Queen Mary, University of London

School of Physics and Astronomy

Physics in Techniques

Conduction Band

Gap

Valence Band

Γ   P   Z   Γ   Q   Z   L   Γ   F
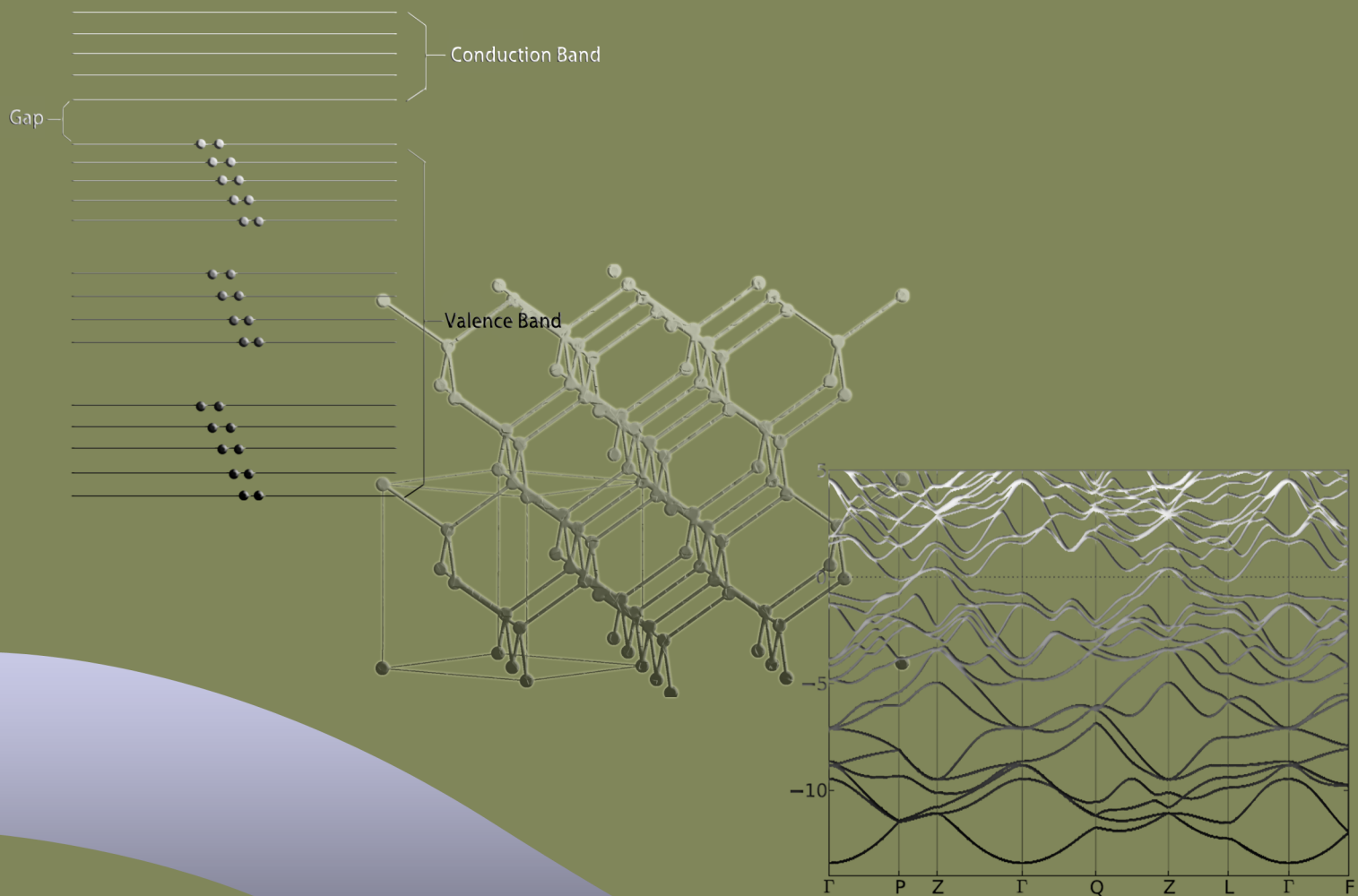
X-ray Photoelectron Spectroscopy – XPS

The basic formula for XPS spectroscopy is:

$$E_{binding} = E_{photon} - (E_{kinetic} + \phi) \tag{1-1}$$

where $E_{binding}$ is electron binding energy for specific material, E_{photon} is the incoming X-ray energy, $E_{kinetic}$ is the energy of photoelectron, and ϕ is the work-function of facility (NOT the material! It corresponds to any energy loss caused by the facility. For more about work-function of material, refer to Work-Function in this article). For different materials, plotting intensity against corresponding $E_{binding}$ or $E_{kinetic}$ can give us information about surface chemical status.

