Chip Inspection Technology

X-Ray Diffraction (XRD) Analysis

Why XRD

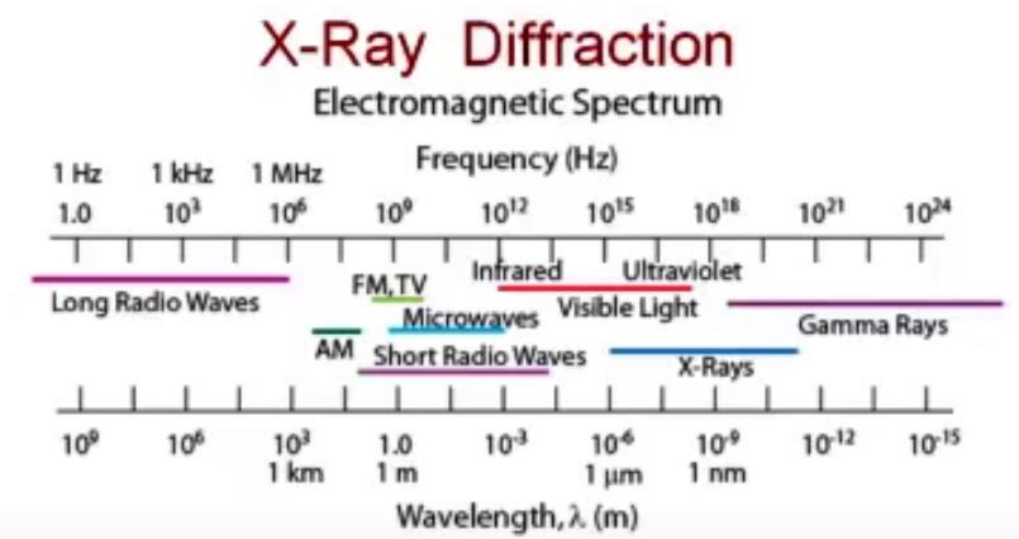
- When the size of IC components continues to shrink with Moore's Law, and reaches the physical limit and cannot be shrunk anymore, the solution is to change the materials used.
- You can improve the low power consumption and high frequency characteristics of the components by replacing materials with more suitable properties.
- In the semiconductor manufacturing process, hundreds of process steps are involved. Once the materials are changed, you must consider:
  - ✓ whether the process equipment also needs to be changed.
  - ✓ whether the samples produced after the equipment change are usable and stable in quality meet the original IC design specifications.
- During the development period of selecting new materials and the production verification after confirming material changes, it is necessary to conduct a series of strict material analysis and control on this material to confirm whether it meets the required characteristic requirements.

Why XRD

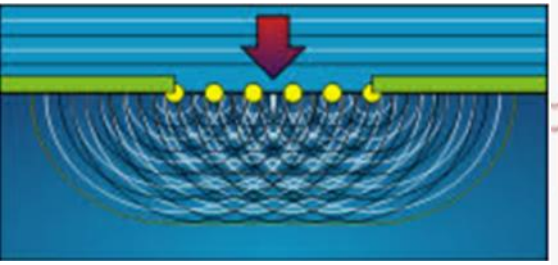
XRD plays an important role in wafer raw material inspection.

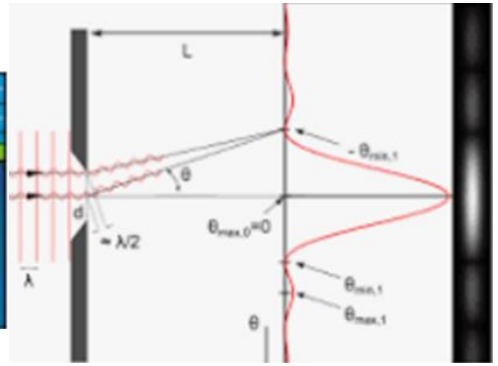
- Non-destructive analysis
  - ✓XRD is a non-destructive analytical instrument. It generates a pattern through the diffraction of X-rays and crystals, and compares it with the pattern database to deduce the arrangement structure of the material crystals, the way the crystals are arranged, and the size of nanocrystals, as well as the crystallinity of single crystal and polycrystalline thin film materials Analysis etc.
- Crystal structure analysis
  - ✓XRD can be used to evaluate the arrangement of crystals and determine whether the crystals have a neatly stacked structure. This is crucial for the research and development stages such as wafer manufacturing and LED manufacturing.
- Film characteristic analysis
  - ✓XRD can further obtain the film thickness, sample surface, layer-to-layer interface roughness and the electron density of the film. It even enables analysis of multilayer films, with total thickness limited to less than 500 nm.
- High precision and high strength
  - ✓The XRD introduced by iST is equipped with the XRR (thin film X-ray reflection) function, which can achieve an accuracy of 0.1 nm thickness and provides an excellent tool for non-destructive analysis of thin film material properties.
- In short, XRD can not only ensure the integrity of the crystal structure during wafer raw material testing, but also deeply explore the characteristics of thin films, providing important support for material research and process optimization.

