

## DETERMINATION OF THE ENERGY GAP OF SEMICONDUCTORS BY MEANS OF OPTICAL ABSORPTION

During the process of optical absorption a photon may excite an electron from the valence band to the conduction band. As intraband transitions are not possible in undoped materials, this kind of processes marks the onset of the optical absorption processes in these materials (i.e. they are transparent for photons with energy below the minimum required to promote an electron from the valence to the conduction band). By measuring optical absorption the band structure of the valence and conduction band can be partially revealed.

In this experiment we shall measure the optical absorption spectra of thin slices of Ge and Si in order to find out the energy gap of these two materials using an optical absorption spectrophotometer. The basic rationale behind this apparatus is the following: A light source (a filament lamp for the infrared-visible region and a deuterium lamp for the UV range), a system of mirrors to conduct the light, a monochromator to select the desired wavelength and finally a detector (a phototube in the VIS-UV range and a PbS photodiode in the IR).

When a beam of light  $\alpha$  penetrates into a material the absorption coefficient  $\alpha(h\nu)$  is defined in the following terms:

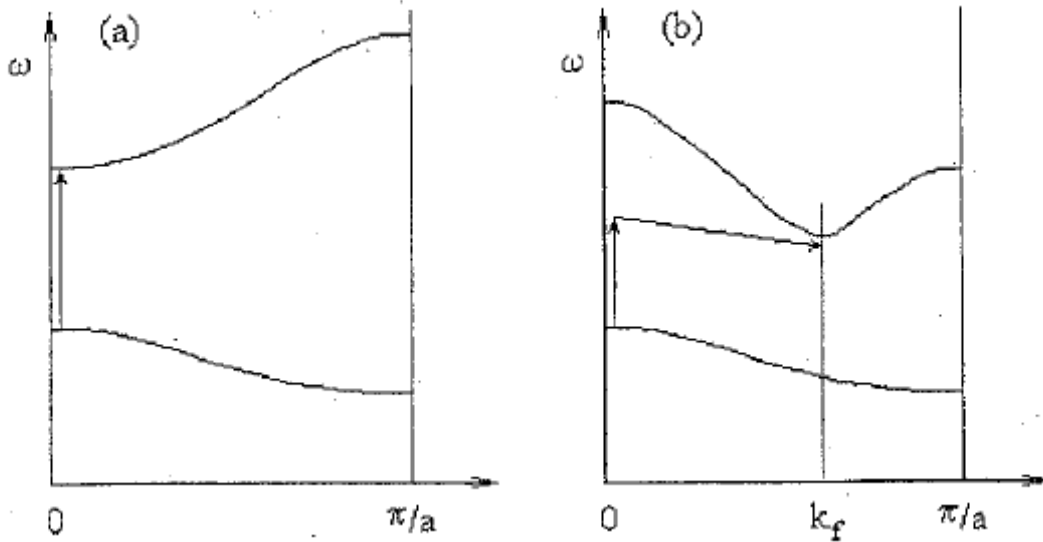
$$\alpha(h\nu) = \frac{1}{I(h\nu)} \frac{d(I(h\nu))}{dx}$$

In our spectrophotometer what is actually measured is the Optical Density (OD) which is defined as follows:

$$OD = -\log \frac{I_t}{I_0}$$

where  $I_t$  corresponds to the intensity of the transmitted light and  $I_0$  of the incident light.

In semiconductors with direct energy gap the maximum of the valence band and the minimum of the conduction band correspond to orbitals with  $k=0$ . Given that the momentum of the photon is very small compared to the dimensions of the Brillouin zone the optical transitions are essentially “vertical”. They are called direct transitions. On the other hand, there are indirect gap type semiconductors. For these materials the minima of the conduction band occur at different values of  $k$  than the maximum of the valence band. Given that the photon moment is negligible compared with this mismatch of the electronic crystalline moment this kind of transitions are forbidden. Nevertheless they can take place with the assistance of phonons bridging the difference in the value of  $k$  of the initial and final electronic states. In the figure 1 we show the two types of electronic transitions.



Two kinds of indirect gap transitions may take place: with emission of phonons and at temperatures above 0 K, with absorption of phonons. In either case the conservation of energy and crystalline moment must be preserved, the former giving rise to the following equations for absorption and emission assisted processes ( $E_f$  and  $E_i$  stand for the energy of the final and initial state whereas  $E_p$  corresponds to the energy of the emitted or absorbed phonon):

$$h\nu_e = E_f - E_i + E_p \quad (\text{phonon emitted})$$

$$h\nu_a = E_f - E_i - E_p \quad (\text{phonon absorbed})$$

This kind of processes are formally represented in figure 1(b).

