NMR Imaging in porous media

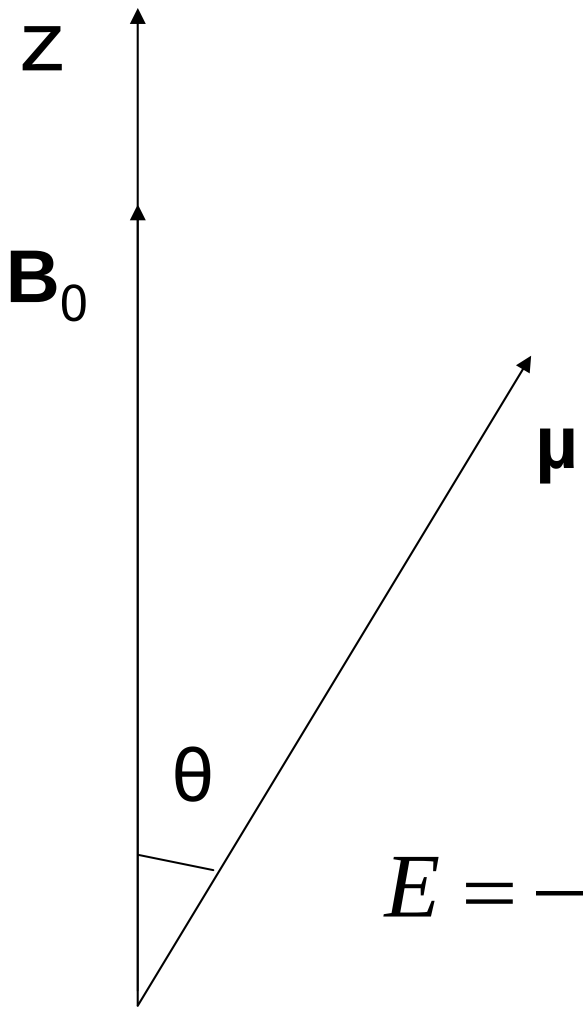
What does NMR give us.

- Chemical structure.
- Molecular structure.
- Interactions between atoms and molecules.
- Incoherent dynamics (fluctuation, rotation, diffusion).
- Coherent flow encoded in a NMR signal.

Basics of NMR.

- Quantum picture: spins and magnetization.
- Classic picture: vector of magnetization.
- Relaxation phenomenon.
- Spin echo.

Magnetic moment of a nucleus.



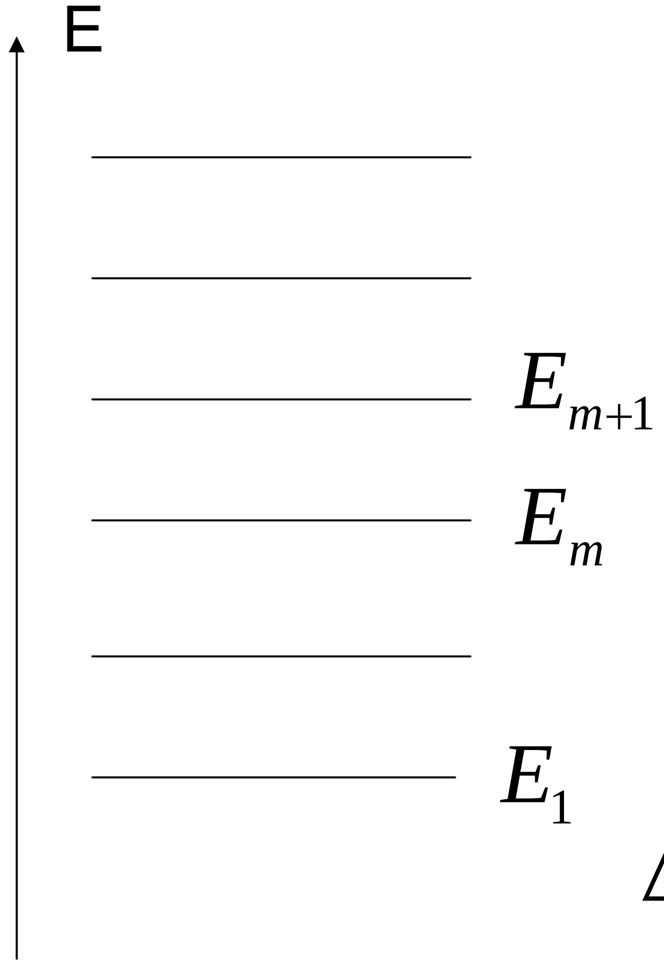
$$p = \hbar \cdot I \quad , \quad \mathrm{I} = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$$

$$\boldsymbol{\mu} = \gamma \cdot \mathbf{p} = \gamma \cdot \hbar \cdot \mathbf{I}$$

P – intrinsic momentum
I – spin
μ - magnetic moment
γ – gyromagnetic ratio

$$E = -(\boldsymbol{\mu}, \mathbf{B_0}) = -\mu \cdot B_0 \cdot \cos\vartheta = -\mu_z B_0$$