Principle of XRD



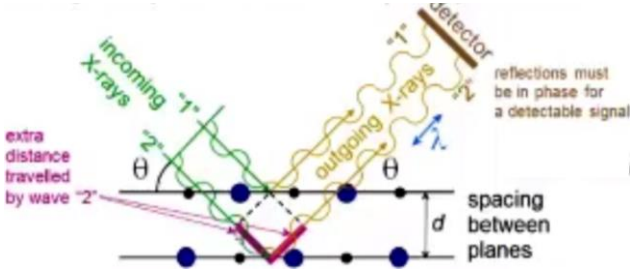
- Diffraction gratings must have spacings comparable to the wavelength of diffracted radiation.
- ~~Can't resolve spacings < λ~~.
- Spacing is the distance between parallel planes of atoms

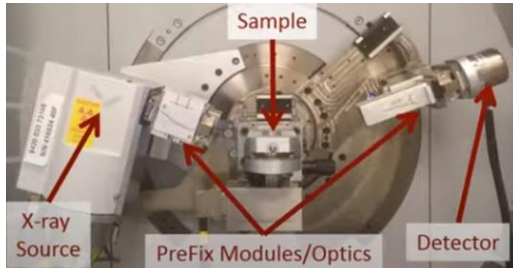




- **Interaction of X-rays with crystals**
  - ✓When a beam of monochromatic X-rays shines on a crystal, the atoms in the crystal scatter the X-rays.
  - ✓Each atom produces scattered waves, which interfere with each other, causing diffraction.
  - ✓The superposition of diffracted waves results in the rays being strengthened in some directions and weakened in other directions.
- **Bragg equation**
  - ✓The relationship between the interplanar spacing of a crystal and the wavelength of incident X-rays is Bragg's equation, which describes the relationship between diffraction angle and interplanar spacing:

$$2d\sin(\theta) = n\lambda$$





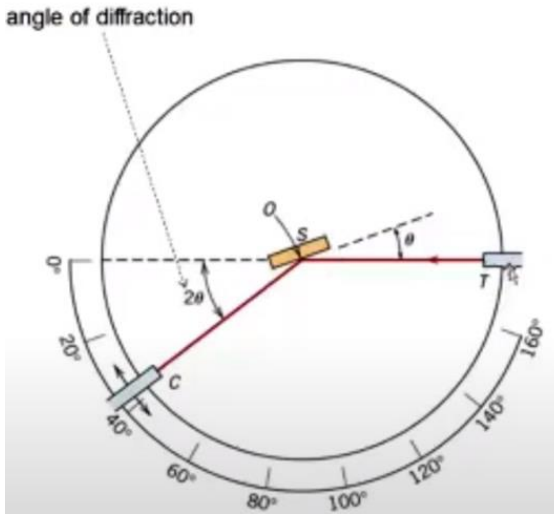
where *d* is the interplanar spacing, *θ* is the Bragg angle, *n* is the reflection order, and *λ* is the wavelength of X-rays.

- **Diffraction pattern**
  - ✓By measuring the diffraction intensity at different angles, the **diffraction pattern of the crystal** can be obtained.
  - ✓The diffraction pattern of each crystal reflects its internal atomic distribution, thereby **reveal the crystal's structure**.