Statistical and quantum mechanics give rise to the following theoretical expressions for the absorption coefficient  $\alpha(h\nu)$ . The calculation takes into account the densities of initial and final states.

The absorption coefficient for a transition mediated by the absorption of a phonon is given by:

$$\alpha_a(h\nu) = \frac{A(h\nu - E_g + E_p)^2}{\exp\frac{E_p}{k_B T} - 1}$$

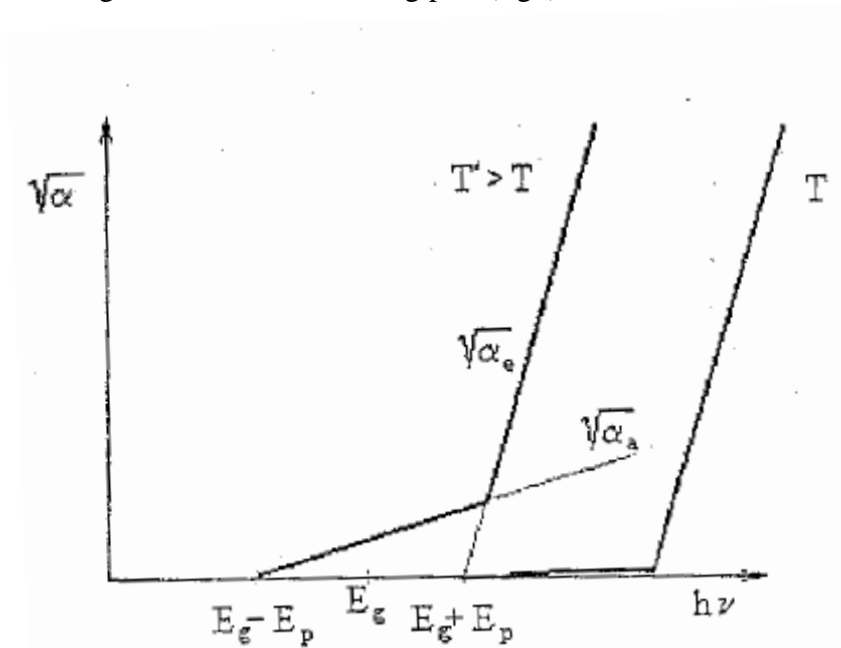
where  $E_g$  is the energy gap and the energy of the photon is such that  $h\nu > E_g - E_p$ .

Correspondingly the absorption coefficient with emission of a phonon is given by:

$$\alpha_e(h\nu) = \frac{A(h\nu - E_g - E_p)^2}{1 - \exp\left(\frac{-E_p}{k_B T}\right)}$$

for photons with  $h\nu > E_g + E_p$ .

If we represent the square root of the absorption coefficient versus the photon energy it should give rise to the following plot (fig2)



At low temperatures the density of phonons is very low and processes with phonon absorption are almost absent. At higher temperatures they start to contribute. Extrapolation to  $\alpha=0$  allows to estimate the values of  $E_g - E_p$  and  $E_g + E_p$  and from that both the energy gap and the phonon energy. The lower the temperature the better this approximation.

Both Ge and Si are indirect gap semiconductors and the fundamental absorption is phonon assisted. In this practice we shall measure the optical absorption of Si between 1300 and 950 nm and that of Ge between 2000 and 1500 nm in order to obtain through the theory outlined above the energy gap of these materials and the energy of the phonon that mediates the transitions.

#### OPTICAL ABSORPTION BY A RARE EARTH COMPOUND

The low lying energy levels of the rare earth atoms are essentially due to the different states of the inner 4f electrons and they only weakly affected by the electrical field produced by other ions in the crystal lattice ("crystal field"). Therefore the absorption spectrum is characteristic of each rare earth.

We have two compounds (both transparent with a slight pink and green colour) of rare earths and we try to identify what is this rare earth in each compound. The experiment consist of measuring the absorption spectrum of both compounds and identifying the

observed peaks of each with the transitions from the ground state to other atomic states, according to the well known quantum rule:

$$\hbar\omega = E_f - E_0,$$

where  $\omega$  is the angular frequency of the photon,  $E_0$  the ground state energy and  $E_f$  the final atomic energy after absorbing a photon. A chart of the energy levels for all rare earths is supplied to identify the transitions with the observed absorption peaks. Please realise that not all transitions are allowed due to the selection rules for photon absorption.

