SWORFISH project

Estimation of mechanical stresses with mid infrared spectroscopy

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COST Action FP0904

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outline

- Goal
- Experiment
- Preliminary results
- Why does it work?
- Conclusions

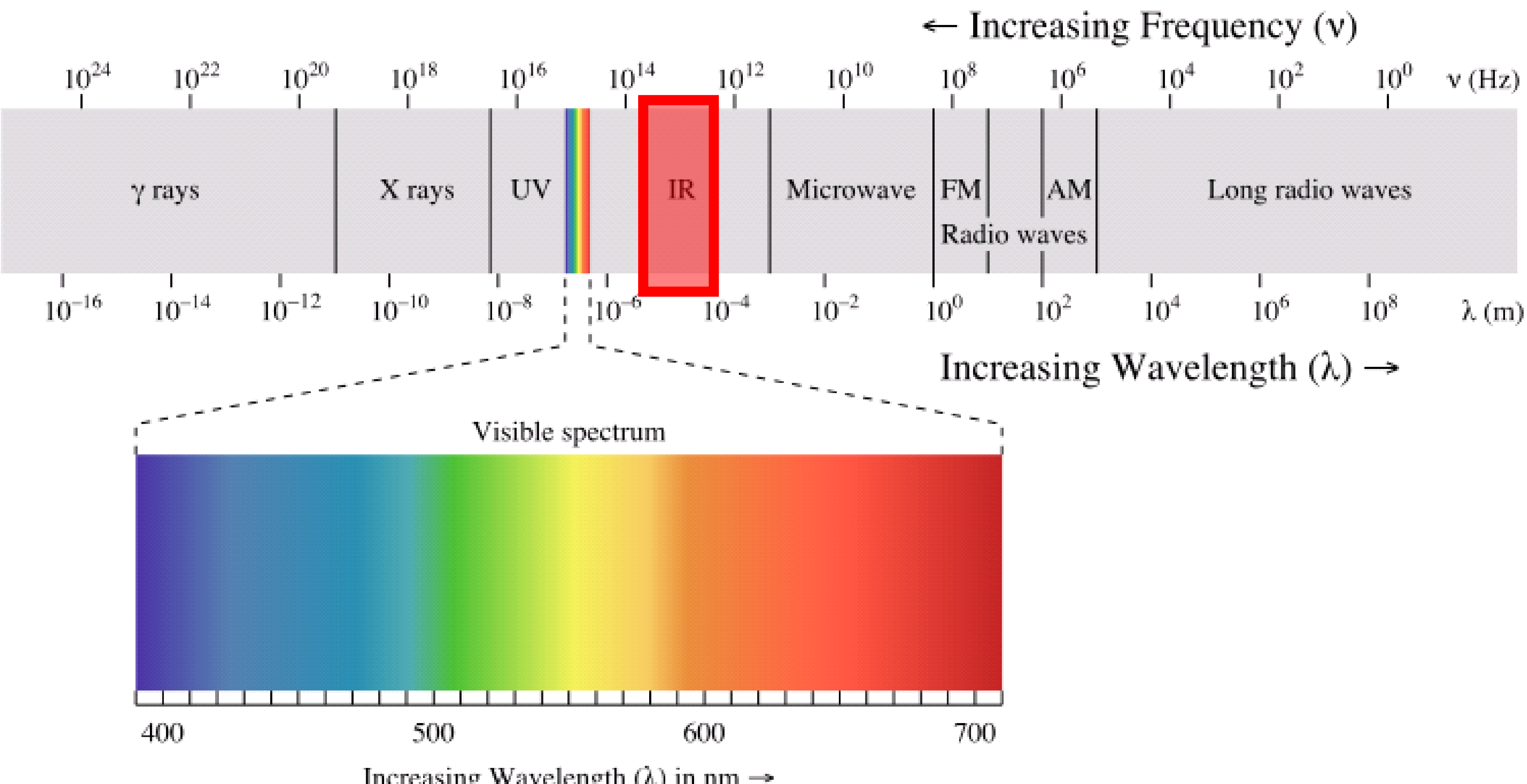
19 slides to the end

Goal

Can any modifications of the material (wood) due to mechanical stresses be noticeable in the infrared spectra?

