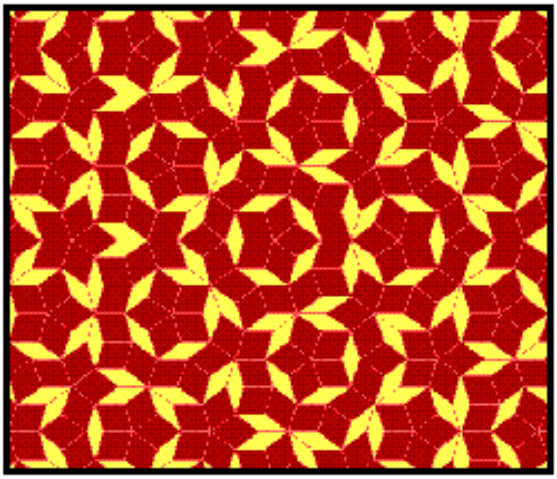

Figure 3 - Rhombic Penrose Tiling (4)

This pattern of tiles is not periodic but still contains some long range order. This long range order can be seen more clearly in Fig. 4 below where lines have been added connecting rhombus with parallel edges. The ordering of large and small gaps creates part of the Fibonacci sequence as shown earlier (2).

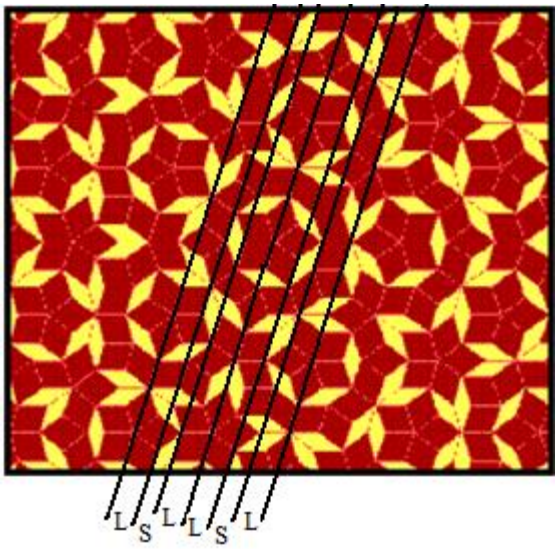

Figure 4 - Penrose tiling with Periodicy shown

1.2 Icosahedral Quasicrystals

Since their discovery quasicrystals with various symmetries have been discovered. The Ag-In-Yb quasicrystal that is being analysed in this project is an icosahedal quasicrystal. These quasicrystals get their name from the icosahedron because they share the same axis of symmetry. They both have 6 x 5-fold, 10 x 3-fold and 15 x 2-fold axes. Fig. 5 shows an icosahedron with some of the symmetry axis labelled. In this project surfaces cut perpendicular to the 3 fold and 2 fold plane have been analysed.

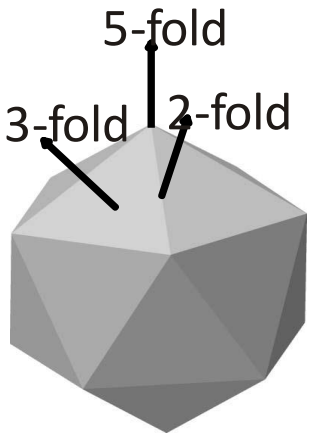

Figure 5 - Icosahedron with symmetry axis

1.3 Structure of *i*-Ag-In-Yb

The atomic structure of *i*-Ag-In-Yb is identical to that of *i*-Cd-Yb. In *i*-Ag-In-Yb Cd is replaced by equal percentages of Ag and In. The reason for scanning *i*-Ag-In-Yb instead of *i*-Cd-Yb is that Cd is unstable in UHV conditions as it evaporates at annealing temperatures (5). In this project, experimental data collected is compared with theoretical data for the *i*-Cd-Yb quasicrystal as both quasicrystals fit the same theoretical structure and atomic arrangement.

In 2000 the binary *i*-$Cd_{5.7}Yb$ quasicrystal was discovered (6) and at the end of 2006 a journal article was published containing the full atomic structure of the quasicrystal (7). The *i*-Cd-Yb quasicrystal is made up of three building blocks shown in Fig. 6. The rhombic triacontahedral (RTH) on the left is made up of another four sub-shells shown in Fig. 7. The RTH makes up 93.8% of all of the atoms in the quasicrystal (7).

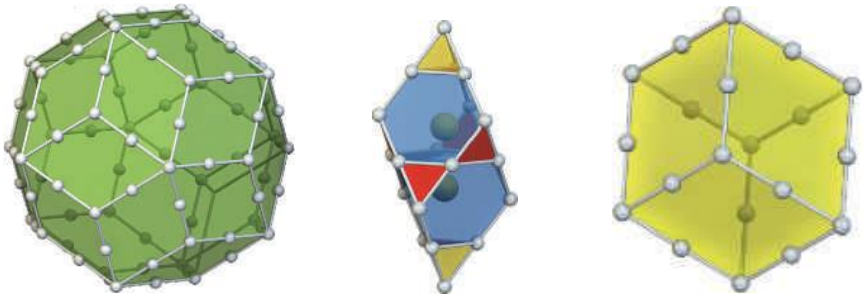

Figure 6 – Building blocks of *i*-Cd-Yb quasicrystal from left to right: Rhombic Triacontrahedral (92 atoms, 0.78nm radius), Acute Rhombohedron, Obtuse Rhombohedron (7)

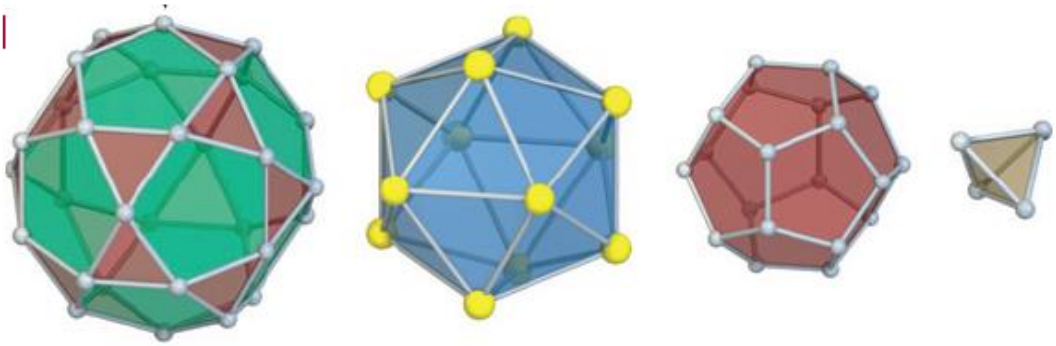

Figure 7 - Building blocks of RTH from left to right: Icosidodecahedron (30 Cd Atoms R=0.65nm), Icosahedron (12 Yb Atoms R=0.56nm), Dodecahedron (20 Cd Atoms R=0.46nm), Tetrahedron (4 Cd Atoms) (7)

2. Experimental method and programs for data analysis

2.1 Low Energy Electron Diffraction (LEED)

LEED is a technique that can be used to produce a diffraction pattern related to the Fourier transform of the atomic arrangement on the surface. This pattern gives very useful information related to the symmetry of a quasicrystal and is also a good measure of the quality of surface structure. If a clear diffraction pattern is shown then surface is well ordered. Electrons are fired from a hot filament at the quasicrystal sample surface at a low energy typically from 20-500eV. The electrons are then backscattered onto a high voltage biased florescent screen (typically about 5keV) displaying a diffraction pattern (8). Fig. 8 shows a diagram of a typical LEED and Fig. 9 shows diffraction patterns from 2, 3 and 5 fold quasicrystals. These will be referred to later in comparison to Fourier transforms of STM images.