Common XRD data analysis methods

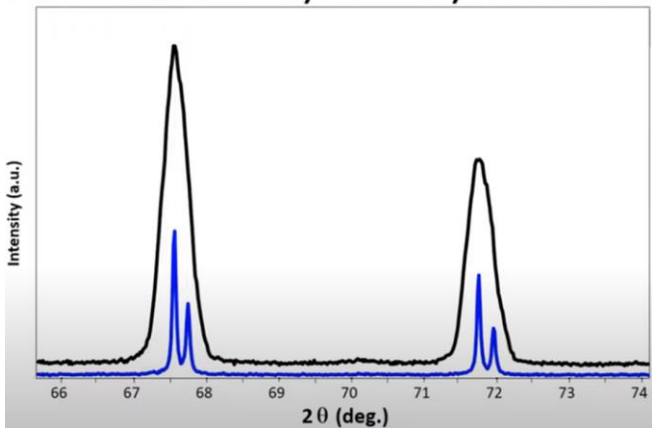
- Phase characterization
  - ✓Compare the measured diffraction pattern of the sample with the standard PDF card to determine the phase present in the sample. This is one of the most common applications of XRD.
- Determine the unit cell parameters
  - ✓By analyzing the position and intensity of the diffraction peak, calculate the unit cell parameters, such as lattice constant, unit cell volume, etc.
- Crystal orientation analysis
  - ✓XRD can be used to evaluate the orientation of crystals and determine whether the crystals have a neat stacking structure.
- Grain size calculation
  - ✓By analyzing the half-maximum width of the diffraction peak, the size of the grain can be estimated.
- Quantitative calculation of physical phases
  - ✓Calculate the content of different phases in the sample based on the intensity of the diffraction peaks.
- X-ray diffraction analysis generates a pattern through the diffraction of X-rays and crystals, and compares it with the pattern database to deduce the arrangement structure of the material's crystals, the way the crystals are arranged, the size of the nanocrystals, and the size of the single crystal.

Diffractometers

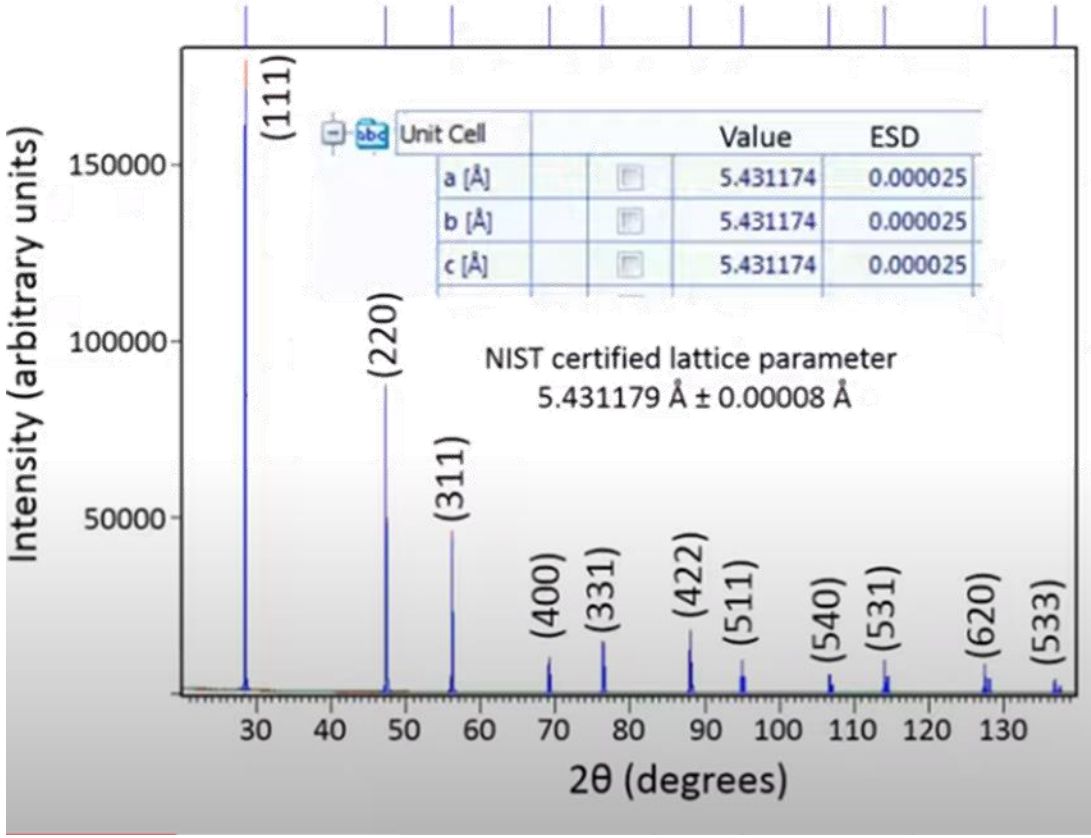


If you had a single crystal specimen, you would have to move your sample more. But if you have a polycrystalline specimen or a powder, then you have a large number of random orientations to see diffraction from all possible planes.