Electromagnetic spectrum

λ= 3 to 30μm or 4000 to 4000cm^{-1}



http://en.wikipedia.org/wiki/Image:EM_spectrum.svg

MID INFRARED SPECTROSCOPY

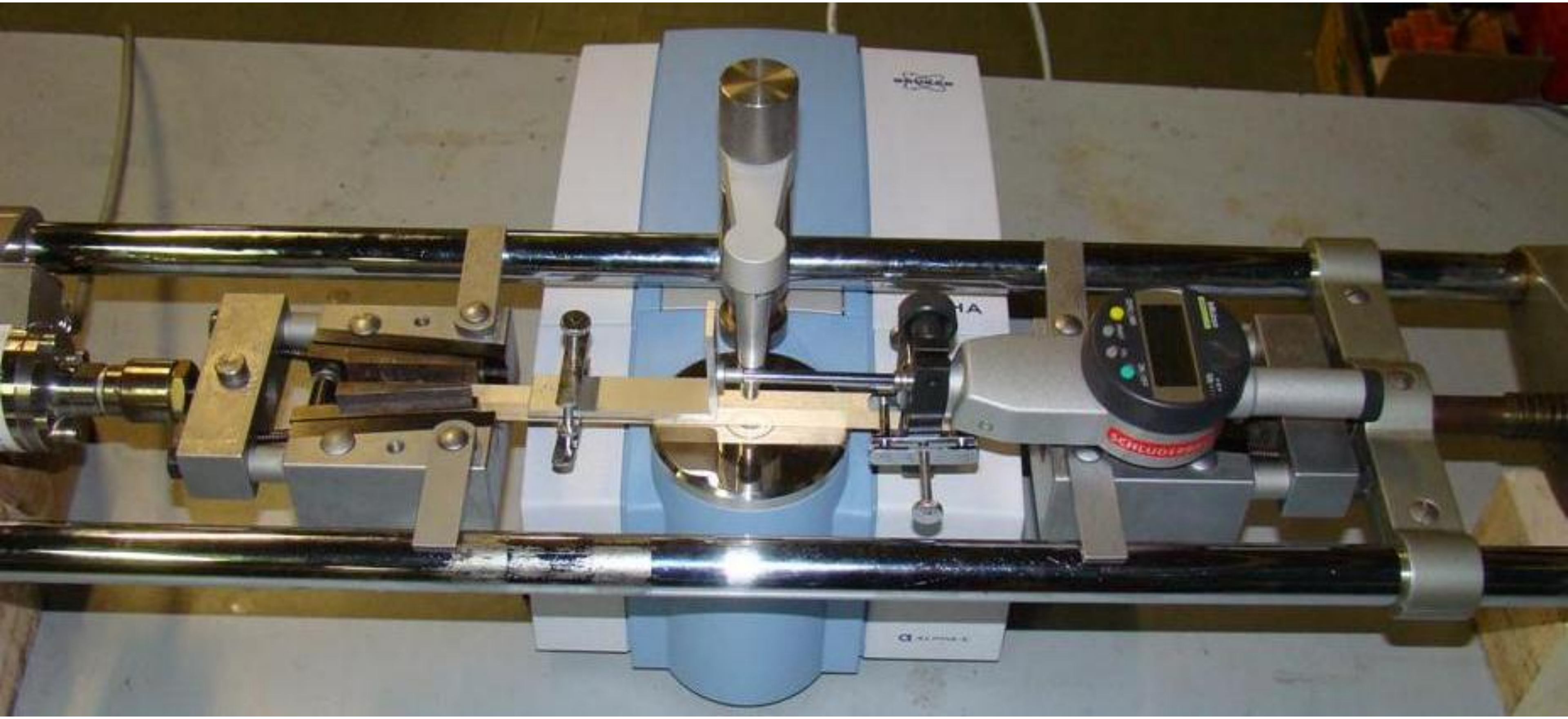
- FT-ATR-MIR (Fourier transform attenuated total reflectance mid infrared) spectrometer Alpha produced by Bruker Optics GmbH
- ZnCr cristal
- spectral range: 4000 cm^{-1} to 600 cm^{-1}
- spectral resolution: 4 cm^{-1}
- each spectrum has been computed as an average of 50 successive measurements
- the sample was pressed to the crystal surface with a constant pressure during the spectra acquisition (whole test)

Materials

- Larch (Larix sp.) wooden blocks
- without defects
- 10 mm x 10 mm x 340 mm (width x thickness x length)
- moisture content: ~9%
- density: 450 kg/m^3
- surfaces refreshed before testing assuring a clean and smooth surface