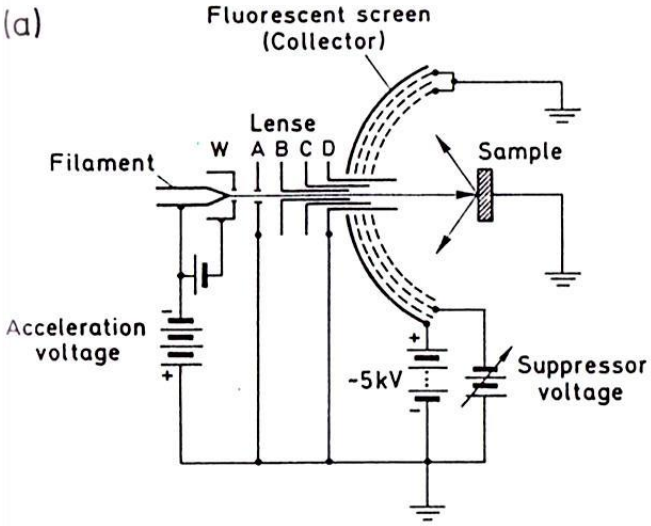

Figure 8 - Diagram of LEED (8)

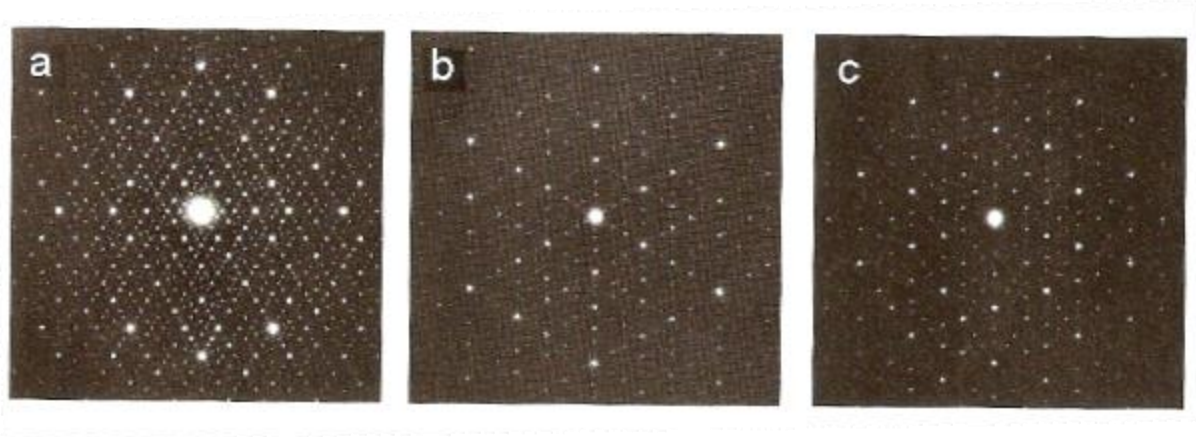

Figure 9 – Electron Diffraction Patterns: (a) Twofold (b) Threefold (c) Fivefold (9)

2.2 Scanning Tunnelling Microscope (STM)

The method used for imaging the surface of quasicrystal in this project is scanning tunnelling microscopy. It enables acquisition of 3D images of a sample to atomic scale. This method requires an ultra high vacuum to work. It uses the concept of quantum mechanic tunnelling to image the surface. The technique involves moving an atomically sharp metallic conducting tip very close to the surface that is to be imaged. A voltage difference is then applied between the two which allows electrons to tunnel through the vacuum, creating an electric signal called the tunnelling current. This current is a function of tip position, applied voltage and the local density of states of a sample and so – as the applied voltage and tip position are known - can be used to create an image of the sample (10).

This technique requires very clean surfaces of a sample and also very stable surroundings to obtain a good image of a surface so can be tricky to carry out.

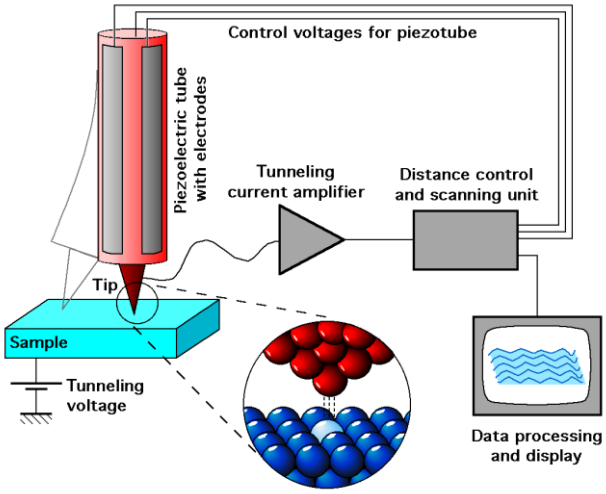

Figure 10 - Schematic of STM (10)

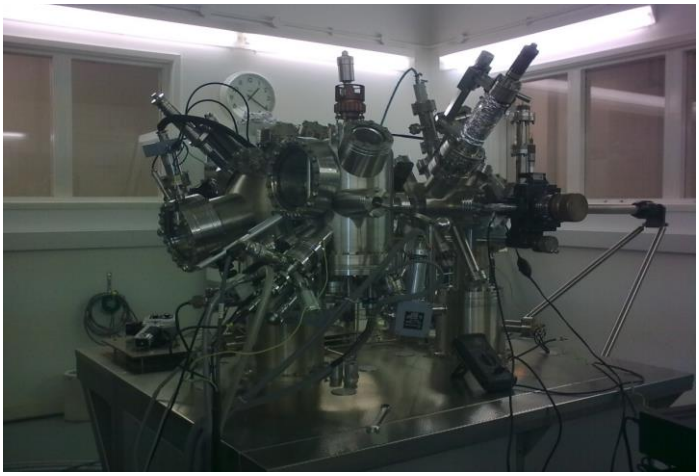

Figure 11 - UHV chamber at Liverpool SSRC. Contains LEED and STM

2.3 WsXm

WsXm is an image analysis program that can be used to view and to measure various features of the STM images. Using this program it is possible to view the images in either 2D top-down view or in 3D. It employs a histogram method for measuring step heights on the quasicrystal surface. This method totals the height of the different levels and then displays the heights in the form of a histogram. If used correctly there will be two peaks, the distance between corresponds to the step height. The program can also be used to obtain a fast Fourier transform of STM images, which if a good enough quality image is used can show a pattern similar to LEED patterns which show symmetry and long range order.

2.4 IGOR Pro

Igor is a piece of data analysis software. It can be used to model atomic systems. In this project a premade file was used with the theoretical model for the *i*-Cd-Yb quasicrystal shown earlier. This program allows a view of atomic arrangement in 3 dimensions, so can be used to view atomic arrangement on planes that are most likely to be that of bulk terminations. It is also possible to obtain theoretical values for step heights on the surface of quasicrystals by extracting values for cluster centres into excel and calculating the distance between points.

3. Method of Data Analysis

Images were provided taken from STM sessions scanning an *i*-Ag-In-Yb quasicrystal cut along the two fold axis and also images taken when a similar quasicrystal was cut along the three fold axis. All the three fold images analysed were taken in the Liverpool Surface Science Research Centre (SSRC) by Peter Nugent. The two fold images that were analysed were all taken by Peter Nugent with involvements by HR Sharma. Some were taken in the Liverpool SSRC and the other images were taken in the National Institute for Materials Science (NIMS), Tsukuba, Japan.

Upon obtaining the images they were looked through and images with larger scale showing steps / terraces were separated from those of atomic resolution. Both large scale and high resolution images are shown on the next page in Fig. 12.

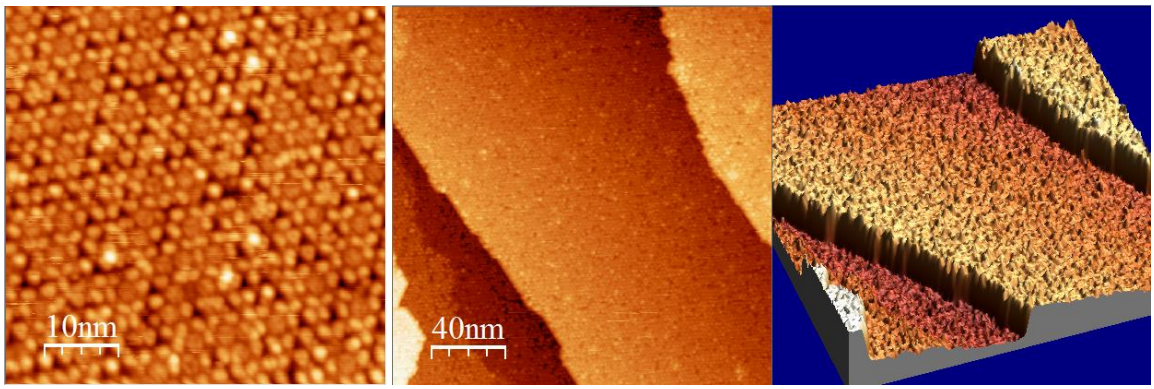

Figure 12 – From Left to Right: 3 Fold STM at atomic resolution, 3 Fold STM with steps 2D and 3D

Once the data had been separated, all of large scale images showing step heights were analyzed individually using WsXm. A local plane function was then used to calibrate the program. Once this was done a section of the image was zoomed into with as much of the step in question as possible in. The histogram method as mentioned earlier was then employed. Each step height was checked at least twice to check an error giving drastically different results had occurred. As can be seen in Fig. 12 above in the 3D image, each level is not flat so this method is much more accurate than the line scan method in which only a line of points are taken into consideration. The histogram method counts all the points with a certain height and displays them in histogram form as shown in Fig. 13. Two markers are manually selected to select the middle of each peak – each peak corresponding to a different level on the quasicrystal surface – and WsXm calculates distance in between these two points resulting in a value for step height. This data was recorded separately for the two fold and the three fold data.

