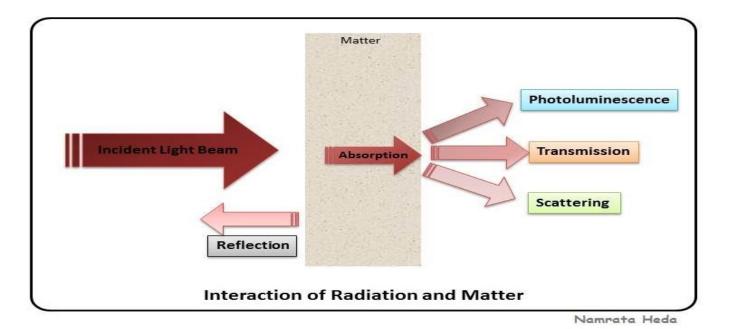
UV –Visible-NIR Spectroscopy Dr. Rakesh Kr Singh Nanoscience and Nanotechnology Center Aryabhatta Knowledge University, Patna <u>www.drrakeshsingh.com</u> 24 April 2020

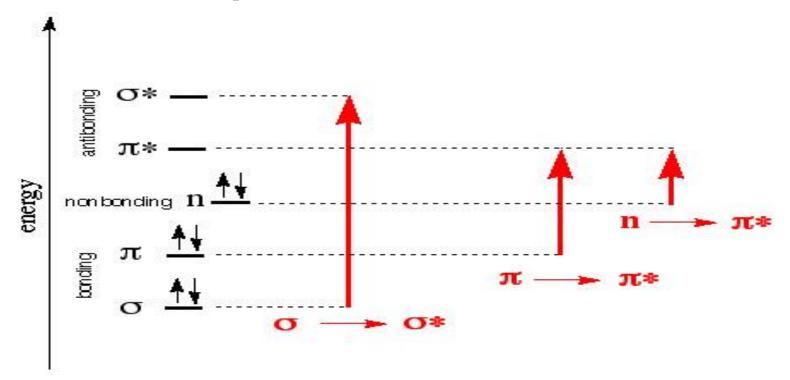
## **Spectroscopy – General Introduction**

- Spectroscopy is the study of interaction of electromagnetic radiation in all its form with materials including nanomaterils, Food, Bimaterials etc
- This interaction leads to Transmission, absorption, emission of electromagnetic radiation by atoms and molecules through excitation. This spectrum shows of intensity of absorbed or emitted radiation by materials verses wavelength



#### **Possible Transitions**

Materials/ Molecules containing  $\pi$ -electrons or non-bonding electrons (n-electrons) can absorb energy in the form of ultraviolet or visible light and further to excite these electrons to higher anti-bonding molecular orbitals. The more easily excited the electrons, the longer the wavelength of light it absorbs. Possible transitions are  $\pi$ - $\pi$ \*, n- $\pi$ \*,  $\sigma$ - $\sigma$ \*, and n- $\sigma$ \*), and  $\sigma$ - $\sigma$ \* > n- $\sigma$ \* >  $\pi$ - $\pi$ \* > n- $\pi$ \*. Electronics, Vibranational, Rotational spectra involved in this transition.

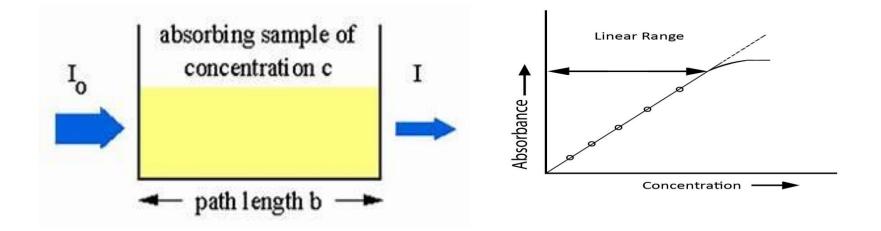


## **Basic Principal**

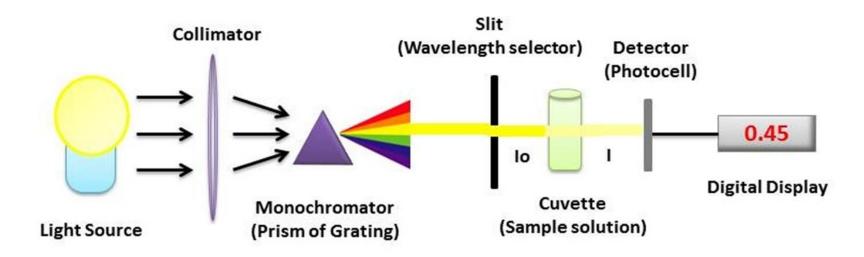
UV spectroscopy based on the Beer-Lambert law, which states that absorbance (A) at particular  $\lambda$  is proportional to the concentration of the molecules (C) in solution, Absorptivity (E) of specific type of molecular vibrations and the path length (L) of the materials holder within the measurement radiation beam . Absorbance is given by