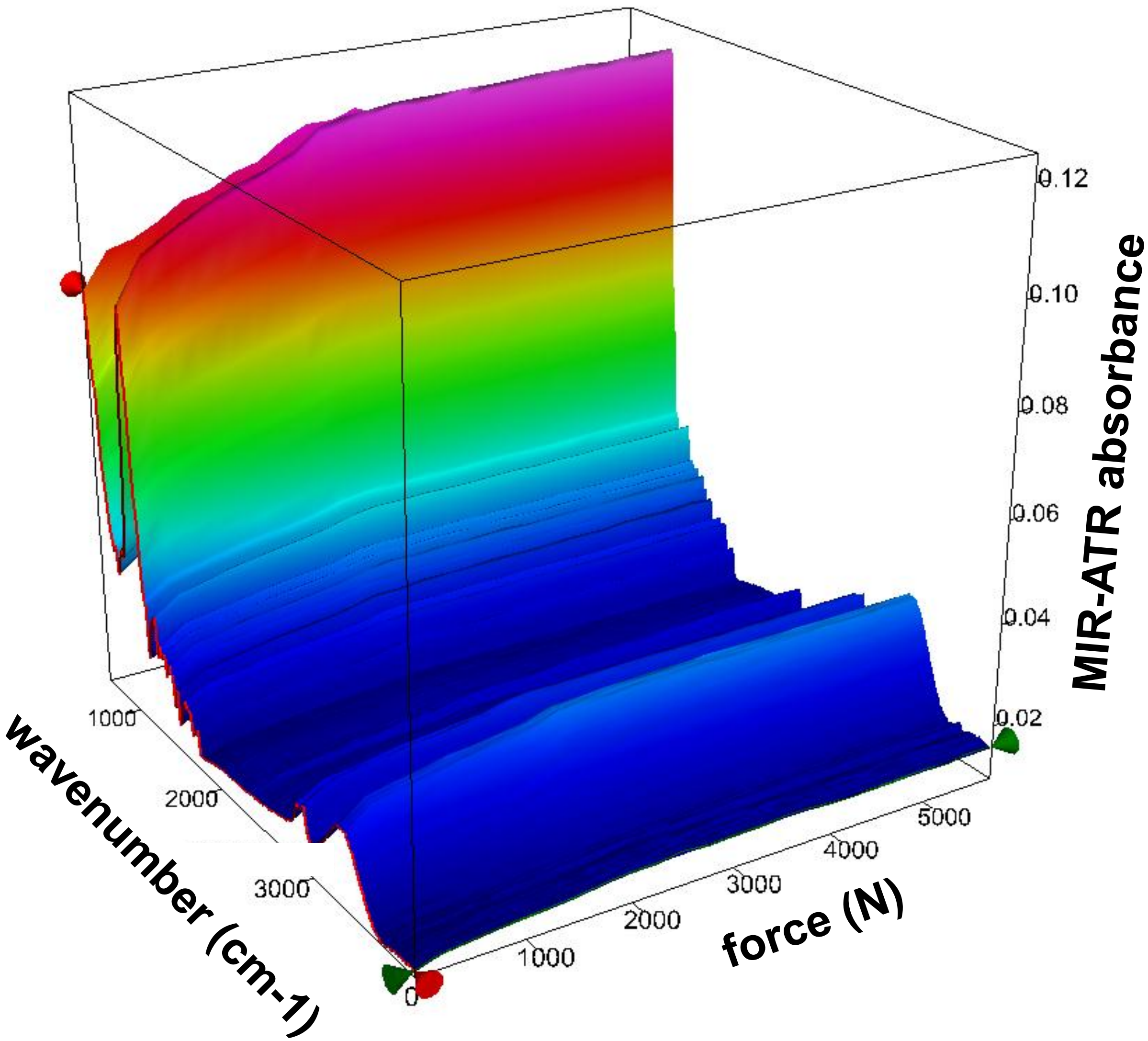
- Measured radial plane
- the workpiece was exposed to varying tension stresses:
    - from 0 N up to 5750 N (the limit of the load cell) with step of 250 N