Some good quality atomic resolution images were selected – an example of which is shown on the left of Fig. 12 – and the technique of fast Fourier transform was used. This enables a check of the long range order of the surface, resulting with an image similar to LEED patterns. This gives confirmation of the type of symmetry displayed in the samples and also will give a quick idea of how ordered the surface is, so to show the best images for use when comparing surface structure with that of theory.

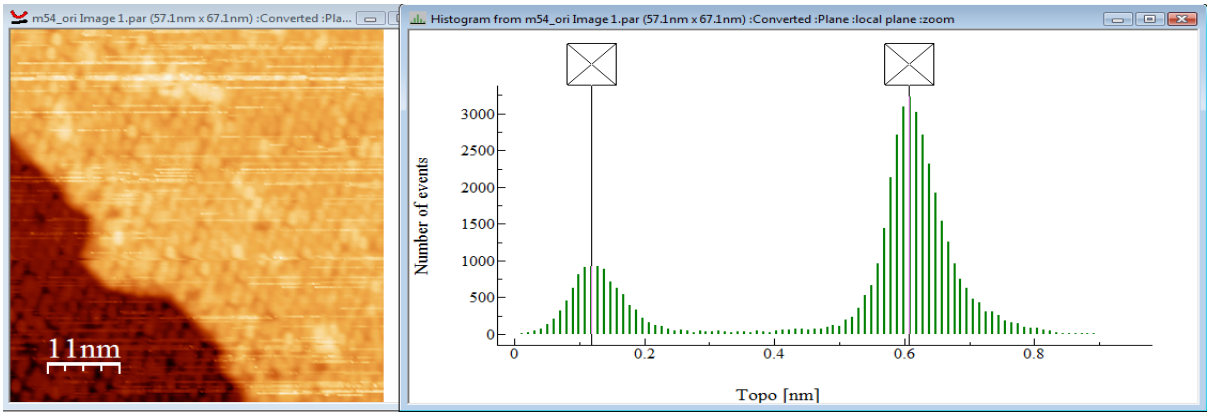

Figure 13 - Histogram method for calculating step height and 2D STM image of QC with 1 step

After all of the step heights were recorded the theoretical data was looked at using IGOR Pro modelling software. The file 'Disp_YbCd_unrelaxed100_ball.pxp' was provided by H R Sharma. This file contained theoretical data for the structure of the *i*-Cd-Yb quasicrystal and data for the 5 fold, 3 fold and 2 fold setup of atoms can be viewed. The file uses a set of axis: X, Y, Z and plots the theoretical positions of atoms in the quasicrystal. The X vs. Y plane is the plane that is scanned during STM sessions and the Z axis is perpendicular to this plane. The program allows data to be viewed in various ways with plots of different axis together. The most useful are the two views shown below in Fig. 14. The view on the left is the Z axis vs. the Density of atoms which shows the positions on the Z axis along with their population of atoms.

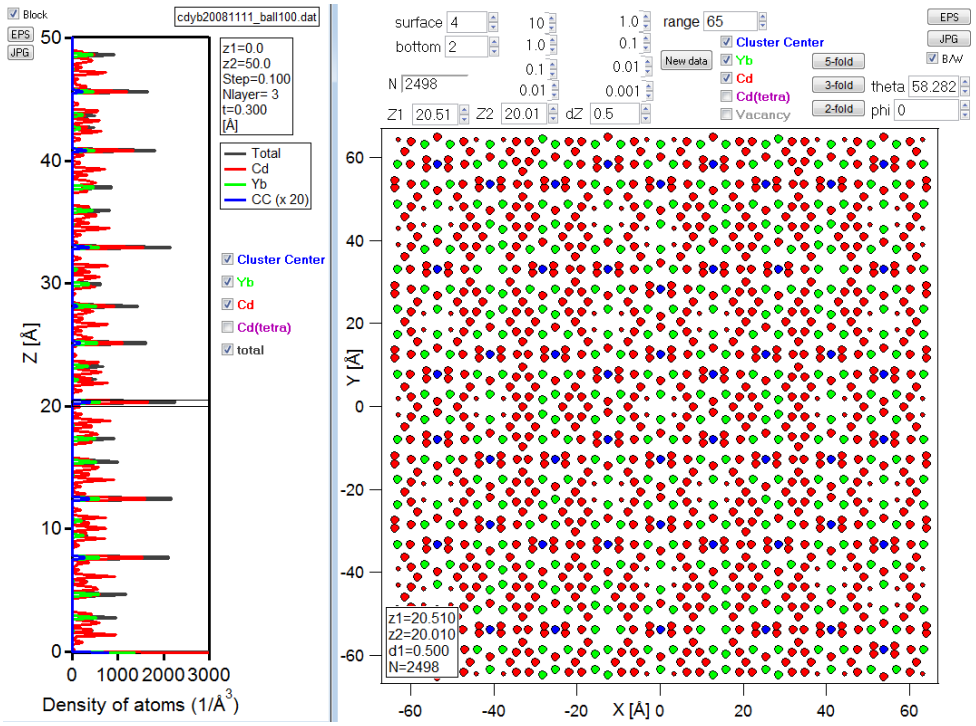

Figure 14 - IGOR Pro, Structure Of 2 fold *i*-Cd-Yb

As can be seen the Z axis positions that coincide with cluster centres have the highest population of atoms. These levels are the most probable levels for a termination. So the difference between two cluster centres would equal the theoretical step height. The Z values for cluster centres for both the twofold and threefold theoretical data were extracted from IGOR pro and using excel the distances between consecutive points were calculated. In both cases the values for theoretical step height repeated to give a few different values for step height. These values were then compared with the values for step heights calculated from the STM images and consistency checks were carried out using the below equation.

$$|x_1 - x_2| < 3\sqrt{\Delta x_1^2 + \Delta x_2^2} \qquad \text{Equation 1}$$

Two independent measurements of the same quantity are said to be consistent if the above conditions apply.

The image on the right in Fig. 14 is the theoretical X vs. Y view of atomic structure for the two fold data at the level of a cluster centre. This can be compared with the atomic scale STM images to look for similarities in surface structure. Any similarities will show agreement with the theoretical model. These comparisons are shown in the comparison with theoretical model sections.

4. Results and Discussion

4.1 3 Fold Surface

4.1.1 Step height distribution

14 STM images taken from different parts of the 3 fold surface were picked out for analysis. From these 14 images 38 step heights were calculated. The step heights found grouped into two sizes, small and large. An example of the different size step heights is shown below in Fig. 15. In this image the line scan method is also shown with a graph to illustrate different size terraces / step heights.

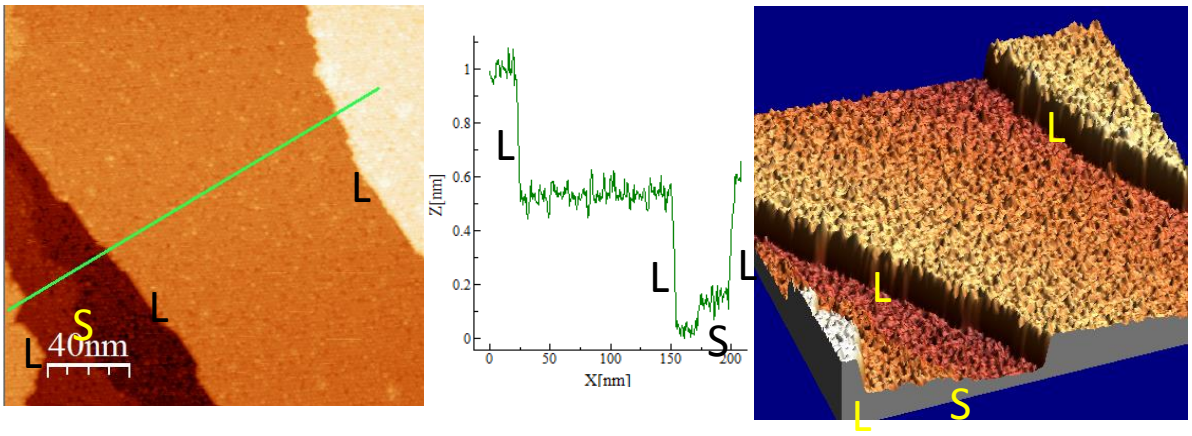

Figure 15 - STM image in 2D and 3D with line scan method shown

There were 25 large step heights found (66%) and 13 small step heights found (34%). The full data set is included in part 1 of the appendix. For each of the two groups of data the average and the standard deviation have been calculated. The standard deviation is the estimation of error on all the values of that data set. Fig. 16 below shows a histogram, plotted with all the step height values collected from the 3 fold images. The bin widths have been set to 0.01 nm. Here it can be seen clearly how the data all groups around 2 points.