$$A = \log (I/Io)$$

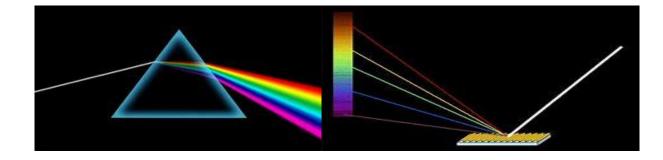
Where I is the intensity of emergent radiation and  $I_0$  is the intensity before incident.



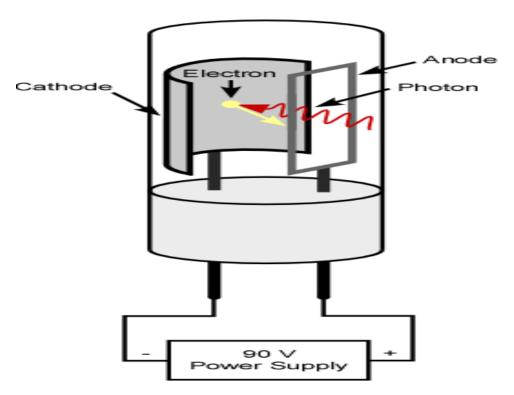
### Instrumentation



Light source used Tungsten filament lamps and Hydrogen-Deuterium lamps.Filters. Interference filters: use constructive and destructive interference to isolate a narrow beam of wavelengths . Absorption filters: Works by selectively absorbing radiation from a narrow region. Finally through prism and grating, monochromatic light allowed to pass to the materials.



# Components of UV-VIS/NIR Detector Cuvette





As Solvents may be Food materiaks, Nanomaterials, Cermics , Magnetic materials etc.

# **\_Instrument care and Precautions**

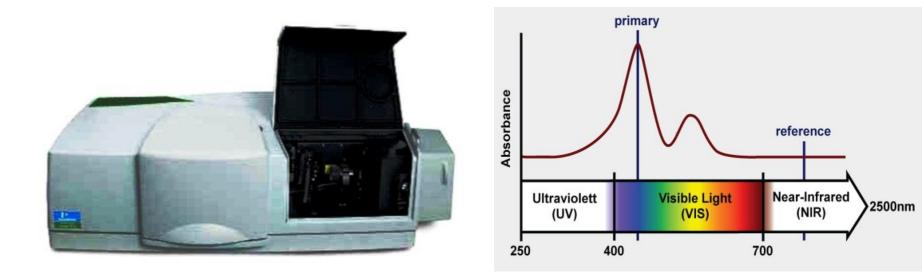
- House the instrument in air conditioned dust free room
- Workbench should be clean
- Instruments should be kept away from vibrations
- Switch off the instruments when not in use to conserve lamp life
- Sample holder should be cleaned properly
- Calibrate instruments performance against references standards at regular interval
- Keep the sample compartment closed during experiment to prevent external light to avoid errors

# **Instrument care and Precautions**

### **Sources of errors May be**

- Environmental factor affecting sample and photometer
- Temperature
- Line voltage fluctuations
- Vibrations
- Contamination
- Software with proper calibrations

#### **UV VIS spectroscopy at Nanotechnology Center, AKU**



(Source:- LAMBDA 950 UV/Vis/NIR manual ACNN, AKU Patna)

(Source:-http://www.kemtrak.com/products\_DCP007.html)

We Can find the position of absorption peak of the examined materials in UV region, Visible region or IR regions. If prepared materials found maximum absorption in IR region. Then the prepared materials are useful for blocking the IR radiation. You can find this results, research finding of ACNN, AKU and his group. Paper detail. doi. http//doi.org/10.1007/s10854-020-02901-1(J. materials science: Materials in Electronics)

