XPS analysis of indium absorption on Ag-In-Yb

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Abstract

In this project we are investigating the composition of the surface of the Ag-In-Yb quasicrystal before and after the deposition of indium mainly to deduce what the indium preferentially bonds to on the quasicrystal surface. We found that is it favours bonding to the indium atoms most strongly and also the Ag atoms which are slightly less favourable but the deposited indium bond to the Yb least favourably.

Introduction

Aperiodic tiling is tiling that is non-periodic and can tile the plane without any overlapping or gaps. In 1619, Johannes Keplar published 'Harmonices Mundi (The Harmony of the World)'. Book 2 of Harmonices Mundi contained a section in which Keplar had attempted to tile the plane aperiodically using pentagons, pentagrams, decagons and other shapes. (see figure 1)

Many people have tried to tile the plane aperiodically since Keplar. In 1961 Hao

Figure 1 - Aperiodic pattern in Keplar's Harmonices

Wang was studying sets of coloured tiles (Wangs tiles) to see if they could tile the plane while following the rule, the touching edges must be the same colour and the tiles couldn't be rotated or reflected. From these tiles Wang conjectured that if the tiles could tile the plane, they would do so periodically. Then in 1964 Robert Burger, a student of Wang, came up with a set of 20,426 tiles that would only tile the plane aperiodically, thus proving Wangs conjecture incorrect. Since Berger came out with his set of aperiodic tiles many mathematicians have found more sets of aperiodic tilings with less and less tiles, going from the original 20,426 down to only 2. The most well-known example of an aperiodic tiling are Penrose tilings.

Penrose tilings, named after Roger Penrose, are the most well-known example of aperiodic tilings. There are three versions of Penrose tilings: original Penrose tiling P1, kite and dart tiling P2 and Rhombus tiling P3. See table 1 below.

	P1 tiling	P2 tiling	P3 tiling
Tiles		72° 144° 72° 144° 72° 36° 72°	
Pattern			

Table 1 – Penrose tilings

Before Penrose tilings there was thought to be only 2-, 3-, 4- and 6-fold symmetry in sets of tiles that can tile the plane but Penrose tilings displayed 5-fold symmetry. Robert Ammann found a set of tiles that displayed 8-fold symmetry at a similar time Penrose tiles were created.

Before quasicrystals were found and accepted by the scientific community, crystals were thought to only be made up of repeating units and thus were periodic. At the time there were thought to be 14 different types of unit cells, called Bravais Lattices discovered in 1848, and up to this point no one had found a crystal that did not fit into these 14-unit cell types. Aperiodic crystals were thought to be impossible as in a crystal the atoms were thought to being arranged locally and an aperiodic pattern seemed to need a long-range coordination so that the pattern did not repeat many thousands of atoms further along in the quasicrystal.

In the early 1980's Paul Steinhardt was modelling how atoms form condensed matter and they found that they like to form icosahedrons. This was unexpected as icosahedrons have 2-, 3- and 5-fold symmetries thought to not be possible in a crystal. Using this and inspiration from Penrose tilings Steinhardt modelled a new type of material, a quasicrystal. The quasicrystal was a 3D analogue of Penrose tilings. They simulated what the x-ray diffraction pattern through this type of crystal would be and they found a pattern with 10 points (See figure 2).

The first quasicrystal that was discovered was found in a study of the Al and Mn alloy Al_6Mn and was found by Daniel Shechtman, Ilan Blech, Denis Gratias and John Cahn. They found that when electrons were diffracted off the Al_6Mn the diffraction pattern had a symmetry forbidden for crystals, 10-fold symmetry (see figure 3). As can be seen the diffraction patterns in figures and are both showing clear 10-fold symmetry, with this discovery and the quasiperiodicity being found, any symmetry in any number of dimensions is possible.