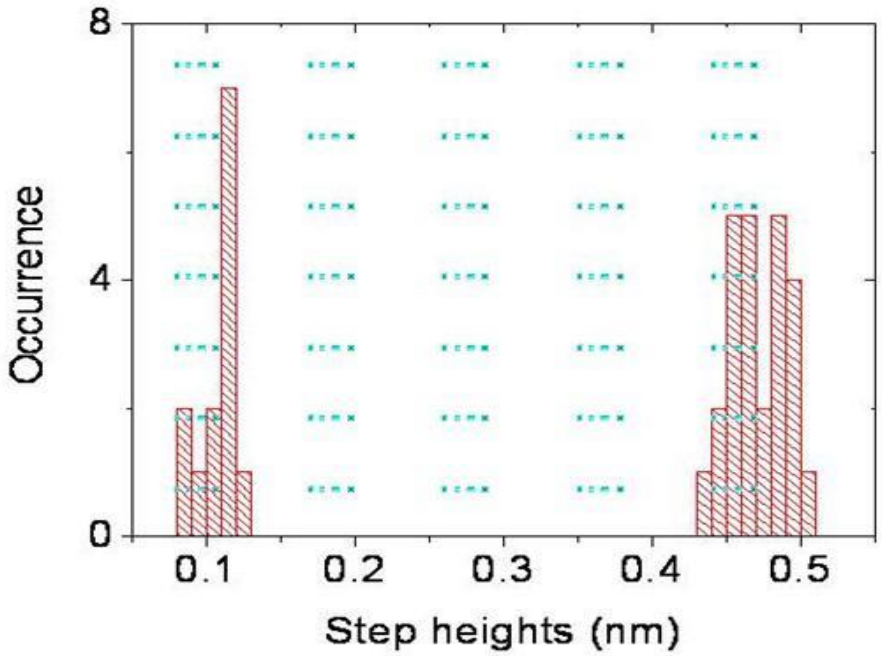

Figure 16 - Histogram of Step Heights found on Surface Of 3-fold Sample

4.1.2 Atomic structure on terraces

Using the fast Fourier transform tool on WsXm some good quality atomic scale images were transformed. Figs. 17-19 show an STM image and corresponding fast Fourier transform. The fast Fourier transform patterns have been zoomed in on so the pattern is easier to view.

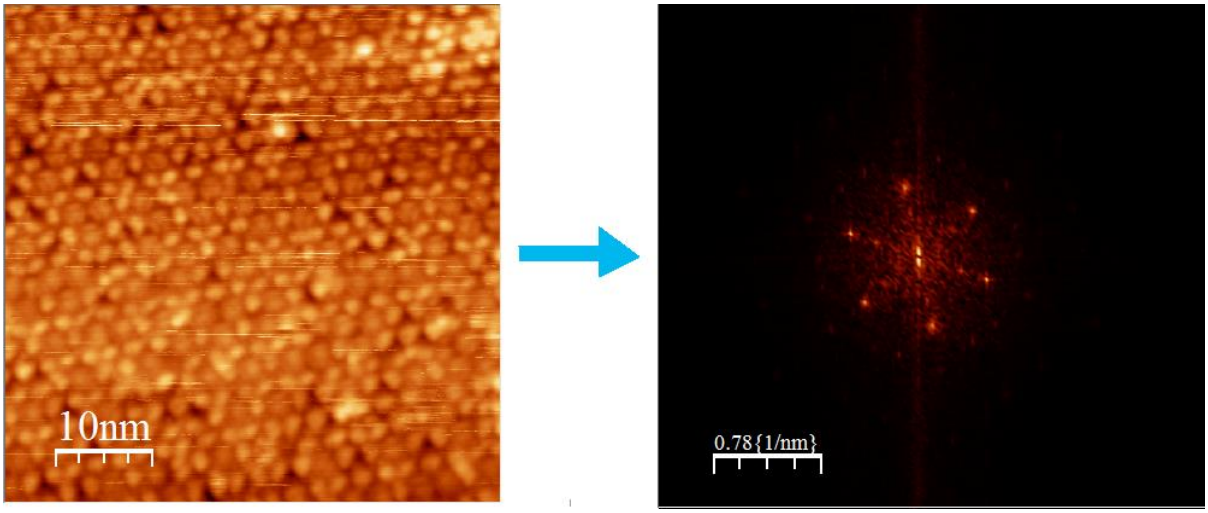

Figure 17

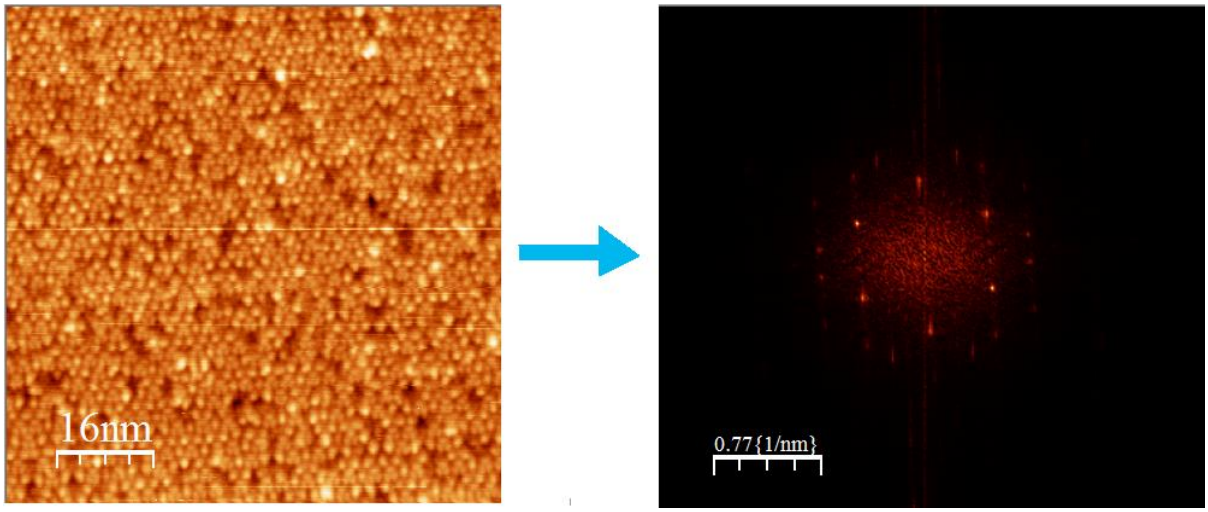

Figure 18

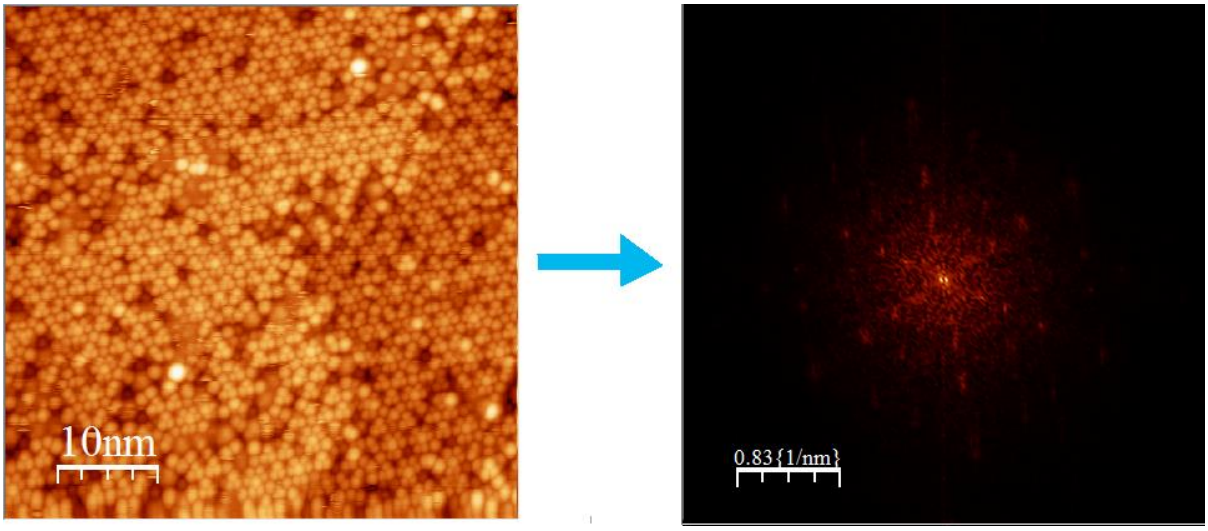

Figure 19

Comparing the fast Fourier transform images above in Fig. 17-19 with the symmetry pattern for 3 fold symmetry in Fig. 9 (b) it is possible to see a lot of similarities. Both show 6 bright dots in a hexagon shape and although the images above have some background it is enough to show that the surface structure of the quasicrystal has some long range order and exhibits 3 fold symmetry.