Peak Breadth Analysis – Crystallite Size



Polycrystalline Powders or Solid Pieces
Phase Identification & Lattice Parameters

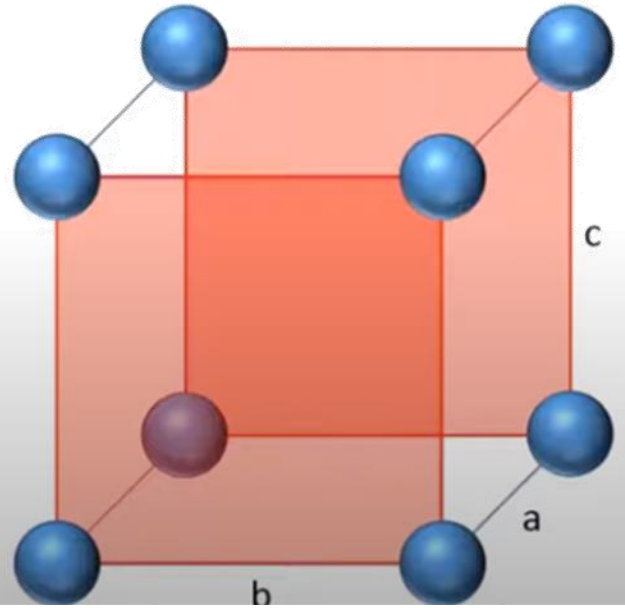


$n\lambda = 2d(\sin\theta)$

Peak Location → θ

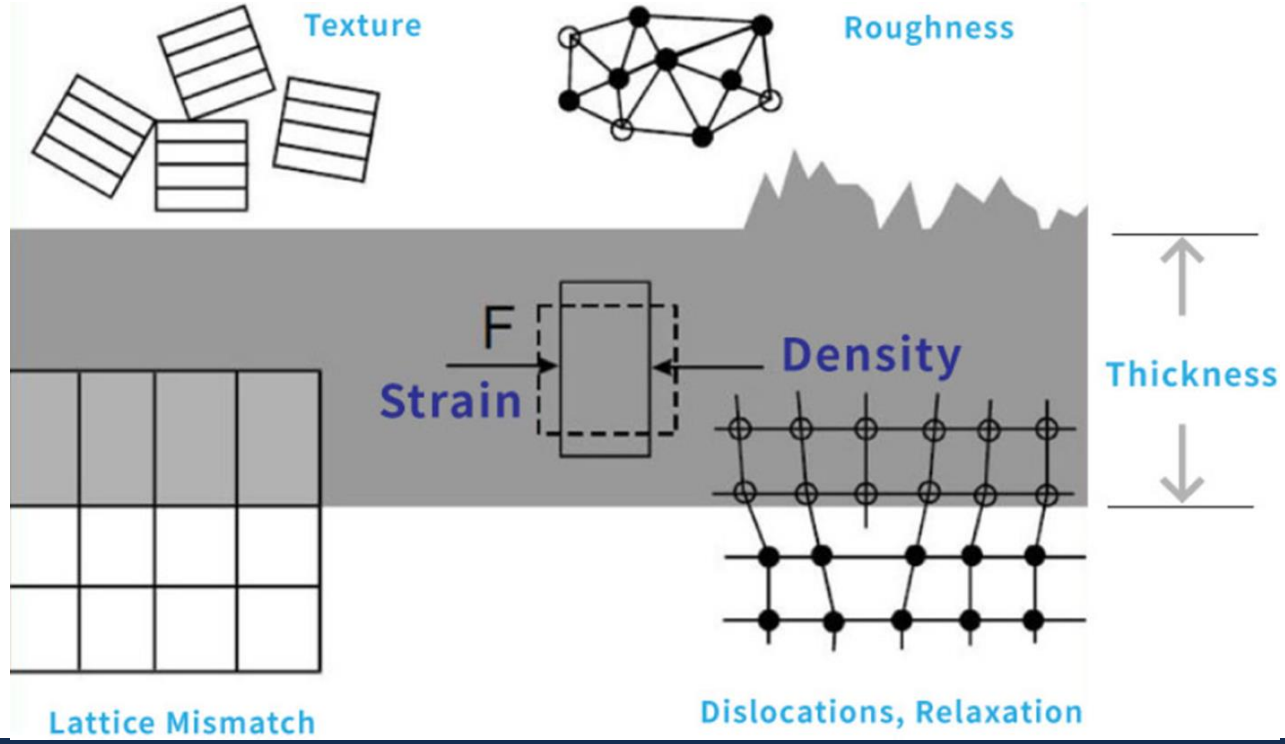
Solve for d-spacing → distance between planes