Experimental set-up

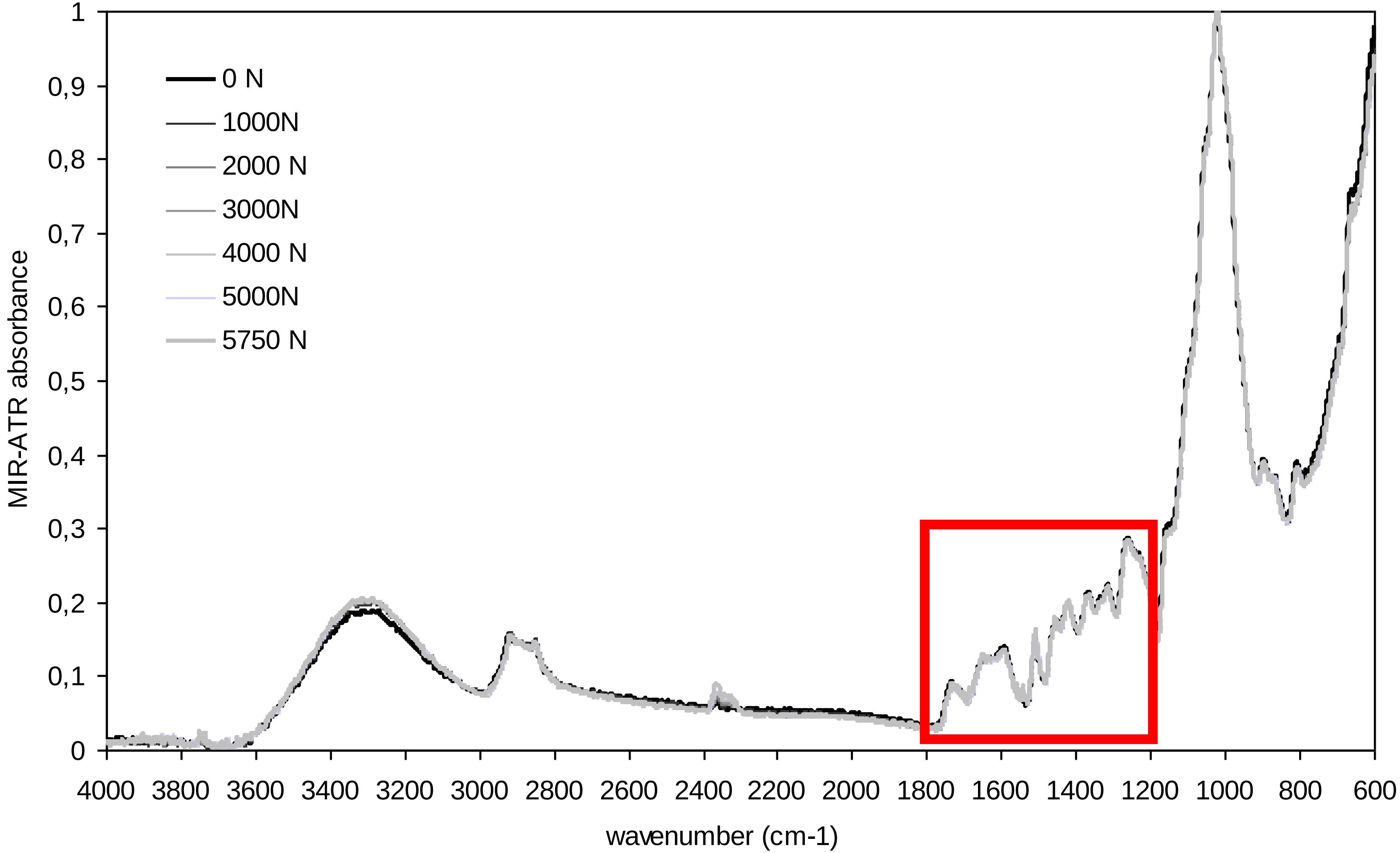


Preliminary results

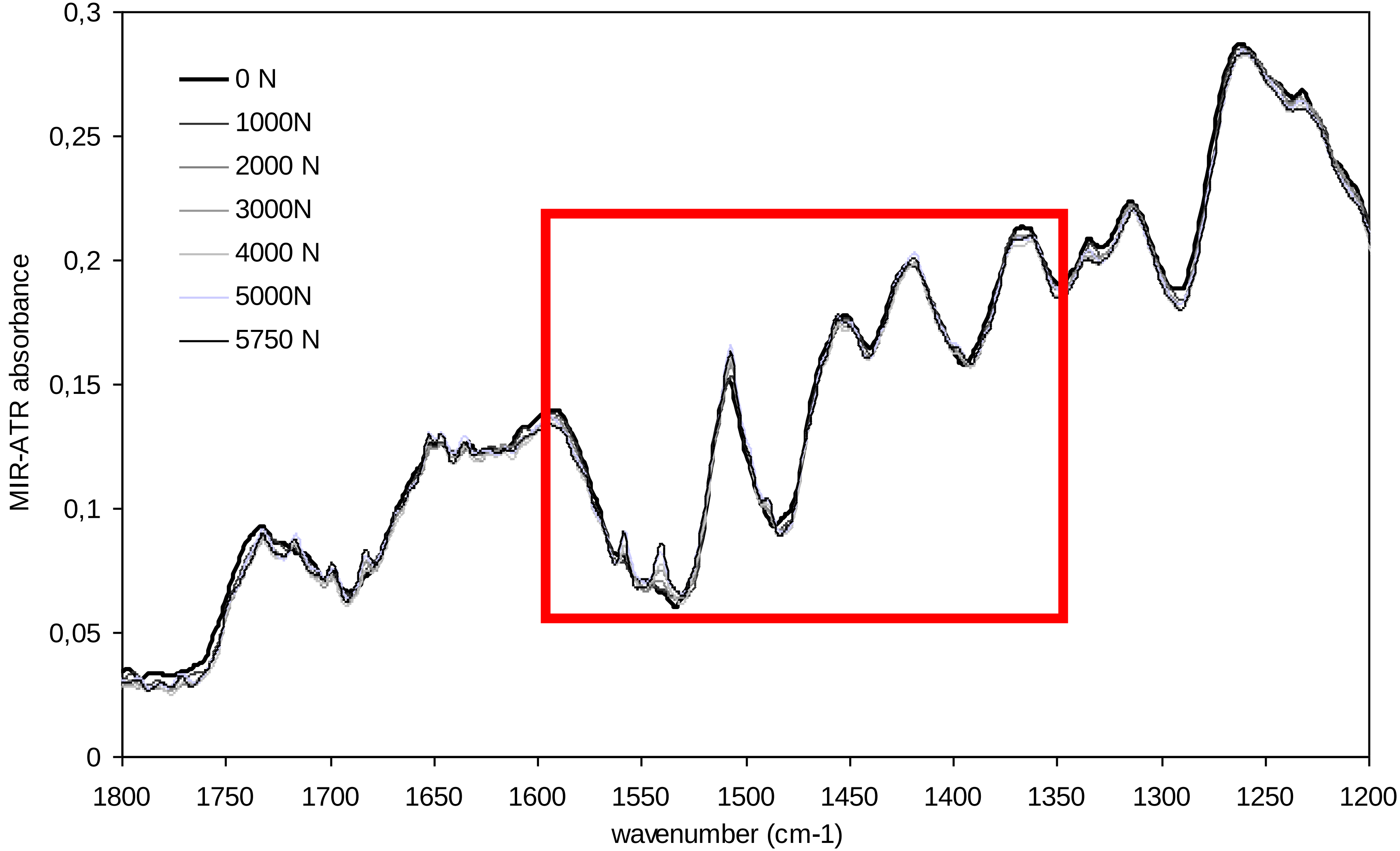
Changes to the MIR-ATR spectra during tension test (raw spectra)