4.1.3 Comparison with theoretical model

Step Heights

By extracting the positions of cluster centres along the Z axis into excel the theoretical step heights were calculated. In Fig. 20 the graph of Z axis against the density of atoms is shown. The theoretical step heights are the distance between successive points as indicated with L, M and S.

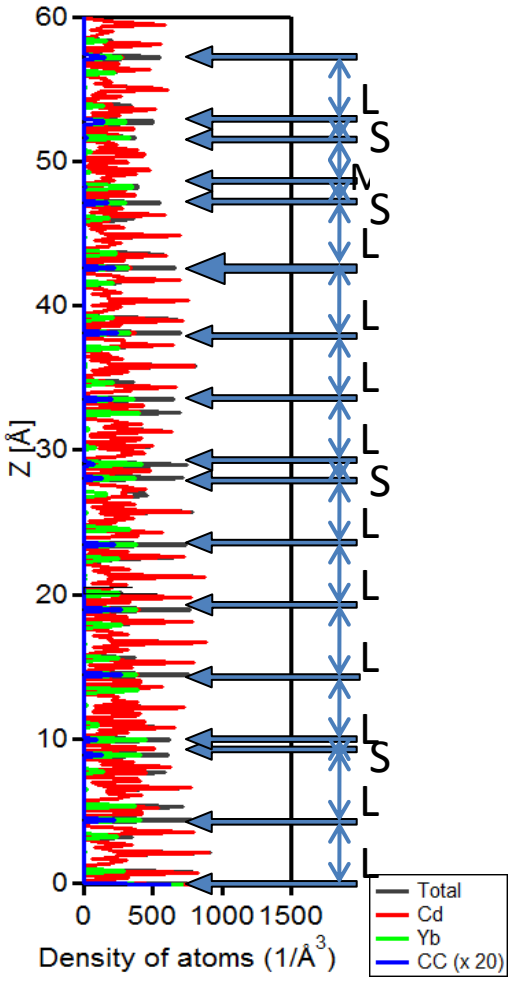

Figure 20 - Z axis Vs Density of Atoms with cluster centres shown (3 Fold)

Overall there were 54 step heights in the theoretical model and these were all one of 3 different values shown in the table below. Listed in the table is also the percentage of the total steps that that step height corresponds to.

Step Height	Step Height Size (nm)	Number Of Steps Found	Percentage of Total Steps (%)
L	0.452	36	66.7
M	0.345	4	7.4
S	0.107	14	25.9

For comparison the table below has been included with the average step height results that were calculated from the STM images.

Step Height	Average Step Height (nm)	Error (nm)	Percentage of total step heights (%)
L	0.471	0.019	65.8
M	----	----	----
S	0.108	0.013	34.2

No medium step heights were found in the measurements of the STM images. The reason for this would be due to rarity. They occur less frequently due to the arrangement of atoms on the medium termination being less dense than on large or small terminations. The less dense arrangement requires more energy and therefore is less preferable. A comparison between medium and large cluster centre levels has been shown in Fig. 21.

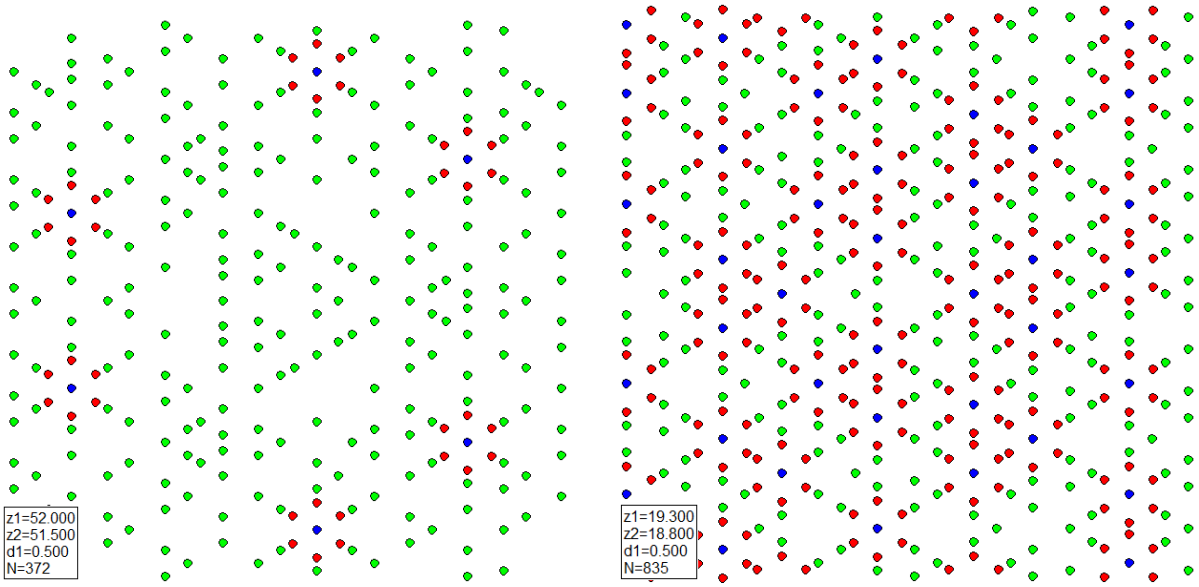

Figure 21 - Left - arrangement of atoms on medium step. Right - On Large step

In the theoretical model only 7.4% of the steps had medium step height and as only 38 step heights were recorded from the threefold images it is not surprising that no steps with such heights were found.

The percentages of large and small step height found from experimental data match well with theoretical data with more large steps occurring than small ones.

Using equation 1 shown earlier a consistency check will be performed between the theoretical values for step height and those found from analysing STM images. The error on the theoretical data will be taken as zero.

Large step height: $x_1 = (0.471 \pm 0.019)$ nm $x_2 = (0.452 \pm 0)$ nm

$$|0.471 - 0.452| < 3\sqrt{0.019^2 + 0^2}$$

$$0.019 < 0.057$$

Small step height: $x_1 = (0.108 \pm 0.013)$ nm $x_2 = (0.107 \pm 0)$ nm

$$|0.108 - 0.107| < 3\sqrt{0.013^2 + 0^2}$$

$$0.001 < 0.039$$

For both large and small step heights the experimental values proved consistent with theoretical values.

Surface Structure Comparison

Using IGOR pro to view the theoretical surface structure at a cluster centre it is possible to compare theoretical structure with atomic scale STM images. In Fig. 22 some similarities have been shown. Using red, blue and green dots some surface structure that was seen to be similar to the theoretical model was marked on. There are a lot of similarities to be seen in the way the atoms have arranged themselves into little triangles (green dots) and hexagons (red/blue dots). Also the three hexagons that have been shown that arranged in a triangle as the theory dictates.

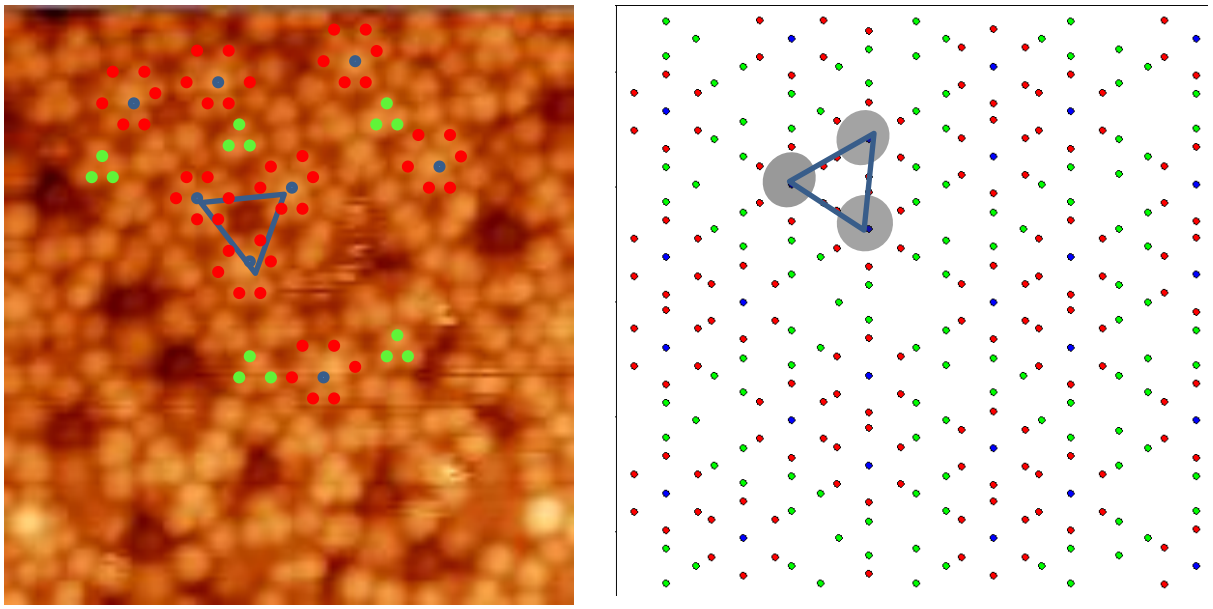

Figure 22 - Comparison between theoretical surface structure and STM images 10 x 10nm.