Transitions



$$E_m = -\frac{m\mu B_0}{I}$$

μ – maximum projection of **μ**

$$\mathrm{m} = \mathrm{I}, \mathrm{I}\text{-}1, \ldots, \text{-}(\mathrm{I}\text{-}1), \text{-}\mathrm{I}$$

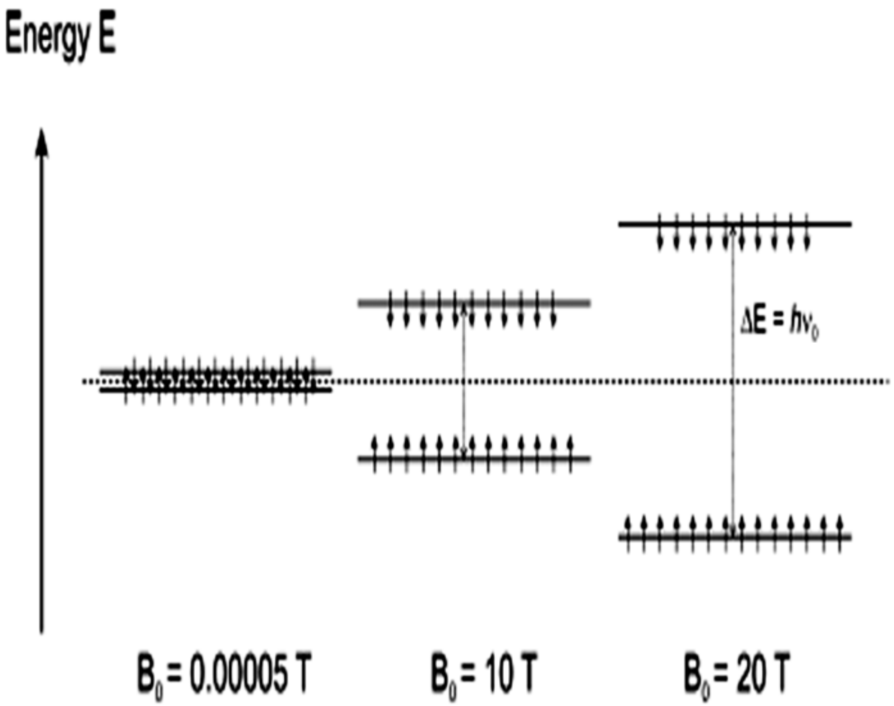
$$\Delta E = |E_m - E_{m+1}| = \frac{\mu B_0}{I}$$

$$\Delta E = \hbar\omega_0 \Rightarrow \omega_0 = \gamma B_0$$

Magnetization and spins.

$I = \frac{1}{2} \Rightarrow 2I + 1 = 2$ **orientations**

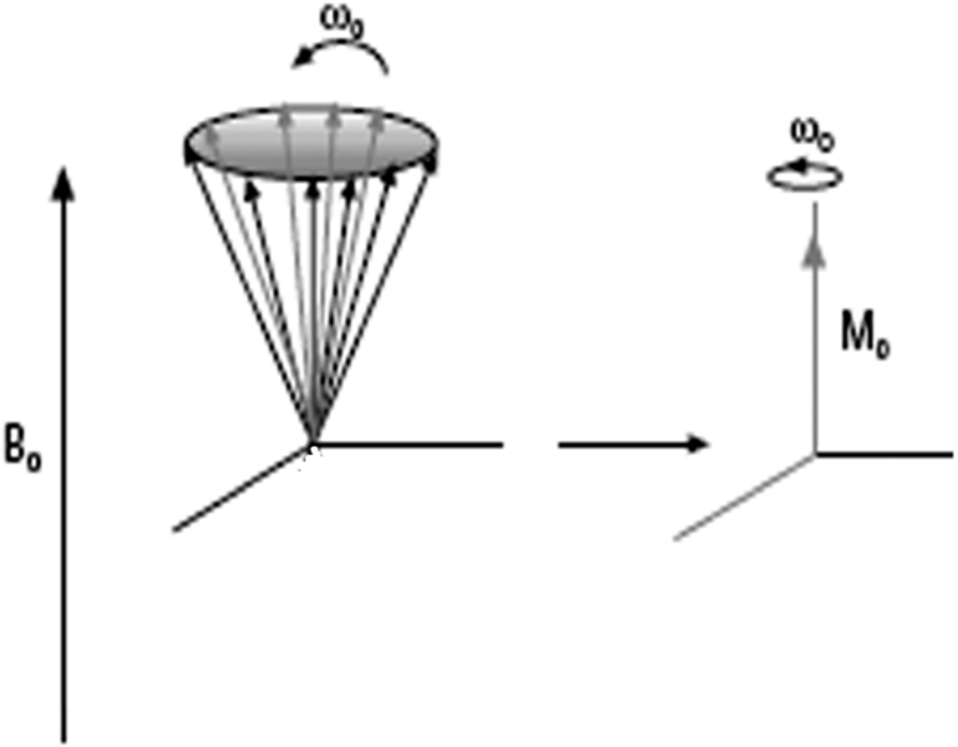
$$\frac{n_{-\frac{1}{2}}}{n_{+\frac{1}{2}}} = exp\left(-\frac{\hbar\omega_0}{k_B T}\right)$$



