

# X-Ray Diffraction & Scanning Probe Microscopy Assessment

Instructor's Guide

## Matching

Match the word with the best definition.

- |                 |                                  |   |
|-----------------|----------------------------------|---|
| <u><b>D</b></u> | 1. diffraction                   | a. an instrument that can image atoms and operates by sensing the force between the surface atoms of a sample and a probe tip   |
| <u><b>H</b></u> | 2. atom                          | b. an instrument that can image atoms by the quantum mechanical tunneling of tunneling effect electrons between an electrically conducting atomic tip and a substrate |
| <u><b>K</b></u> | 3. rastering                     | c. energy of the most weakly bound electrons in a metal   |
| <u><b>G</b></u> | 4. tunneling effect              | d. the scattering of light from a regular array, producing constructive and destructive interference  |
| <u><b>L</b></u> | 5. X-ray                         | e. opposition to the flow of electric current   |
| <u><b>J</b></u> | 6. piezoelectric material        | f. visible light-based method of investigating atomic arrangements at a macroscopic level   |
| <u><b>A</b></u> | 7. AFM                           | g. the movement of an electron due to its wave nature through a classical barrier   |
| <u><b>B</b></u> | 8. STM                           | h. the smallest unit of a chemical element  |
| <u><b>E</b></u> | 9. electrical resistance         | i. radiant energy that exhibits wavelike behavior and travels through space at the speed of light in a vacuum   |
| <u><b>I</b></u> | 10. electromagnetic radiation    | j. material that distorts when a voltage is applied to it   |
| <u><b>F</b></u> | 11. optical transform experiment | k. scanning back and forth across the surface of a material   |
| <u><b>C</b></u> | 12. Fermi Energy                 | l. electromagnetic radiation with a wavelength of about the size of an atom   |



18. a.) What is the frequency of an X-ray with a wavelength of 1.54 angstroms, the wavelength produced by an X-ray tube with a copper target? (The speed of light is  $2.998 \times 10^8$  m/s.)

$$c = \lambda\nu$$

$$(2.998 \times 10^8 \text{ m/s}) = (\nu)(1.54 \text{ angstroms})(1 \times 10^{-10} \text{ m/ angstrom})$$

$$\nu = 1.95 \times 10^{18} \text{ s}^{-1}$$

- b.) What is the frequency of an X-ray with a wavelength of 0.7107 angstroms, the wavelength produced by an X-ray tube with a molybdenum target?

$$c = \lambda\nu$$

$$(2.998 \times 10^8 \text{ m/s}) = (\nu)(0.7107 \text{ angstroms})(1 \times 10^{-10} \text{ m/ angstrom})$$

$$\nu = 4.218 \times 10^{18} \text{ s}^{-1}$$

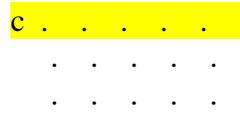
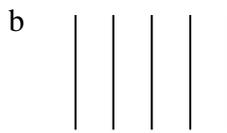
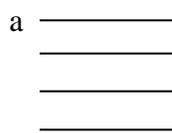
19. What is the frequency of a 670 nm red laser?

$$c = \lambda\nu$$

$$(2.998 \times 10^8 \text{ m/s}) = (\nu)(670 \text{ nm})(1 \times 10^{-9} \text{ m/nm})$$

$$\nu = 4.47 \times 10^{14} \text{ s}^{-1}$$

20. Sketch a qualitative representation of the diffraction pattern produced by the following two-dimensional arrays.



**Vertical spots**

**Horizontal spots**

**Square pattern of spots**

21. Sketch a qualitative representation that shows the difference in the diffraction pattern produced by the following pairs of two-dimensional arrays.



**The smaller square array gives the larger square diffraction pattern.**



The pattern on the left gives a square diffraction pattern; the array on the right gives a rectangular diffraction pattern with the long distance between spots in the horizontal direction.



Both arrays give rectangular diffraction patterns. The array on the left will give a diffraction pattern with the longer edge of the rectangle in the vertical direction. The array on the right will produce a diffraction pattern with the longer edge of the rectangle in the horizontal direction.



An array of lines gives a series of dots in the diffraction pattern. The horizontal pattern of lines will give a diffraction pattern consisting of a set of spots running in the vertical direction, and the vertical array of lines gives a diffraction pattern consisting of a set of spots in the horizontal direction.

22. Why must X-rays be used in crystal-structure determinations rather than visible light?

In order for diffraction to occur, the wavelength of incident radiation must be approximately the same as the spacing of the atoms. Atomic separations are typically a few angstroms. X-rays, with wavelengths of about one angstrom, are a far better match to interatomic spacings than visible light ( $\lambda \sim 4,000$  angstroms to 7,000 angstroms).

23. Why does X-ray diffraction give more information about the three-dimensional structure of a crystalline solid than does scanning tunneling microscopy?

The STM can only collect two-dimensional information. The penetrating nature of X-rays and subsequent diffraction of various planes of atoms adds information in the third dimension.

24. Use the Bragg equation to explain the observation that as the spacing between the atoms decreases, the spacings in the resulting diffraction pattern increase.

For a given order of diffraction ( $n$  value), as  $d$  becomes smaller,  $\sin \theta$  must become larger to satisfy the Bragg equation:  $2d(\sin \theta) = n\lambda$ . Thus, as  $\sin \theta$  and  $\theta$  increase, the observed spacing of the spots in a diffraction pattern increases.

25. Briefly explain how the STM works.

**The STM is an instrument that moves a probe tip terminating in a single atom over a surface that is within Angstroms of it. It maps out the contours of the features of the surface, using differences in height at constant current or in electrical current at constant height. Electrostatic forces hold the electrons on the surface of any material, and this acts as a barrier for preventing the electrons from escaping. However, if another material, such as the probe tip is brought close enough to the surface, the electron can escape from the surface into the tip (or vice versa, depending on the direction of the applied voltage) through the quantum mechanical phenomenon of tunneling. A computer typically sends instructions to the tip, and the tip rasters over the surface and creates a complete image of the surface with atomic resolution.**