Another feature noticed of the surface structure of the quasicrystal was the fact that the distance between 'holes' seemed to repeat with 2 lengths of intervals in a given direction. This is shown on the next page in Fig. 23. The lengths corresponding to the coloured arrows are as follows:

Blue	4.2 nm
Yellow	2.3 nm
Green	4.6 nm
White	7.1 nm

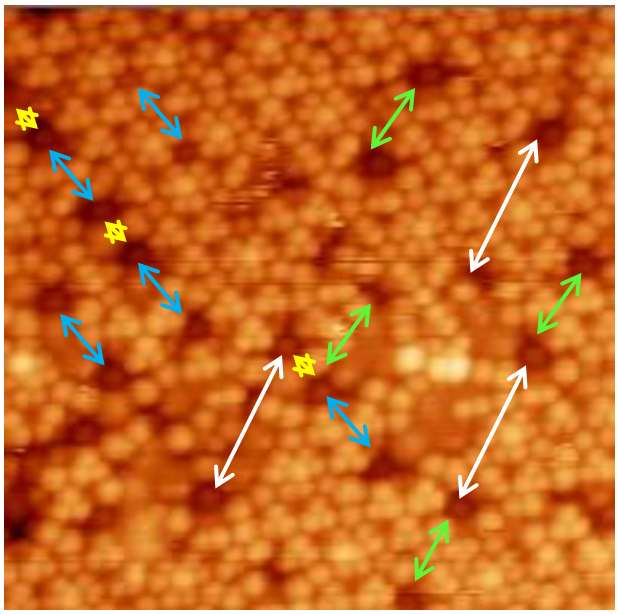

Figure 23 - 3 fold STM image showing 'holes' and distances between.

As shown by the coloured arrows in the above image the lengths of spacing repeat in each direction. This is a sign of long range order on the surface of the quasicrystal. The theoretical model also displays similar behaviour with holes separating themselves with 2 different distances along a line. This has been shown in Fig. 24 below. The black dots indicate a hole and along each line there appears to be two different distances of separation.

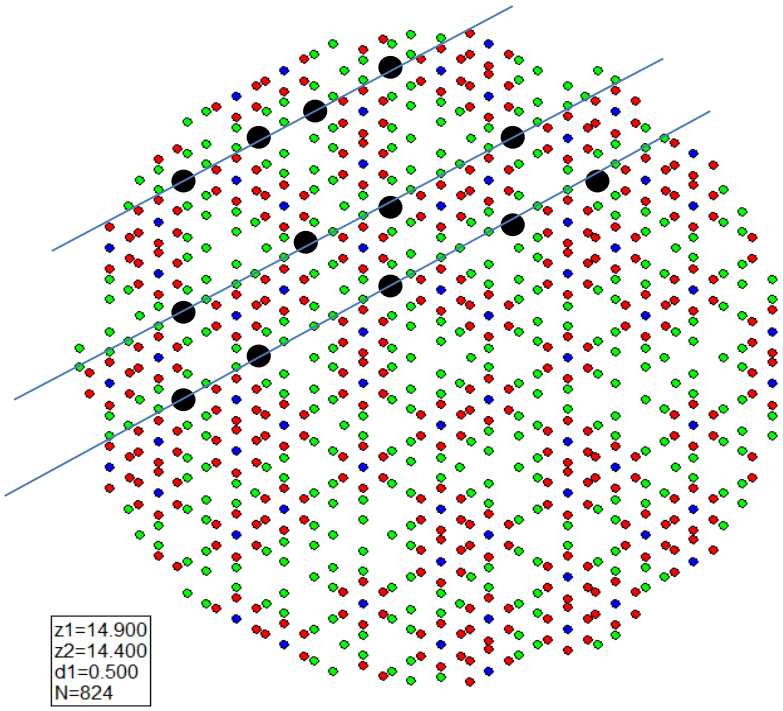

Figure 24 - Atomic arrangement at cluster centre level with distances between holes

4.2 2 Fold Surface

4.2.1 Step height distribution

17 large scale images were picked out from the provided two fold images. From these 80 step heights were recorded. The full results can be found in part 2 of the appendix. The majority of step heights recorded fitted into 3 groups: large, medium and small. There were also 11 out of the 80 step heights recorded that were larger than these three groups and these points have not been included in the averages. These step heights seemed to be combinations of the large, medium and small step heights bunched together. These results are shown in part 3 of the appendix along with suggestions for the combined steps.

From the 69 step heights recorded above 28 were large step heights (41%), 25 were medium step heights (36%) and 16 were small step heights (23%). The error, as before has been taken as the standard deviation on each group of step heights. It was noticed that the total of the averages of both the small and medium step heights when added together equals a value very close to the large step height. 0.466 (M) + 0.277 (S) = 0.743 ~ L

Displayed below in Fig. 25 is a histogram of the above data. The bin widths are 0.01nm. The three groups of step height can be seen although the large step heights are more spread out than medium and small. This is reflected in the large error on the large step heights.

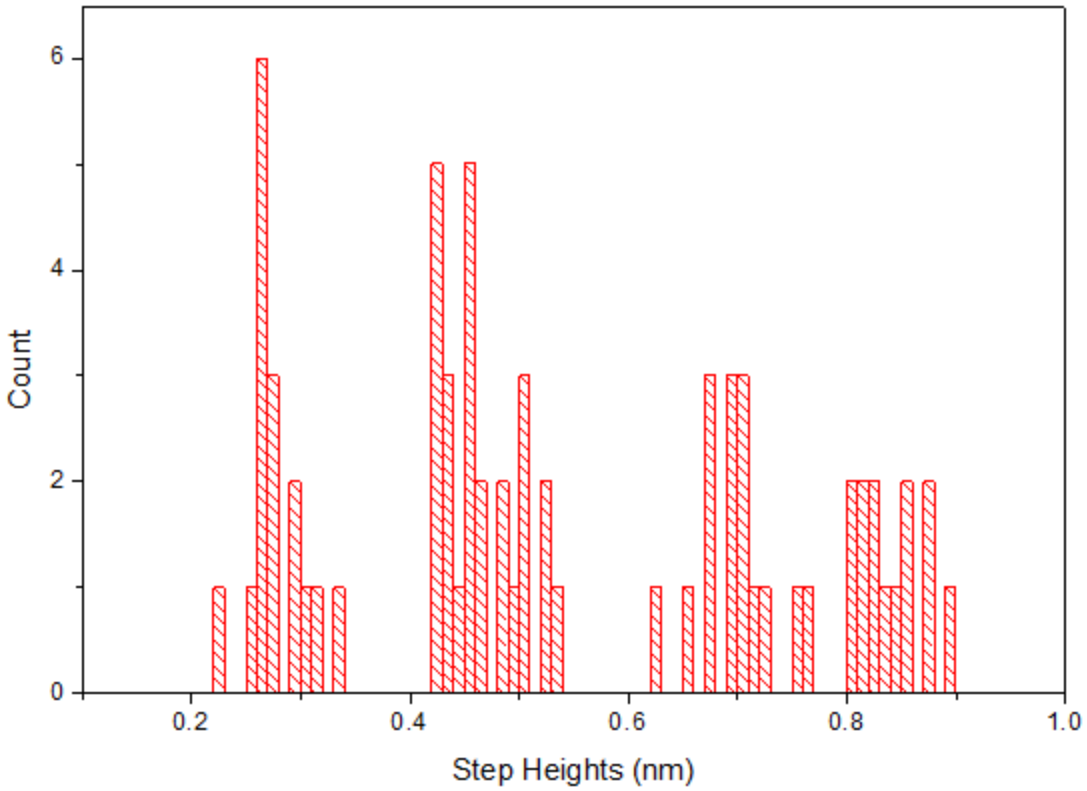

Figure 25 - Histogram of Step Heights found on Surface Of 2-fold Sample

4.2.2 Atomic structure on terraces

Below in Figs. 26-28 some images taken at the surface of the two fold quasicrystal at high resolution are shown along with their fast Fourier transforms. These images were picked out because they showed some surface structure and gave a fast Fourier transform with a good pattern that can be compared to the LEED images in Fig.9 (a).

