Infra-Red (IR)
&
Fourier Transform Infra-Red (FT-IR) Spectroscopy
Session 4

IR Spectrometer: IR Spectrophotometer

- Dispersive IR:

✓ traditional

✓ double beam: reference & sample

- Fourier Transform IR: FT-IR:

✓ modern

✓ mono beam

✓ FT operation on interferogram: if on sum of accumulated intereferogram:

✓ better signal to noise ratio

✓ greater speed

✓ greater sensitivity

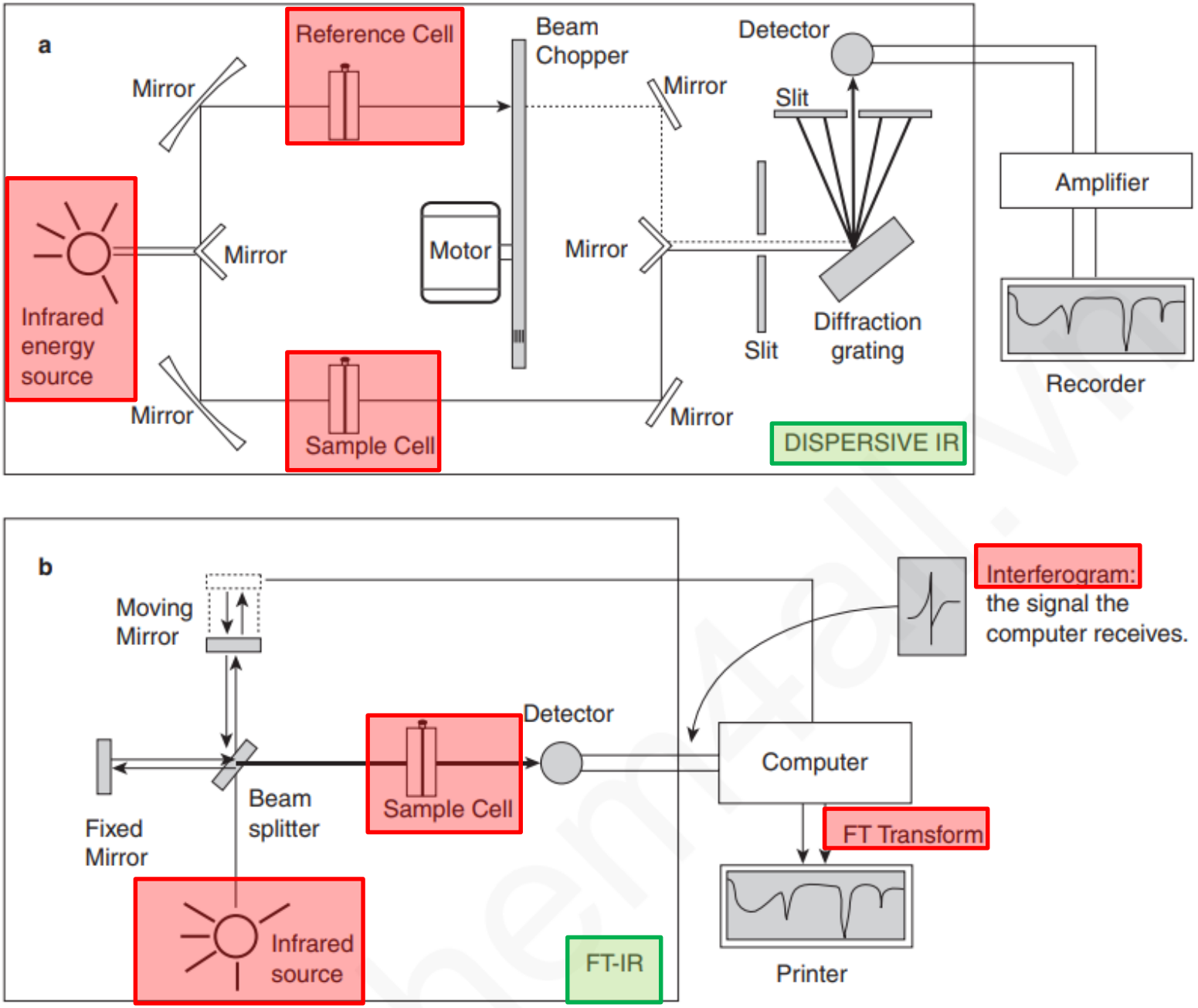
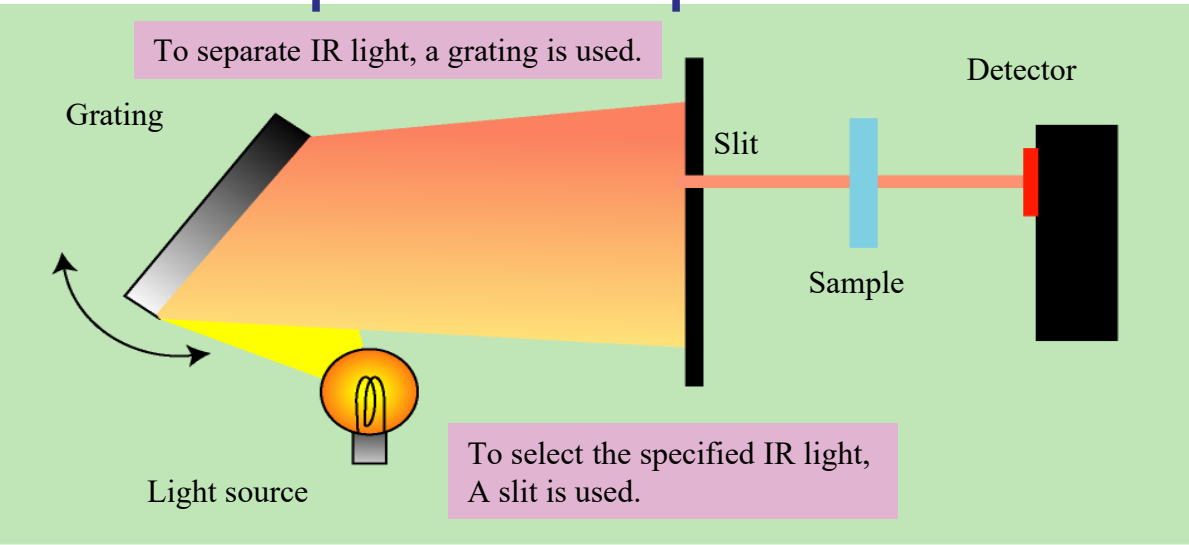