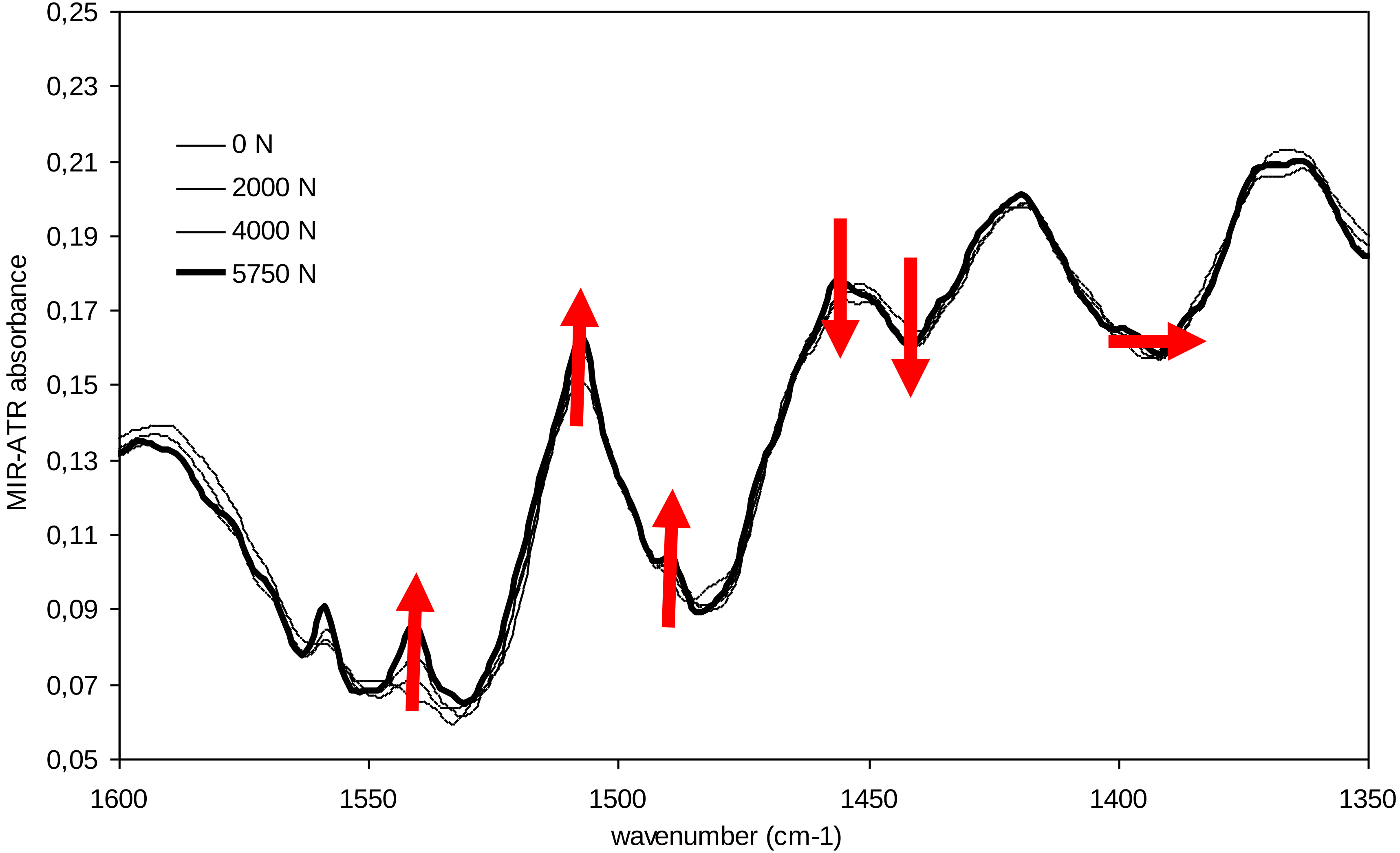
Spectra after normalization in a whole range