Distance between planes → lattice parameters

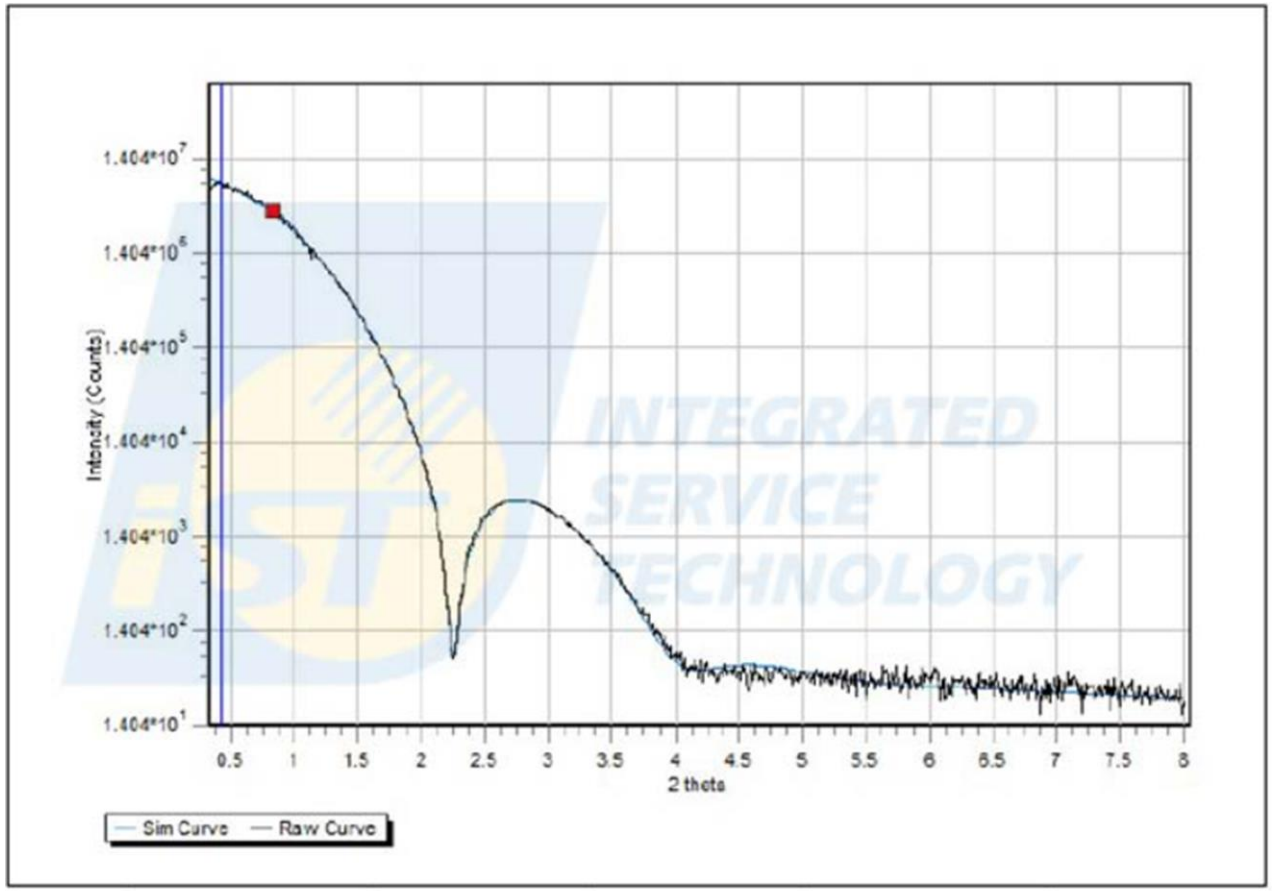


XRD +XRR(X-Ray Reflectivity)

- XRD uses the principle of diffraction, while XRR is the reflection pattern of XRD, which can further obtain
  - ✓the thickness of the film (ex. accuracy up to 0.1nm thickness)
  - ✓the interface roughness of the sample surface, layer and layer
  - ✓the electron density of the film
  - ✓the multi-layer film analysis (the total thickness is limited, ex. less than 500nm)
  - ✓non-destructive analysis of film material properties



XRR spectrum and fitting analysis results of extremely thin metal film Ru grown by ALD



N	R	Material	Cell input	Thickness	Roughness	Density T
1	1	Ru	density	4.334	0.641	13.286
SUB	1	SiO2_a	density	0.000	0.562	2.1960

(from Integrated Service Technology, Inc)

Reference link

10 minutes to learn XRD
https://www.youtube.com/watch?v=dzHrVPmYJ5c

What is X-ray diffraction?1
https://www.youtube.com/watch?v=QHMzFUo0NL

What is X-ray diffraction?2
https://www.youtube.com/watch?v=93bTw8Xcc8M

Introduction to X-ray Diffraction
https://www.youtube.com/watch?v=n5qZMgOnsAs

Thanks for your listening