For this experiment the recommended range of wavelength is from 2000 nm to 325 nm.

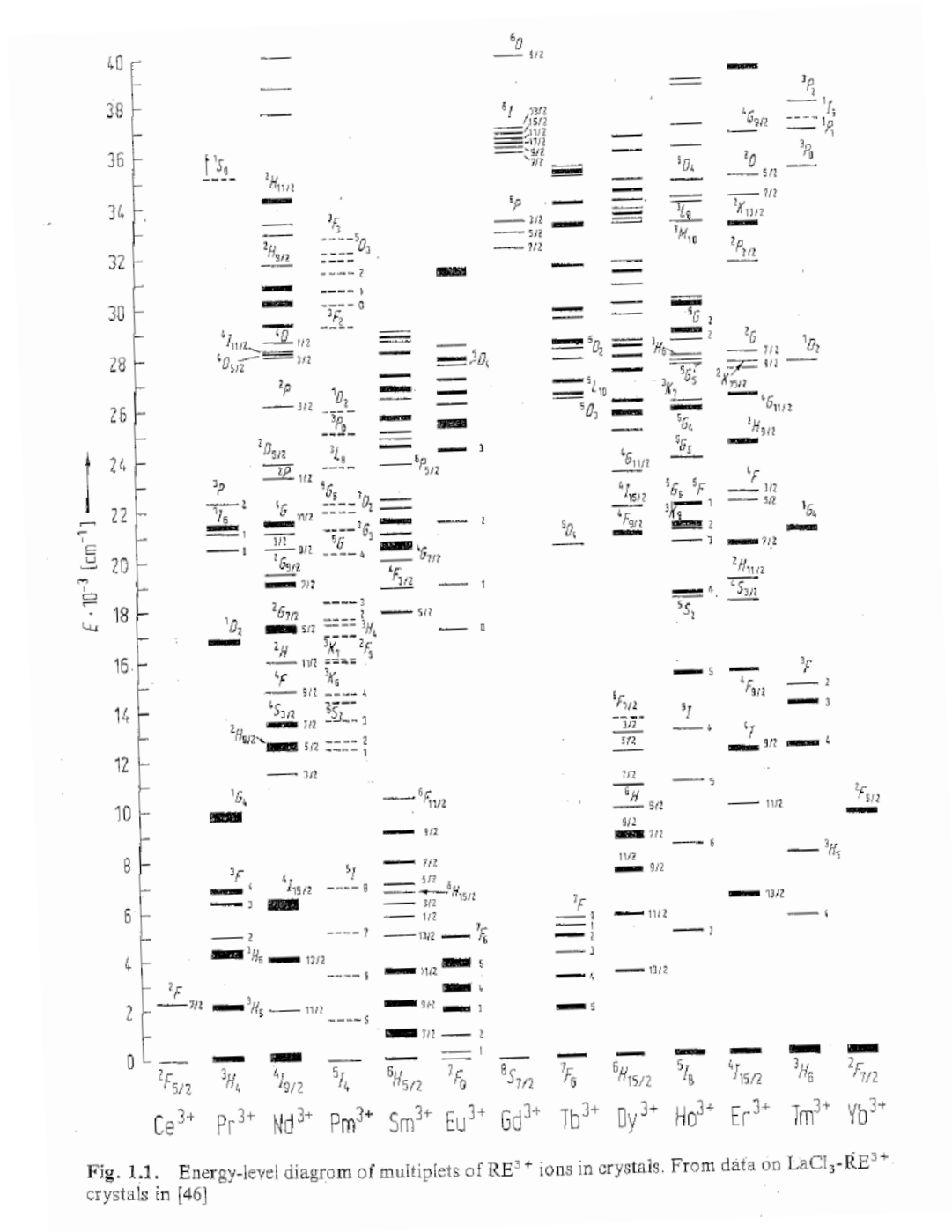
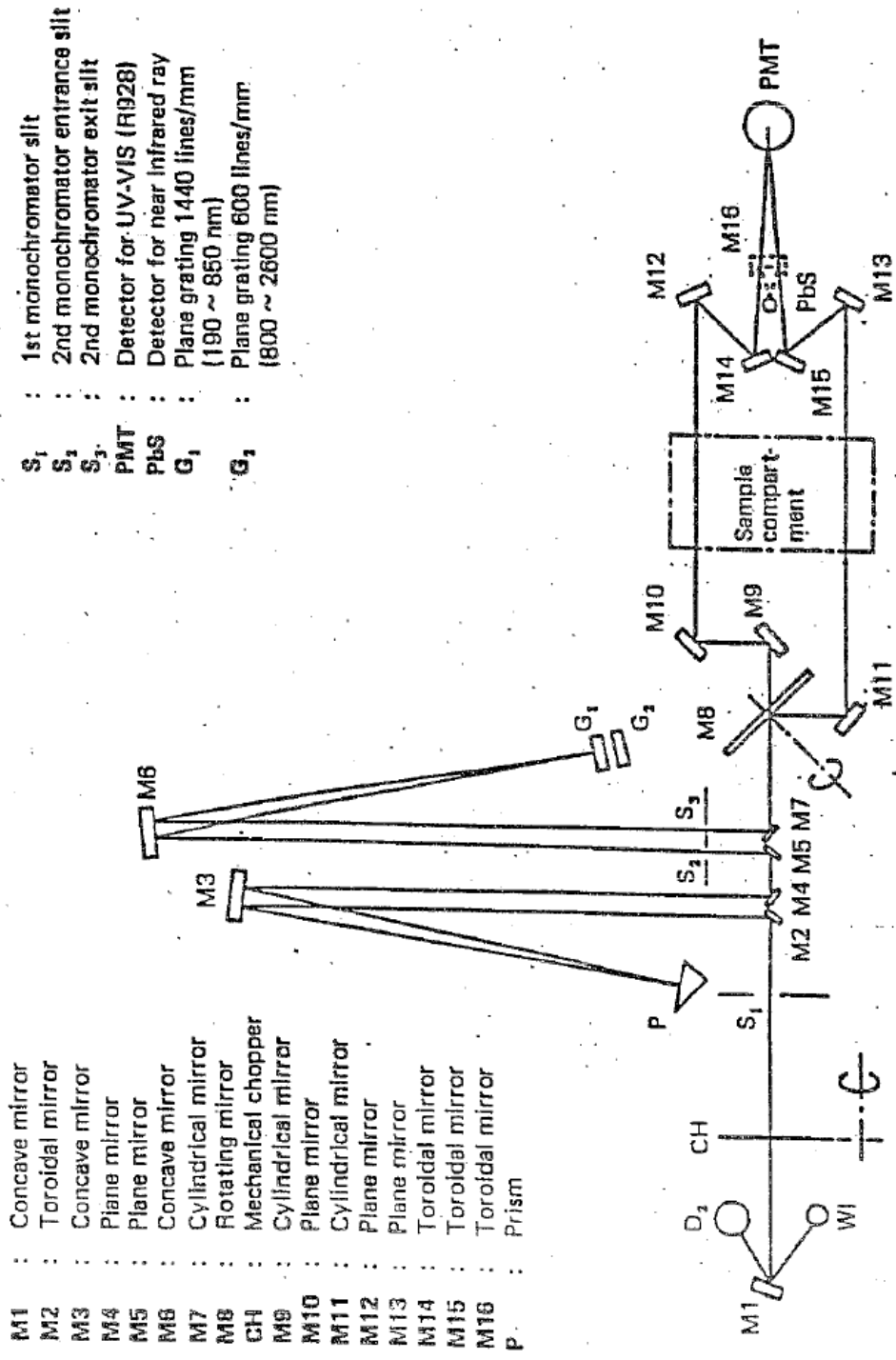


Fig. 1.1. Energy-level diagram of multiplets of RE<sup>3+</sup> ions in crystals. From data on LaCl<sub>3</sub>-RE<sup>3+</sup> crystals in [46]



- M1 : Concave mirror
- M2 : Toroidal mirror
- M3 : Concave mirror
- M4 : Plane mirror
- M5 : Concave mirror
- M6 : Cylindrical mirror
- M7 : Rotating mirror
- M8 : Mechanical chopper
- M9 : Cylindrical mirror
- M10 : Plane mirror
- M11 : Cylindrical mirror
- M12 : Plane mirror
- M13 : Plane mirror
- M14 : Toroidal mirror
- M15 : Toroidal mirror
- M16 : Toroidal mirror
- P : Prism

- S<sub>1</sub> : 1st monochromator slit
- S<sub>2</sub> : 2nd monochromator entrance slit
- S<sub>3</sub> : 2nd monochromator exit slit
- PMT : Detector for UV-VIS (R928)
- PbS : Detector for near infrared ray
- G<sub>1</sub> : Plane grating 1440 lines/mm (190 ~ 850 nm)
- G<sub>2</sub> : Plane grating 600 lines/mm (800 ~ 2600 nm)

Fig. 2-2 Optical Layout of Model U-3400