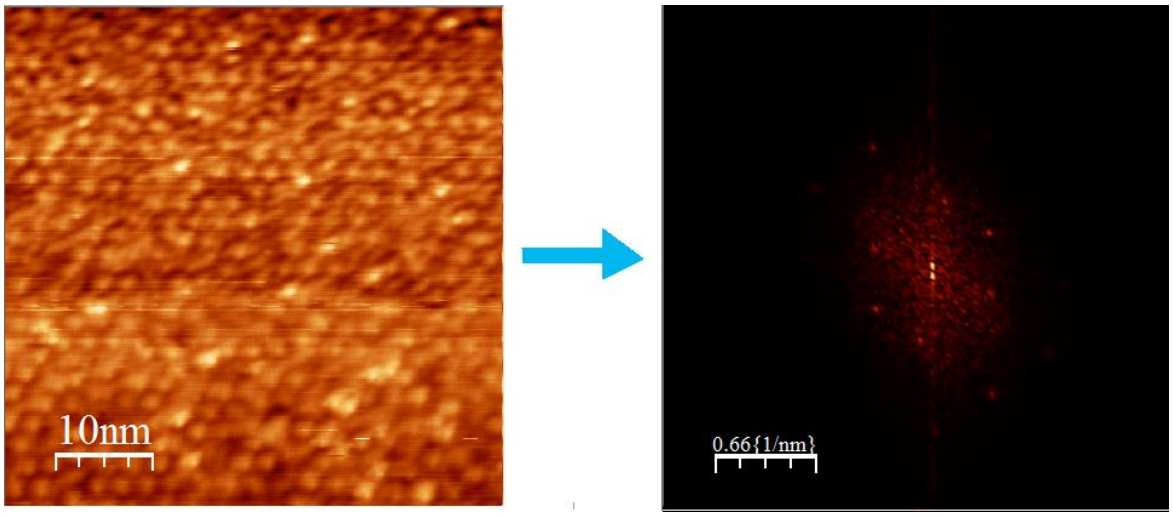

Figure 26

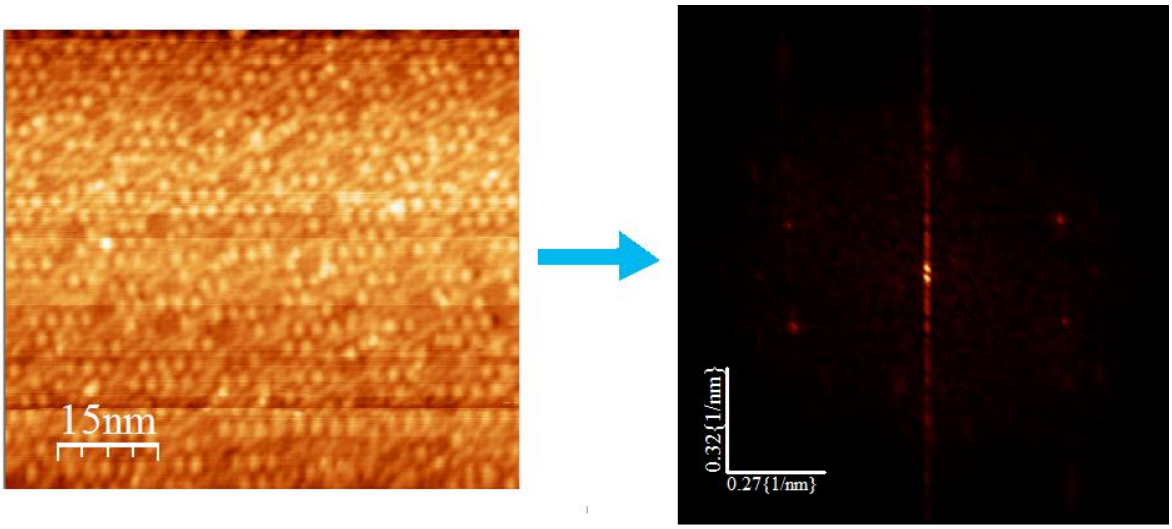

Figure 27

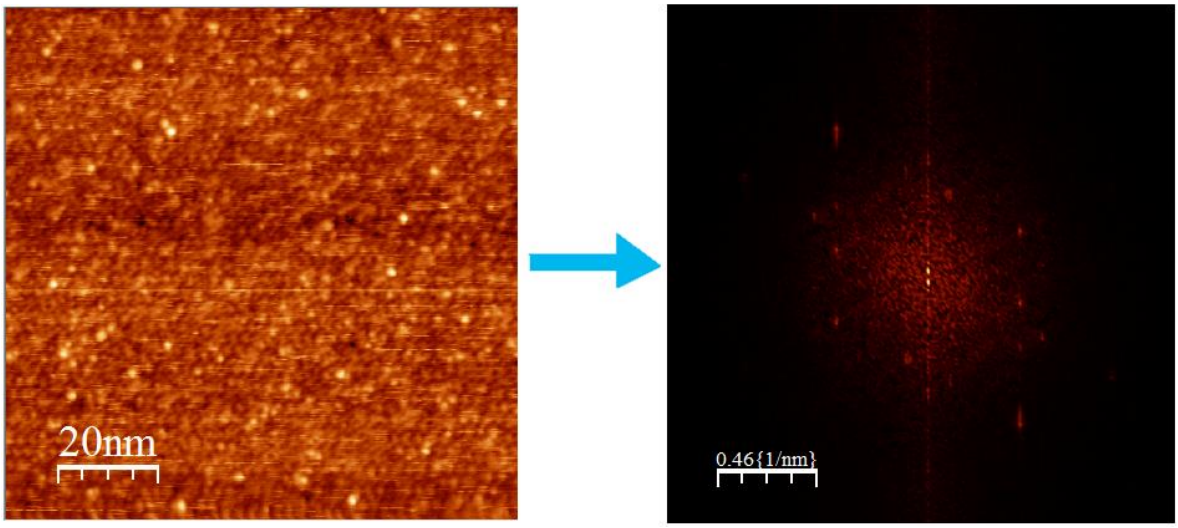

Figure 28

It's possible to see some similarities between the above images and image (a) in Fig. 9. All three images show four bright spots creating a rectangle around the middle. These appear to be in similar to the four dots marked in blue in Fig. 29 below. Figs. 26 and 28 also show bright dots which are in the same position as the dots marked in red and blue below.

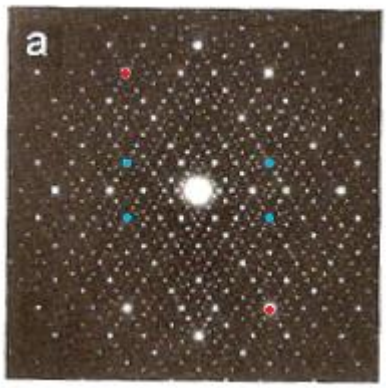

Figure 29 - 2 fold LEED Pattern

4.2.3 Comparison with theoretical model

Step Heights

By extracting the positions of cluster centres along the Z axis into excel the theoretical step heights were calculated. In Fig. 30 below the graph of Z axis against the density of atoms is shown for the 2 fold quasicrystal.

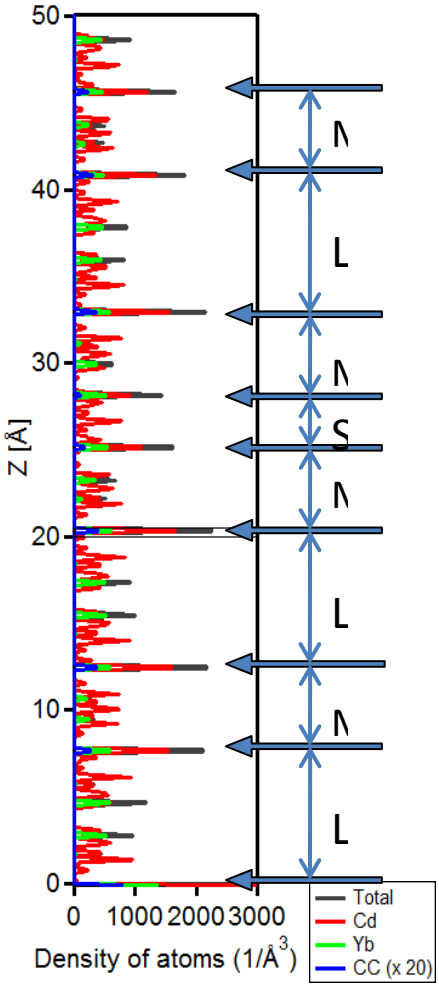

Figure 30 - Z axis Vs Density of Atoms with cluster centres shown (2 Fold)

Overall there were 35 step heights in the theoretical model and these were all one of 3 different values shown in the table below. Listed in the table is also the percentage of the total steps that that step height corresponds to.