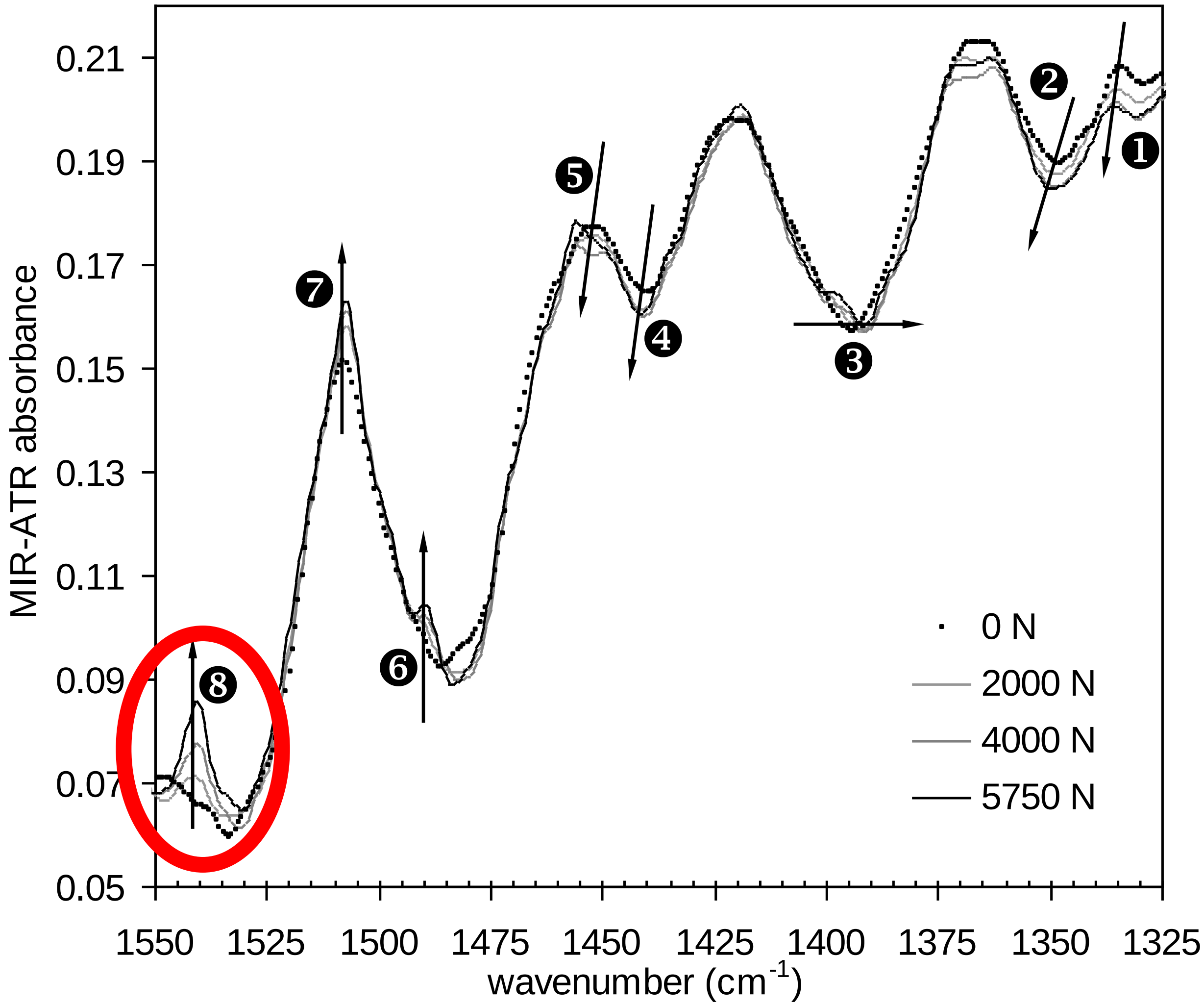
“fingerprint” region



Changes to the spectra due to mechanical stresses



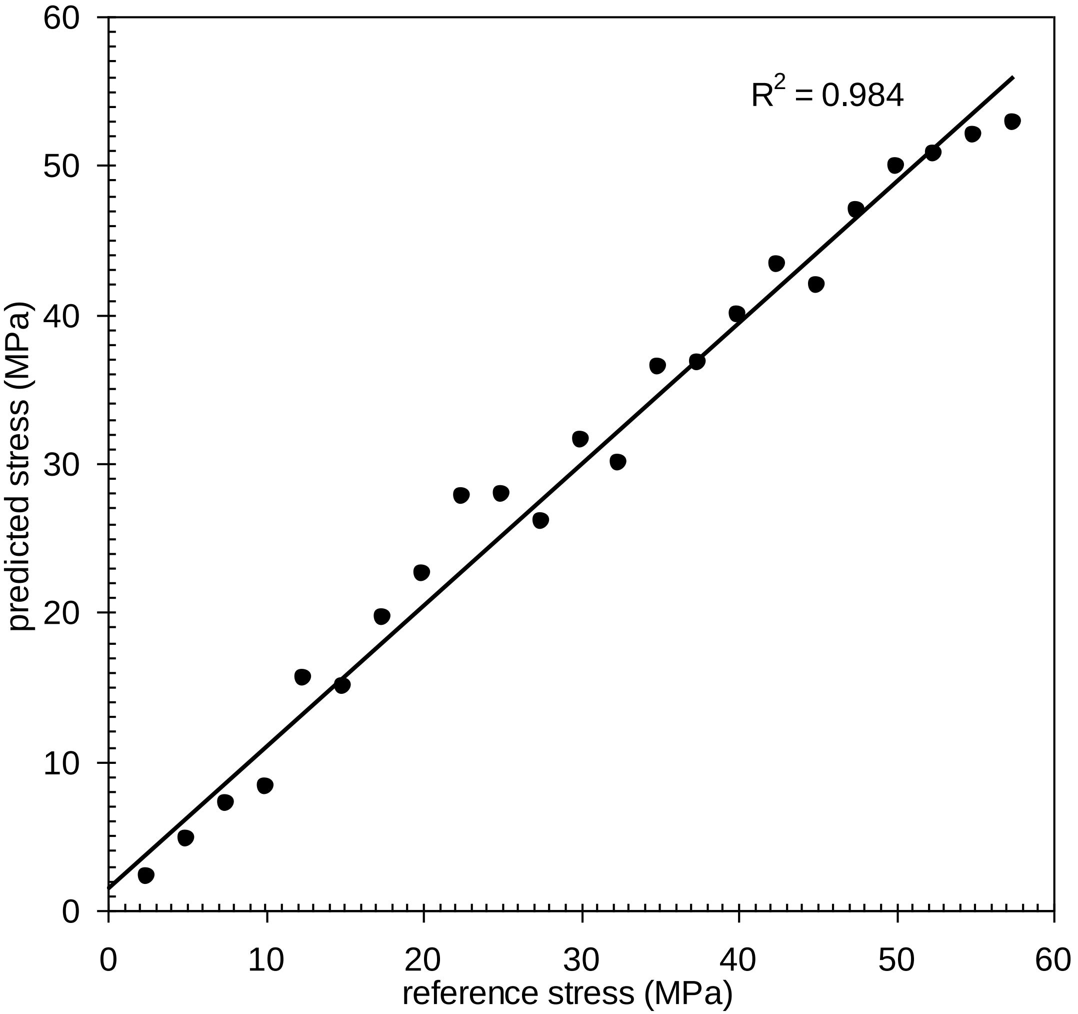
Detailed interpretation…



❶, ❷, ❸ and ❼; aromatic structures of lignin ❹ and ❻; cellulose

❺; CH deformation in both lignin and carbohydrates ❽; probably lignin

PLS (Partial Least Squares) prediction of the tensile stresses by MIR



Straight line subtraction
Range: 1782-1317, 1203-1086 cm^{-1}
Rank 2

Calibration

R^2 = 99.38
RMSEE = 146 N
RPD = 12.7

Validation

r^2 = 98.33
RMSCV = 224 N
RPD = 7.74
Bias = 8.69

How is it possible?

Our hypothesis; do you agree???