The quasicrystal we will be investigating in this report is a Ag-In-Yb quasicrystal. The Ag-In-Yb quasicrystal is formed by rhombic triacontahedron clusters. There have been multiple papers about the



^Figure 2 - theoretical prediction of a 10-fold



^Figure 3 - Experimental of a 10fold diffraction pattern from Al₆Mn

structure of the surface of the Ag-In-Yb quasicrystal. The rhombic triacontahedron clusters are made up of 5 successive atomic shells (See figure 4), which can be mapped with P1 Penrose tiling, with a few Yb 'glue atoms' between shells. In a study from 2018 'Growth of a bismuth thin film on the five-fold surface of the icosahedral Ag-In-Yb quasicrystal' ^[3], it showed that the deposited bismuth atoms would fill the empty sites of the atomic shells of the rhombic triacontahedron and continue the quasiperiodic structure of the Ag-In-Yb quasicrystal. This was interesting because if this is also possible with other elements it would mean there are many new allotropes of elements, with unknown and possibly useful physical properties.



^Figure 4 - Successive atomic shells that make up the rhombic triacontahedron clusters

The technique used to analyse the surface of the Ag-In-Yb quasicrystal in this investigation is X-ray Photoelectron Spectroscopy, XPS. XPS uses x-rays incident on the quasicrystal surface that, through the photoelectric effect, are ejected from the surface of the quasicrystal. These ejected electrons have a kinetic energy that can be incident on a detector and measured. From this we can identify; the elements on the surface, metallic and insulating features, chemical composition of the surface, surface alloying (core level shifts), depth profiling and thin film growth modes. In this investigation we will focus on chemical composition, surface composition and alloying.

The data we get from the detector after XPS is in the form of a spectra of binding energy against counts per second (electron intensity). The XPS spectrum consists of the following features: Photoelectric peaks, Background, Plasmon peaks, Oxide peaks, Satellite peaks and Auger peaks (See figure 5). We do not need to worry about the Oxide peaks as our surface was sputtered under ultra-high-vacuum and annealed so any oxidation would have been removed. In this investigation we are most interested in the metal peaks so ignore the valence and auger peaks. In the spectra we see peak splitting due to the spin of the electrons, we will see in the Aq-In-Yb spectra different peaks for the 3d_{3/2} and 3d_{5/2} electron binding energies. The background in the spectra is due to the inelastically scattered electrons, the background is greater at higher binding energy due to this.



<u>Methodology</u>

Due to the Covid-19 pandemic we were unable to go into the labs to see how the data is taken or take any data ourselves, so we were provided data that had been taken prepandemic, specifically in this investigation from 2014 and 2015. The quasicrystal was grown by the Bridgman method, the sample will have been cut perpendicular to the five-fold axis and polished using diamond paste to 0.25µm. Before the spectra was taken the surface needs to be cleaned to minimise any impurities present on the quasicrystal surface. This is done by repeated cycles of sputtering and annealing under ultra-high vacuum. After sputtering In and Yb is depleted on the quasicrystal surface and the annealing recovers the bulk composition of the quasicrystal surface.

After the surface has been cleaned it is put into the analyser to take the measurement. CasaXPS only takes VAMAS (.vms) files so the files that the analyser give need to be converted to this file type (See appendix [3] for how to convert to accepted file type). CasaXPS is the programme that will be used to fit and extract meaningful quantities from the measured spectra this is a guide on how I used CasaXPS to get meaningful values from the spectra, a more general but comprehensive guide can be found in the appendix of the paper 'Surface of Intermetallics: Quasicrystals and beyond'^[3] Using CasaXPS:

- 1. Open CasaXPS application using the open icon.
 - This should give you a screen like this of opened spectra. This is a survey scan.

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- 2. Press the element library icon in the toolbar as seen here.
 - Window 1 should appear. Then press the periodic table tab at the top to get the window 2.



• Then press the 'Find Peaks' button. This should select some element that the programme thinks are present in the survey scan. If there are unwanted elements highlighted, you can deselect them manually by clicking the appropriate element icon/s.

• As in this investigation we are looking at the In deposition on a Ag-In-Yb quasicrystal our periodic table should look like this, with only the Ag, In and Yb selected. When 'Find Peaks' button is used it may select some elements that are not in the sample, just deselect these so only elements present are selected.