Work-Function

The formula to calculate work-function of material is:

$$W = -e\phi - E_f \tag{2-1}$$

where ϕ is the electrostatic potential in vacuum near the surface of material, and $-e\phi$ together means the energy level of electron near the surface. And E_f is the Fermi level (electrochemical potential) of the material. So the work-function defines the energy needed to kick the electron from Fermi level to the surface state. Here it should be noticed the difference between work-function and the so-called ionization energy. The ionization energy refers to the energy needed to kick the electron out of the material to continuum state (corresponding energy level is always regarded as the 0 reference level).

Raman G-band & D-band

The G-band and D-band Raman mode specifically refers to the vibration mode for Carbon related material. G-band is specifically for graphene vibration mode and D-band refers to the mode when there is defect within graphene.

Radial Breathing Raman Mode (RBM)

Here specifically, RBM Raman mode refers to one of the vibration modes for tube like structure, e.g. carbon nanotube. This vibration mode is depicted in the following graph:
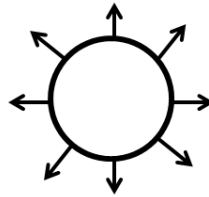

Figure 1. The illustration for RBM Raman mode.

Introduction To Mössbauer Spectroscopy

In this section, Mössbauer spectroscopy will be briefly introduced without going deep into details. Only several key points concerning the understanding of Mössbauer spectroscopy will be given. First of all, Mössbauer spectroscopy concerns the energy level of nuclei only. The basic physics image for Mössbauer spectroscopy is the emission from energy level transition of one nuclei is resonantly absorbed by another nuclei. Thinking about the energy level for electrons, where we have orbital and spin angular momentum, so finally we have fine structure for electron which contributes to Zeeman effect. For nuclei, although we cannot directly say we have orbital angular momentum for nuclei, we can still imagine 'something' coupling with nuclei spin angular momentum (the nuclei indeed has spin angular momentum), leading to fine energy level for nuclei (analogue to fine structure of electron energy level). It is just the fine structure of nuclei that contributes to what is detected by Mössbauer spectroscopy. Furthermore, if we compare Mössbauer spectroscopy to NMR (which also concerns with the quantum state of nuclei), the focus of these two spectroscopy is different. As stated above, Mössbauer spectroscopy concerns with only nuclei energy level, however, NMR focuses on the coupling between nuclei spin and electron angular momentum!

Another key point for Mössbauer spectroscopy is the condition when we can detect the Mössbauer signal. When gamma-ray is emitted from the exciter, it will push back the exciter itself (called 'recoil' effect), thus leading to the reduction of gamma-ray compared to corresponding nuclei energy level difference. And also the recoil effect could again reduce the energy of excited gamma-ray when it reaches the absorber. Thus normally we cannot easily observe Mössbauer effect. It is just the solving of recoil problem using crystal structure framework restriction that wins Mössbauer the 1961 Nobel Prize in Physics. However, then we have the motion restriction for nuclei, it is still difficult to observe Mössbauer effect for many isotope due to their high energy gamma-ray. And also the long lifetime of nuclei excited state is another crucial condition for observation and application of Mössbauer effect. Since if the nuclei excited state lifetime is so short that it will go back to ground state before the resonant absorption occurs, we cannot detect the resonance at all!

Last but not least, if we want to use Mössbauer effect as a kind of spectroscopy, only the Mössbauer resonant absorption cannot tell any information except element distinguishing. Actually, in specific system, the interaction of detected nuclei with its surrounding environment makes Mössbauer effect very sensitive spectroscopy. The type of interaction includes isomer shift, quadruple splitting and magnetic splitting, which can be used to detect different valence state, magnetic properties, etc.

For detailed introduction to Mössbauer spectroscopy mechanism, useful explanation and application, refer to the online material: Introduction To Mössbauer Spectroscopy.