Statement 1

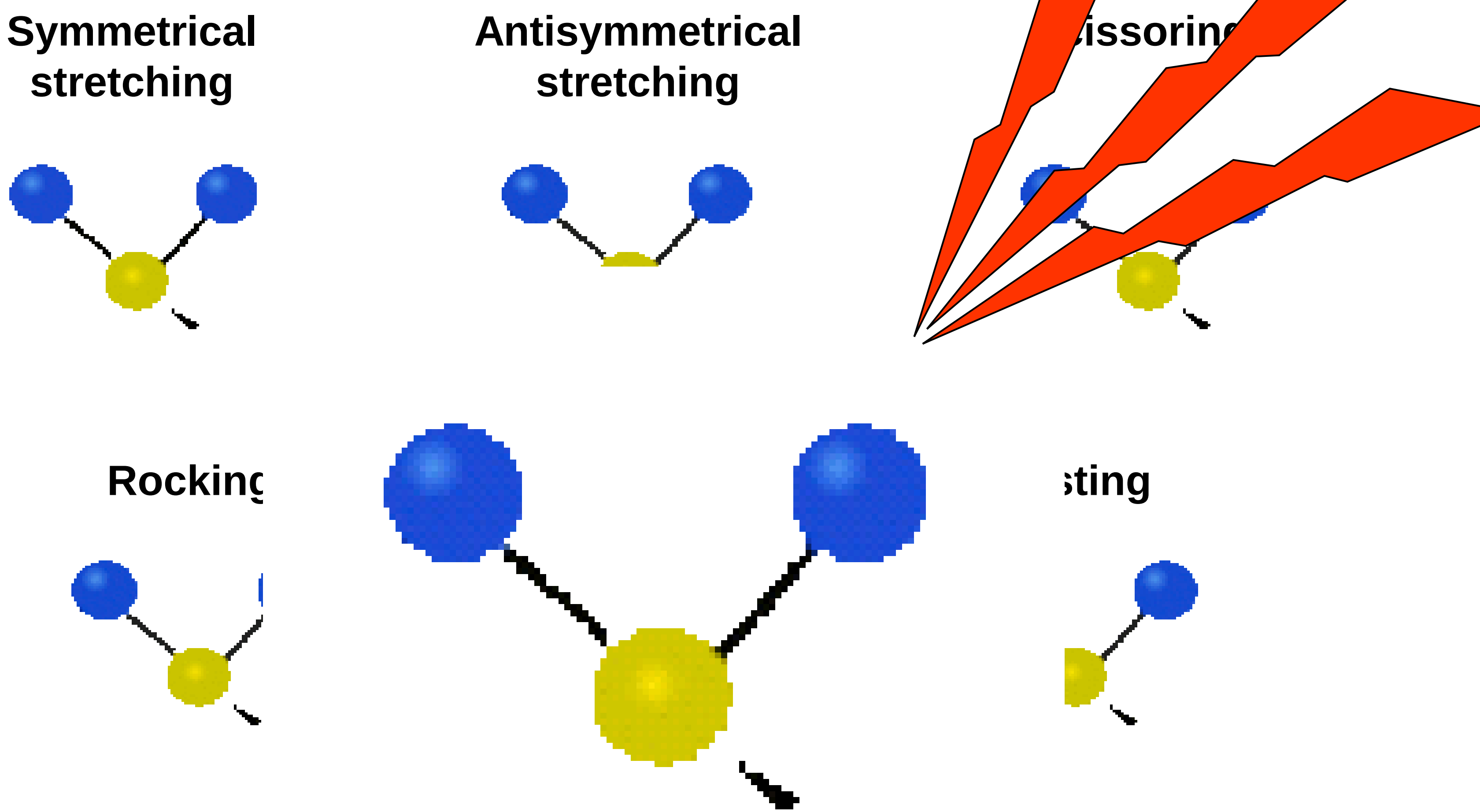
The great advantage of infrared spectroscopy is its ability to determine the chemical composition (of wood). It is sensitive enough to differentiate the sources of molecular vibrations and even to link the spectra with the peculiar functional groups (such as hydroxyl, methyl, etc.).

Statement 2

As mentioned above, the variations of the spectra due to mechanical stresses can be revealed as amplitude or wavenumber shift (or both)…

…but what is a source of spectra?!

Source of spectra

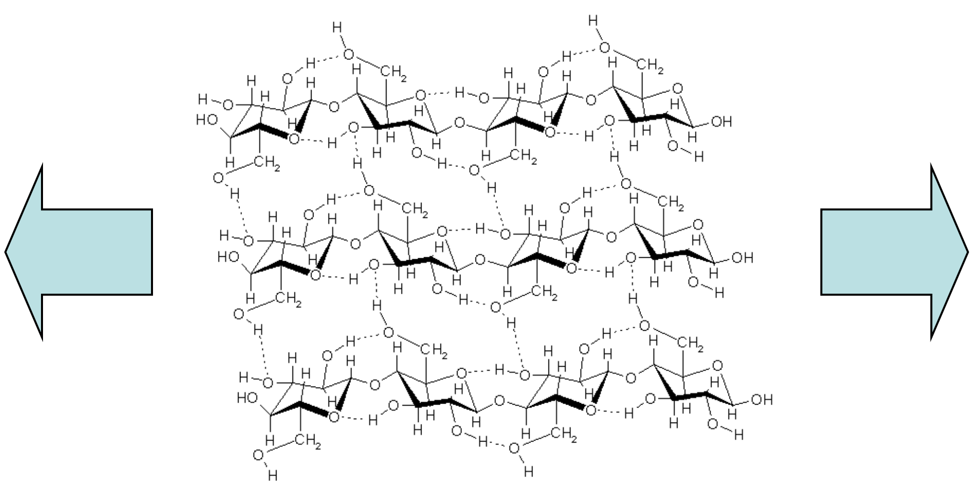


The MIR (and NIR) spectra are characterized by the assignment of the absorption bands to overtones and combinations of fundamental vibrations associated with C-H, O-H, and N-H bonds (having dipole momentum)

http://en.wikipedia.org/wiki/Infrared_spectroscopy

Wood chemistry

- Mechanical properties of timber are highly related to its chemical composition:
  - cellulose: crucial role for resisting tensile stresses (covalent bonding within the pyranose rings and other functional groups)
  - lignin is stiffening wooden structures, especially in compression.
  - hemicelluloses links together both, cellulose and lignin
- due to mechanical stresses (and related deformations) the interaction between constitutive elements of wood changes, proportionally to the stresses applied



CONCLUSIONS

- prediction of the mechanical stress on the basis of the mid-infrared spectra **seems to be possible**
- detailed interpretation of the changes to constitutive components, (and its interrelations) is a **key challenge**
- … the method presented here requires much more work and further improvements - **additional intensive research**

Implementation of infrared techniques in to mechanical testing of wood provides very essential supplement to the typical information collected during standard tests:

It extends the human perception into something we can not see

ACKNOWLEDGEMENT

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