 Now looking at figure X, it should have vertical lines indicating the binding energies of the various electrons with labels showing which shell they are from and their orbital spin. As can be seen it has labelled all binding energies of Ag, In and Yb electrons. For this investigation we are focusing on the Ag 3d_{3/2}, Ag 3d_{5/2}, In 3d_{3/2}, In 3d5/2, Yb 4d_{3/2} and Yb 4d_{5/2} core electrons.



Figure 7 - Survey scan labelled with all electron binding energies displayed with lines indicating their position.

- 3. We now need to create regions that we want to look at so we can calculate relative intensities. To do this we press the 'create regions' button of either window 1 or 2 and it will create regions, highlighted in green, at the desired binding energies. Once the regions are created, I pressed the 'Clear All Elements' button in window 2 as the newly formed regions will be labelled so it is easier to see what is going on to remove the rest of the labelled peaks not in the regions.
 - As can be seen in the top left of the below spectra, position, full width at half maximum, area and atomic percentage have been automatically calculated for the generated regions, we are going to improve the regions and introduce a background to the data in step 4 so this data can be ignored in this step as we will get more accurate values when we have manually fitted the regions. See below the survey scan with regions.



Figure 8- Spectra with automatically generated regions highlighted in green.

Regions labelled from leftright: In 3d, Ag 3d, Yb 4d.

- These are the regions that the programme auto selected when we pressed the 'Create Regions' button. See appendix [1] to see enlarged highlighted regions. They are not very well fit so we will add more regions in step 4 and manually manipulate the boundaries of the current regions in order to accurately calculate a suitable background.
- 4. As we are interested in both the 3/2 and the 5/2 angular momentum quantum number for the 3d in the Ag and In peaks and the 4d in the Yb peak we need to fit regions to each of the corresponding peaks.
 - To do this we must press on the quantification parameters icon in the toolbar. As seen here.

• This should open this window making sure that you are on the regions tab. You should be able to see the three pre-existing regions that we have generated when we pressed the 'create regions' button in the previous part. Make sure that the row labelled 'BG Type' all filled in with Shirley background type. We will use this window to create more regions.



- we now need to zoom in on the spectrum where we can see the existing region labelled by In 3d. We can do this by using the cursor to draw a square around the region we want to zoom in on and then press the zoom in icon as seen here.
- Once we zoom down the right region click the create button in the quantification parameters window. This should create a region that spans both the peaks, we want to use cursor to move the boundaries of the region to appropriately fit in each peak as seen below.

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Figure 9 - Spectra with manually selected regions for In 3d_{3/2} and In 3d_{5/2} peaks.

- When this new region is created, a new column in the quantification parameters window will be made, label this column with the appropriate element, orbital and angular momentum quantum number. The quickest way to find out which electron is responsible for the peak is to go back to window 2 and select the element that you are trying to fit from the periodic table, this should show which electron is responsible for the peak and thus how you should label the region.
- Repeat Step 4 for the Ag and Yb peaks. There should now be six different regions in the quantification parameters window. See appendix [2] for Ag and Yb manually fitted regions.
- 5. We are now going to create three more regions each one will span both peaks of each element this will help us get a total area under the peaks. we want to zoom in on a set of two peaks, now press the create region button in the quantification parameters window and use your cursor to drag the boundaries of the newly created region to be fitting in both existing regions. This is an example.



Figure 10 - Spectra with manually fitted regions.

- Ask can be seen from figure 10, the newly created region plus boundaries that are just outside the outer boundaries of the individual regions, we want to name this region 'Indium total', as for this example is with Indium. Repeat this process for silver and ytterbium peaks.
- Now open the quantification parameters window on the region tab, on the row labelled 'BG Type' all the columns should have Shirley background, we now want to change the column that represents the total region of each element, change the background type to 'Skip', to save time you can just type SK into the box and press enter and it should auto fill Skip. This background type is used because it prevents any change in the background so will retain the Shirley background defined in the separate peaks.