Step Height	Step Height Size (nm)	Number Of Steps Found	Percentage of Total Steps (%)
L	0.783	11	31.4
M	0.484	17	48.6

S	0.299	7	20.0

For comparison the table below has been included with the average step height results that were calculated from the STM images.

Step Height	Average Step Height (nm)	Error (nm)	Percentage of total step heights (%)
L	0.764	0.080	40.6
M	0.466	0.035	36.2
S	0.277	0.027	23.2

As in the theoretical model the experimental step heights fitted into 3 groups of large, medium and small.

In the experimental data more large step heights were found than medium ones which does not agree with theoretical data where almost 50% of step heights are medium. The percentage of step heights found that were small is similar to that in the theoretical model with a difference of only 3.2%

The theoretical values for small and medium step heights sum together to give the large step height exactly – 0.299 (S) + 0.484 (M) = 0.783 (L). It was noted earlier that when the medium and small step heights were added together for the experimental data it gave a value close to that of the large step height.

Using equation 1 a consistency check will be performed between the theoretical values for step height and those found from analysing STM images. The error on the theoretical data will be taken as zero.

Large step height: $x_1 = (0.764 \pm 0.080)$ nm $x_2 = (0.783 \pm 0)$ nm

$$|0.764 - 0.783| < 3\sqrt{0.080^2 + 0^2}$$

$$0.019 < 0.240$$

Medium step height: $x_1 = (0.466 \pm 0.035)$ nm $\quad x_2 = (0.484 \pm 0)$ nm

$$|0.466 - 0.484| < 3\sqrt{0.035^2 + 0^2}$$

$$|0.018| < 0.105$$

Small step height: $x_1 = (0.277 \pm 0.027)$ nm $\quad x_2 = (0.299 \pm 0)$ nm

$$|0.277 - 0.299| < 3\sqrt{0.027^2 + 0^2}$$

$$0.022 < 0.081$$

All three experimental step heights were consistent with their corresponding theoretical step height. This shows good agreement with theoretical data.

Surface Structure Comparison

Unfortunately after looking through all the images, none were found of good enough quality to compare atomic structure as was done for the 3 fold surface images. Instead a technique was used which involved filtering the fast Fourier transform of an image of the surface of a quasicrystal, then taking the inverse of the filtered Fourier transform. This image was then combined with the original image to enhance certain structural features. This output image is shown below in Fig. 31 along with the theoretical structure.

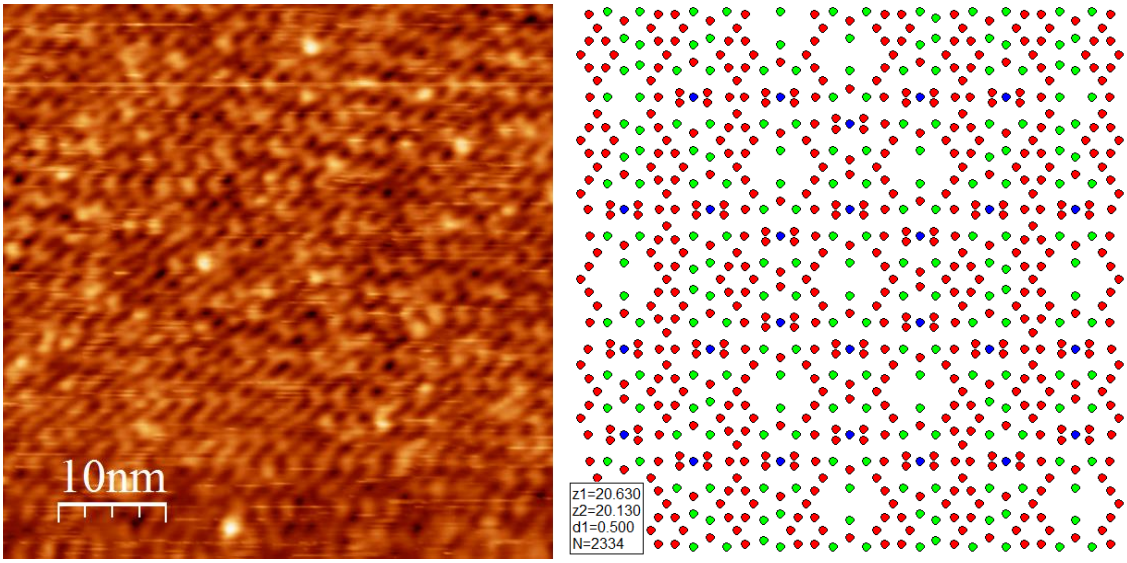

Figure 31 – Left, 2 fold surface combined with inverse of Filtered FFT. Right – Theoretical model

Although no individual atoms can be seen in the STM image, it is possible to see a 'zigzag' pattern similar to that of the theoretical model. It is also possible to see some holes which appear in lines which would agree with the theoretical model.

5. Conclusion

In conclusion it can be seen that experimental data from both the threefold and twofold quasicrystals agrees to a good extent with theoretical data. The consistency between experimental and theoretical values for step height show good agreement and are consistent for both two and threefold. This also shows that it was correct to assume that terminations occurred in levels intersecting cluster centres. For both threefold and twofold samples the fast Fourier transforms display patterns comparable to that of electron diffraction patterns showing that long range order exists on the sample surfaces. The threefold surface showed many features that were similar to the theoretical model and the distance between holes on the surface showed some long range order. Upon comparing the twofold STM surface image combined with the inverse of the Fourier transform it appeared that some surface structure was similar. However higher resolution images with more detail are required for a proper comparison.

If this study was to be repeated again, the improvements that could be made would be to analyse a larger number of images to have at least 100 step heights of both twofold and threefold surfaces to compare with theory. Some higher resolution images of the twofold

quasicrystal would also be required to properly compare with theoretical data and so better quality Fourier transforms could be obtained. It would also be preferable to compare some of the surface features to a relaxed model for theoretical structure, as only the unrelaxed model was used in this study.

This study could be brought forward by looking into the use of the *i*-Ag-In-Yb quasicrystal surface as templates for growth of single element quasiperiodic material.

During this project I have learnt a great deal about quasicrystals and their structure. I learnt about structure on the surface (including terminations and step heights) and aperiodicity in structures. I used programs including WsXm and IGOR which I did not know how to use before to analyse data. I have also gained experience in the lab of methods such as LEED and STM, and learnt about some of the difficulties (very clean surface, stable conditions) in implementing such techniques.

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7. Appendix

1 - 3 Fold Data

Below the step heights recorded for the 3 fold surface. The results have been split into two columns, as the step heights obtained fitted into two groups. Each group has been ordered from highest to lowest.

Large Step Heights (nm)
0.500

Small Step Heights (nm)
0.127

0.497
0.497
0.494
0.493
0.488
0.487
0.487
0.482
0.480
0.473
0.472
0.469
0.469
0.467
0.462
0.462
0.459
0.459
0.458
0.454
0.454
0.445
0.443
0.432

Average
0.471
Standard Deviation
0.019

0.119
0.118
0.116
0.115
0.113
0.110
0.110
0.108
0.105
0.097
0.088
0.083

Average
0.108
Standard Deviation
0.013

2 - 2 Fold Data

Below are the step heights recorded for the 2 fold surface. They have been grouped into three sets: large, medium and small. They have been listed from highest to lowest.

Large Step Heights (nm)
0.895
0.875
0.875
0.859

Medium Step Heights (nm)
0.530
0.529
0.520
0.509

Small Step Heights (nm)
0.331
0.317
0.303
0.299

0.857
0.849
0.834
0.822
0.822
0.818
0.817
0.804
0.800
0.769
0.752
0.721
0.718
0.708
0.708
0.700
0.697
0.696
0.691
0.676
0.672
0.671
0.654
0.624

Average
0.764
Standard Deviation
0.080

0.506
0.503
0.498
0.486
0.485
0.467
0.465
0.457
0.456
0.453
0.451
0.450
0.449
0.437
0.432
0.432
0.429
0.429
0.427
0.426
0.425

Average
0.466
Standard Deviation
0.035

0.296
0.279
0.278
0.270
0.265
0.265
0.264
0.263
0.262
0.261
0.250
0.221

Average
0.277
Standard Deviation
0.027

3 - Combinations of Step Heights

In the table below the step heights found that were omitted from the averages are shown. Included are the step heights and a possible combination of steps that could have led to this height.

Combinations of Step Heights	Suggested Combination
1.795	L+L+S
1.214	L+M
1.212	L+M
1.173	L+M

1.162	L+M
1.149	L+M / L+S
1.133	L+M / L+S
1.132	L+M / L+S
1.124	L+M / L+S
1.111	L+M / L+S
1.099	L+M / L+S

L+L+S	1.804
L+M	1.230
L+S	1.040