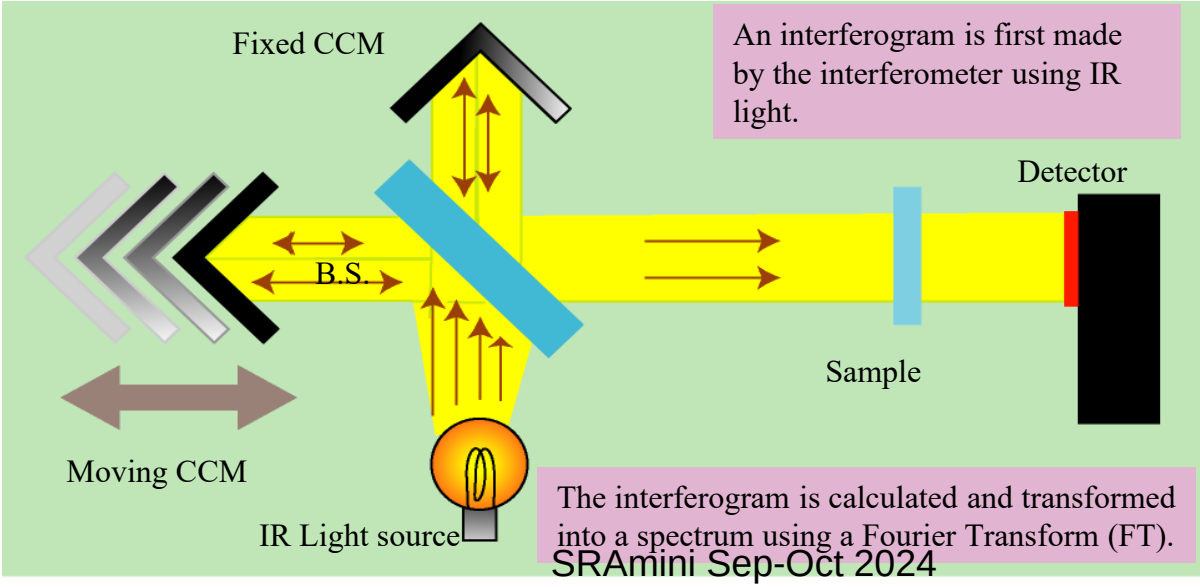
FIGURE 2.3 Schematic diagrams of (a) dispersive and (b) Fourier transform infrared spectrophotometers.