• One the regions are correctly placed and the total regions have been given the 'skip' background type, the table of data in the top left of the spectra should look like this.

Name	Pos.	FWHM	Area	At%
Ag 3d3/2	368.60	1.28	12700.11	9.43
Ag 3d5/2	374.60	1.25	7803.03	4.68
Ag total	368.60	1.28	20486.81	23.73
In 3d3/2	451.10	1.29	10776.79	12.48
In 3d5/2	443.60	1.39	18216.48	10.92
In total	443.60	1.39	28969.94	33.55
Yb 4d3/2	190.60	3.95	865.47	1.00
Yb 4d5/2	181.10	3.40	1394.37	1.61
Yb total	181.10	3.40	2248.40	2.60

- As can be seen from the table we have automatically calculated values of position, full width at half maximum, area and atomic percentage. In the element totals rows, we only need to worry about area as the other three values are incorrect. We can also ignore the final column Which represents atomic percentage as it is incorrect due to the regions overlapping. We can use these values of area to calculate and ratio between silver and Indium and thus determine whether this Spectra is from before Indium is deposited on the surface or afterwards but to get a more accurate area, we will first need to fit align shape to the peaks.
- 6. We now want to fit line shapes to the peaks in order to get a more accurate value of peak area. we do this by going to the component tab of the quantification parameters window this should display a window like this.

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Window 5:

• Now zoom in on a set of two peaks and click the 'Create' button twice in the components tab of the quantification parameters window. This will add two columns to the table in the components tab it should have fitted a line shape to both peaks. It will most likely not be a very good fit at this point, but we will change the parameters to make it fit better. It should look like this.

Window 6.

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 Make sure to label the peaks appropriately. In these fits we are going to be using the Doniach Sunjic line shape also peaks are slightly so asymmetric. to do this we need to go to the row labelled line shape and type in DS(0.01,499) and press return. The Doniach Sunjic is used as the peaks are roughly equally asymmetric. Once the line shape row is changed, we press the 'fit components' button, this should give a fairly good fit. See on the next page the fit we got for In 3d_{3/2} and In 3d_{5/2} following this step.



Figure 11 - shows the difference in the curves with parameters of 0.1and S 0.2



Figure 12 - In $3d_{3/2}$ and In $3d_{5/2}$ peaks fitted with Doniach Sunjic line shapes.

• Repeat step 6 for all elements. Once all peaks have been fitted the residual STD should be reduced. Windows 6 should now have 6 columns each corresponding to a peak. from these columns we are given multiple sets of data including area, full width at half maximum, position and percentage concentration.

<u>Results</u>

I was given 8 spectra to analyse so I followed from steps one to six for each Spectra to determine the area, full width a half maximum, position and percentage concentration. Tables 2-9 will display the data for each peak in each spectrum.

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	13224.3	21444.0	7007.8	10809.0	1314.9	1384.8
FWHM	1.323	1.469	1.213	1.259	4.458	3.255
Position (eV)	451.32	443.75	374.69	368.70	190.66	181.20
Percentage concentration	23.96	38.86	12.70	19.59	2.38	2.51

Table 2: Spectra taken on 16/04/2014. Residual Standard deviation = 0.9922

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	13179.0	20658.2	9053.5	12928.6	2262.5	3011.3
FWHM	1.384	1.469	1.288	1.284	4.700	4.332
Position (eV)	451.25	443.65	374.64	368.63	190.47	181.57
Percentage concentration	21.57	33.81	14.82	21.16	3.70	4.93

Table 3: Spectra taken on 17/04/2014. Residual Standard deviation = 0.9804

Table 4: Spectra taken on 18/04/2014. . Residual Standard deviation = 1.127

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	16240.5	24443.1	9767.8	15200.7	1529.1	1740.3
FWHM	1.404	1.453	1.259	1.323	3.537	3.055
Position (eV)	451.33	443.74	374.69	368.68	190.84	181.36
Percentage concentration	23.56	35.47	14.17	22.06	2.22	2.53