#### Band Gap determination using UV-Visible-NIR spectrum

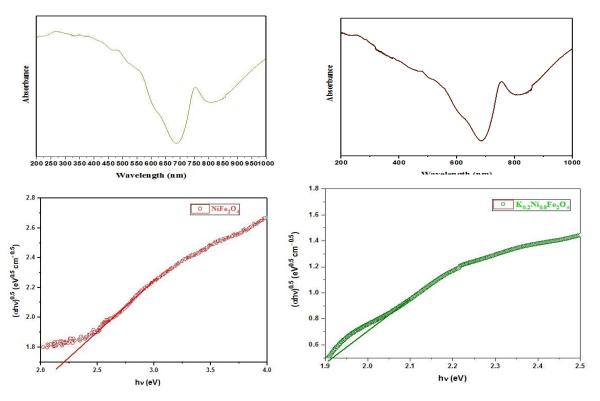


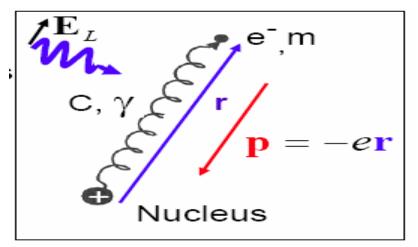
Fig. Tauc plot showing Indirect band gap of NiFe<sub>2</sub>O<sub>4</sub> and Ni<sub>0.8</sub> K<sub>0.2</sub>Fe<sub>2</sub>O<sub>4</sub>

It has been reported that with substitution of monovalent  $K^+$  ion band gap found to decrease from 2.20eV to 1.91eV. There would be a different reason that due to doping of  $K^+$  ion a new energy state can be formed and thus it recombine with lower energy state electron hole pair leading to narrowing in band gap.

Ref- M.Tech project, Nishant Kr, Rakesh Kr Singh, AKU, Patna, Reported for publication in J. of Electronics Matter letter(2020)

#### Surface plsmon resonance(SPR), Optical behavior and Materials Technology

Surface plasmon resonance is the coherent excitation of all the free electrons within the conduction band, leading to an in-phase oscillation. When the size of a metal nanocrystal is smaller than the wavelength of incident radiation, a surface plasmon resonance is generated. The external electric field of an incoming light induces a polarization of the free electrons relative to the cationic lattice. Dipolar oscillation of electrons is created with a certain frequency. Now a days nanomaterials with light emission from plant, yeast, bacteria etc. are being produced widely. Such optical behavior are very important for materials devlopement in cosmetics industry, biological imaging and others.





# **<u>Reference</u>s**

- 1. Fig1-https://www.docsity.com/documents/pages/2017/03/04/a b926e9a485cf5f9cdcfe59e11eb174f.png taken on 16.5.18 at 9:00 pm
- 2. Fig2-http://www.chem.ucla.edu/~bacher/UVvis/electronic\_energy\_diagram.jpg Taken on 16.5.18 at 10:05 pm
- 3. Fig3http://hplc.chem.shu.edu/NEW/Undergrad/Molec\_Spectr/Lambert.html
- 4. Fig4-http://lab-training.com/2014/10/04/beer-lambert-spectroscopicabsorbance- principle/
- 5. Fig5-https://www.biochemden.com/spectrophotometer-instrumentationprinciple/ Taken on 17.5.18 at 7:00 am
- 6. Fig6-https://upload.wikimedia.org/wikipedia/commons/thumb/7/76/Prismrainbow-black-2.svg/1024px-Prism-rainbow-black-2.svg.png taken on 17.5.18 at 8:00am
- Fig7-http://www.inprentus.com/diffraction-gratings/ taken on 18.5.18 at 3:00 pm
- 8. Fig8- https://www.hitachihightech.com/image/global/products/science/tech/ ana /uv/basic/uv\_course5\_01.gif taken on 18.5.18 at 3:15 pm

## **<u>Reference</u>**s

9.Fig9-https://www.slideshare.net/kamransaleh92/best-presentation-of-uv taken on 18.5.18 at 3:20 pm

10. Fig10-www.researchgate.net/publication/225303405

11. Fig11-Tyagi et al. Nano scale Research Letters (2016) 11:362DOI

10.1186/s11671-016-1576-5

12. Fig12-J. Phys. Chem. C, 2009, 113 (11), 4277-4285• DOI: 10.1021/jp8082425

• Publication Date (Web): 24 February 2009 Downloaded from http://pubs.acs.org on March 16, 2009