Comparison Between Dispersion Spectrometer & FTIR



Dispersion Spectrometer

In order to measure an IR spectrum, the dispersion Spectrometer takes several minutes.
Also the detector receives only a few % of the energy of original light source.



FTIR

In order to measure an IR spectrum, FTIR takes only a few seconds.
Moreover, the detector receives up to 50% of the energy of original light source.
(much larger than the dispersion spectrometer.)

FTIR

- Interferometer: device to process the energy sent to sample
- Beam splitter: energy passes through:

✓ separate incoming radiation to two perpendicular beams:

✓ one deflected: which goes to a moving mirror: & returns to beam splitter

✓ one in 90 angle to the first one: which goes to stationary or fixed mirror & returns to beam splitter

✓ two meeting beams cause constructive or destructive interference

✓ motion of mirror causes path length that 2nd beam traverse to vary.

- Interferogram: combined beams containing these interference patterns:

✓ contains all of the radiative energy coming from the source

✓ so has wide range of wavelength

✓ is oriented toward sample by the beam splitter

Sample Preparation in IR Spectroscopy

- Solids: mixed with KBr to prepare sample discs in:

✓ NaCl, KCl, KBr & CsI discs

✓ IR card

✓ Nujol mulls

✓ KBr pellets

- Oil / solutions in optimum solvents (CS_2, CCl_4)

✓ NaCl & KBr discs

✓ ATR: Attenuated Total Reflection (Reflectance)

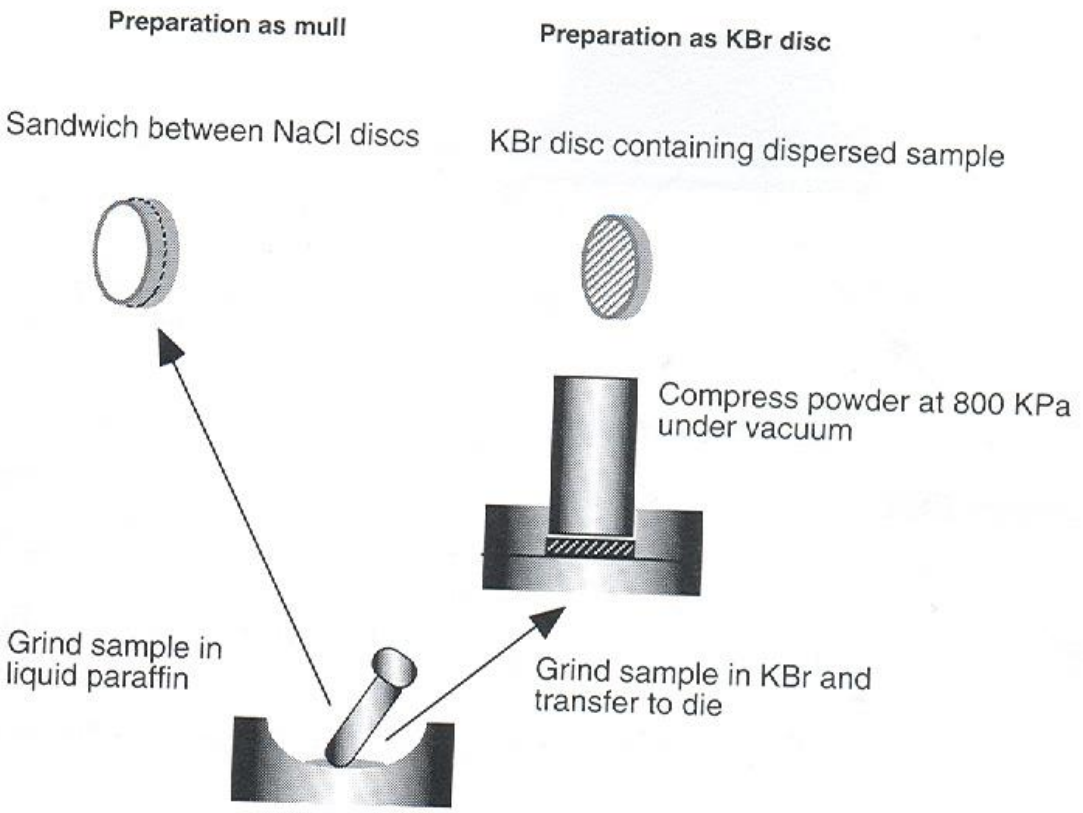
- Instrument subtracts IR spectrum of:

✓ solvent & IR active atmospheric gases (CO_2; H_2O) as background

✓ IR inactive gases of atmosphere: N_2; O_2

Preparation of Sample for IR Spectroscopy

Fig. 5.6
Preparation of samples as discs and mulls.



Attenuated Total Reflectance (ATR)

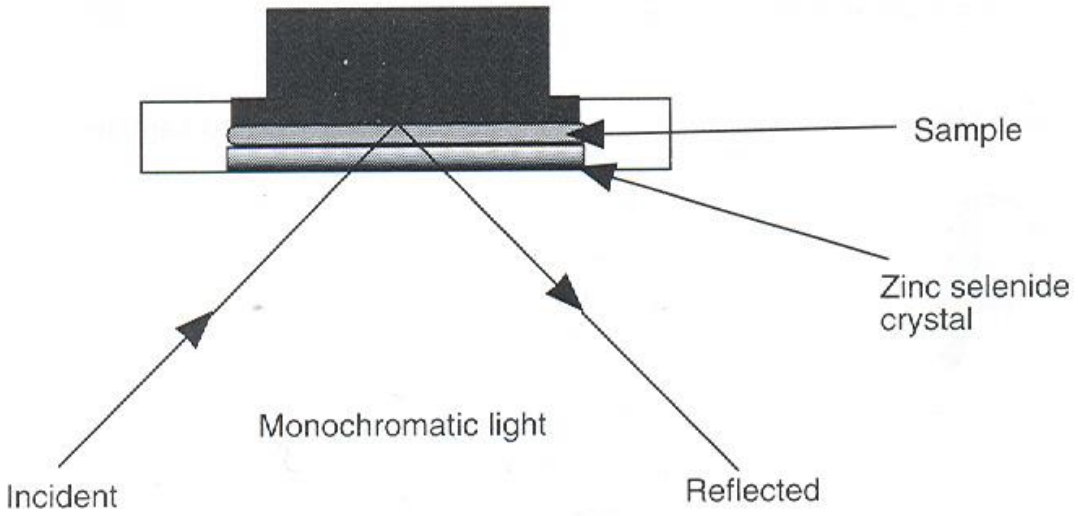


Fig. 5.8
Attachment for analysis of a sample by ATR.

Pathway of IR Radiation through Sample Cell in IR Spectroscopy

- Double beam: in dispersive IR (traditional IR)

✓ one beam is transmitted from sample

✓ second beam is transmitted from reference

- Mono beam: in FTIR:

✓ spectrum is resulted from FT on the interferogram

Output Files in IR Spectroscopy

- Interferogram:

✓ complex signal

✓ wave-like pattern

✓ intensity versus time: time-domain spectrum

- Spectrum:

✓ resulted by mathematical operation (FT) on interferogram

✓ separate individual absorption frequencies from interferogram

✓ intensity versus frequency: frequency-domain spectrum