Table 5: Spectra taken on 02/06/2014. . Residual Standard deviation = 0.9076

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	11641.8	18529.2	8481.9	13148.5	1104.0	1573.0
FWHM	1.270	1.415	1.185	1.255	3.601	3.342
Position (eV)	451.25	443.68	374.64	368.64	190.63	181.17
Percentage concentration	21.37	34.01	15.57	24.14	2.03	2.89

Table 6: Spectra taken on 26/01/15. . Residual Standard deviation = 0.8442

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	8283.6	13497.8	7241.9	10853.6	1460.3	554.8
FWHM	1.325	1.455	1.269	1.285	6.032	1.971
Position (eV)	451.27	443.71	374.64	368.63	190.72	181.06
Percentage concentration	19.77	32.22	17.29	25.91	3.49	1.32

Table 7: Spectra taken on 28/06/2015 1 of 2. . Residual Standard deviation = 1.454

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	32417.2	50553.1	21433.5	32334.3	3355.5	5480.1
FWHM	1.504	1.577	1.363	1.431	3.190	3.243
Position (eV)	451.12	443.51	374.47	368.47	190.58	181.13
Percentage concentration	22.27	34.73	14.72	22.21	2.31	3.76

Table 8: Spectra taken on 28/06/2015 2 of 2. . Residual Standard deviation = 1.175

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	28186.6	44994.4	20383.1	30652.8	3839.7	5256.4
FWHM	1.473	1.596	1.395	1.443	3.630	3.540
Position (eV)	451.07	443.50	374.47	368.47	190.59	181.10
Percentage concentration	21.14	33.75	15.29	22.99	2.88	3.94

	In 3d _{3/2}	In 3d _{5/2}	Ag 3d _{3/2}	Ag 3d _{5/2}	Yb 4d _{3/2}	Yb 4d _{5/2}
Area	28156.3	45310.9	20335.9	30267.5	3690.7	4731.4
FWHM	1.469	1.603	1.391	1.430	3.500	3.317
Position (eV)	451.07	443.50	374.47	368.48	190.56	181.13
Percentage concentration	21.25	34.20	15.35	22.84	2.79	3.57

Table 9: Spectra taken on 29/06/2015. Residual Standard deviation = 1.223

Now to calculate the total area of In, Ag and Yb to calculate a Ag to In ratio.

Table 10: showing the summation of the area of two peaks of each element.

Date of spectra taken	Overall In area	Overall Ag area	Overall Yb area	
16/04/2014	34668.3	17816.8	2699.7	
17/04/2014	33837.2	21982.1	5273.8	
18/04/2014	40683.6	24968.5	3269.4	
02/06/2014	30171.0	21630.4	2677.0	
26/01/2015	21781.4	18095.5	2015.1	
28/01/2015 a	82970.3	53767.8	8835.6	
28/01/2015 b	73181.0	51035.9	9096.1	
29/01/2015	73467.2	50609.4	8422.1	

As these spectra were taken on different days the time they were in the detector was not the same every time. We aren't able to just look at the difference in area between each run due to the differing measurement times but we can use the ratio of Ag to In to determine which scan is before and after deposition of In.

Table 11: showing Ag to In ratio of each spectra.

Date of spectra taken	Ag : In area ratio		
16/04/2014	0.5139		
17/04/2014	0.6496		
18/04/2014	0.6137		
02/06/2014	0.7169		
26/01/2015	0.8308		
28/01/2015 a	0.6480		
28/01/2015 b	0.6974		
29/01/2015	0.6889		

When we graph these ratios, we get.



Discussion

After deposition of indium on the quasicrystal surface we would expect the percentage composition of the quasicrystal that is indium would increase as it occupies the empty sites of the rhombic triacontahedron shells and carry on the quasiperiodic structure of the quasicrystal. If this were the case the ratio of the Ag to In atoms in the spectra would be lower. From this assumption I believe that the spectra taken on the 16/04/2014 is a spectrum that has been taken post indium deposition.

I will compare the position and FWHM of the peaks in the 16/04/2014 spectra with that of 28/01/2015 b, as the mean ratio of the remaining spectra is 0.6921 and 28/01/2015 b has the closest ratio to the mean.

	Position	Position	Difference	FWHM	FWHM	Difference
	(eV)	(eV) Before	in	After	Before	in FWHM
	After indium	indium	position(eV)	indium	indium	
	deposition	deposition		deposition	deposition	
In 3d _{3/2}	451.32	451.07	+0.25	1.323	1.473	-0.150
In 3d _{5/2}	443.75	443.50	+0.25	1.469	1.596	-0.127
Ag 3d _{3/2}	374.69	374.47	+0.22	1.213	1.395	-0.182
Ag 3d _{5/2}	368.70	368.47	+0.23	1.259	1.443	-0.184
Yb 4d _{3/2}	190.66	190.59	+0.07	4.458	3.630	+0.828
Yb 4d _{5/2}	181.20	181.10	+0.10	3.255	3.540	-0.285

Table 12: showing comparison of positions and FWHM before and after deposition of indium on the quasicrystal surface.

As can be seen in table 12, the binding energies of all the peaks are shifted to higher binding energy after Indium deposition. The indium peaks are shifted the most, silver peaks being shifted almost as much, and ytterbium only being shifted a small amount. This could suggest that the Indium deposited on the surface bonds to Indium most favourably, followed closely by Ag and then least favourable Yb. The difference in FWHM between before and after deposited indium shows that the range of energies of electrons emitted is smaller in all but the Yb $4d_{3/2}$ case. I believe that this is an anomaly as in the 28/01/2015b Yb peaks were hard to distinguish so I had to guess where the peaks started and ended.

Conclusion/recommendations

In conclusion the investigation it would have improved the results and analysis if we could have gone into a lab and collected more data so that we could try and see and more convincing difference between ratios of silver to indium in the before and after indium deposition spectra. To carry on this project we could combine the use of XPS with STM and LEED to further investigate the composition of the surface of the Ag-In-Yb quasicrystal.







Figure 17 - Manually fitting regions for Yb $4d_{3/2}$ and Yb $4d_{5/2}$.

[3]. https://lib.dr.iastate.edu/cgi/viewcontent.cgi?article=3821&context=etd

[4]. Growth of a bismuth thin film on the five-fold surface of the icosahedral Ag- In-Yb

quasicrystal - S.S. Hars^a, H.R. Sharma^{*,a}, J.A. Smerdon^b, S. Coates^a, K. Nozawa^C, A.P. Tsai^d, R. McGrath^a

Project Proposal

Week 1 (08/02/2021):

- Project proposal
- Risk Assessment
- Start portfolio of activity log
- Apply for Laptop from uni that can run CasaXPS
- Initial research of XPS and Quasicrystals

Week 2 (15/02/2021):

- Further reading on XPS and Quasicrystals
- Specifically, Ag-In-Yb and In absorption and set up

Week 3 (22/02/2021):

• Familiarise with software CasaXPS

Week 4 (01/03/2021):

- Analysis of data
- Start to plan report and presentation

Week 5 (08/03/2021):

- Analysis of data
- Start to write presentation

Week 6 (15/03/2021):

- Analysis of data
- Continue presentation preparation

3 weeks for easter

(22/03/2021):

- Presentation preparation
- Analysis of data
- Research Latex
- Report writing

(29/03/2021):

- Presentation preparation
- Analysis of data
- Research Latex
- Report writing

(05/04/2021):

- Report writing
- Analysis of data
- Finish presentation and start practicing / writing script

Week 7 (12/04/2021):

- Analysis of data
- Finalise and practice presentation

Week 8 (19/04/2021):

- Final analysis of data
- Presentation (20%)
- Report writing after presentation complete

Week 9 (26/04/2021):

• Report writing

Week 10 (03/05/2021):

• Report writing

Week 11 (10/05/2021):

• Finish report and submit