Because of inhomogeneous population of states, corresponding to different projections of the magnetic moment μ, a substance becomes magnetized.

$$\mathbf{M_0} = N\frac{\gamma^2\hbar^2 I(I+1)}{3k_B T}\mathbf{B_0}$$

Resonance phenomenon (ideal situation).



$$\frac{d\mathbf{M}}{dt} = \gamma\left[\mathbf{M} \times \mathbf{B}\right]$$

$$\boldsymbol{\omega}_0 = -\gamma\mathbf{B}_0$$

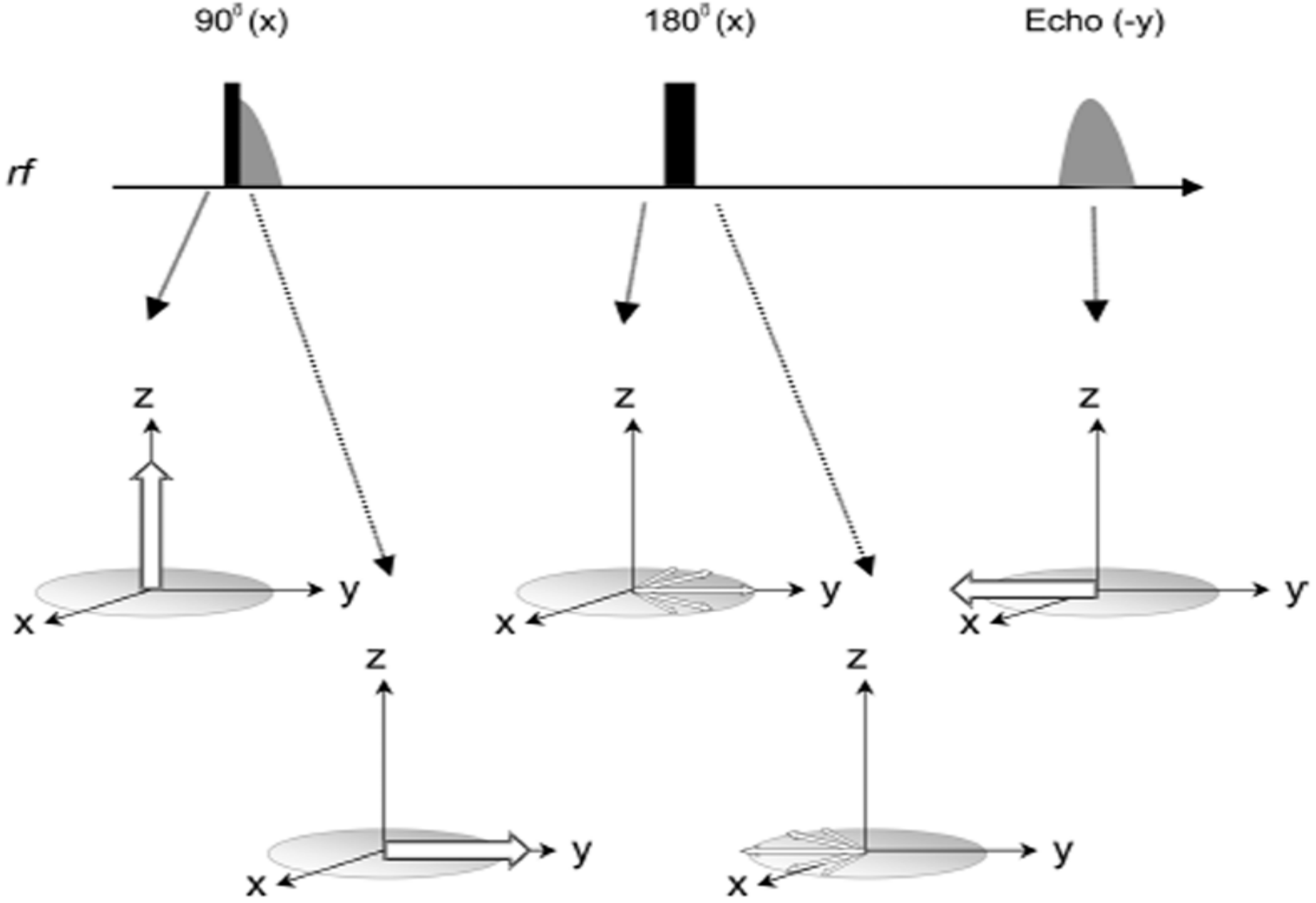
Bloch equation and relaxation times.

$$\frac{dM}{dt} = \gamma[M, B] - e_x \frac{M_x}{T_2} - e_y \frac{M_y}{T_2} - e_z \frac{M_z - M_0}{T_1}$$

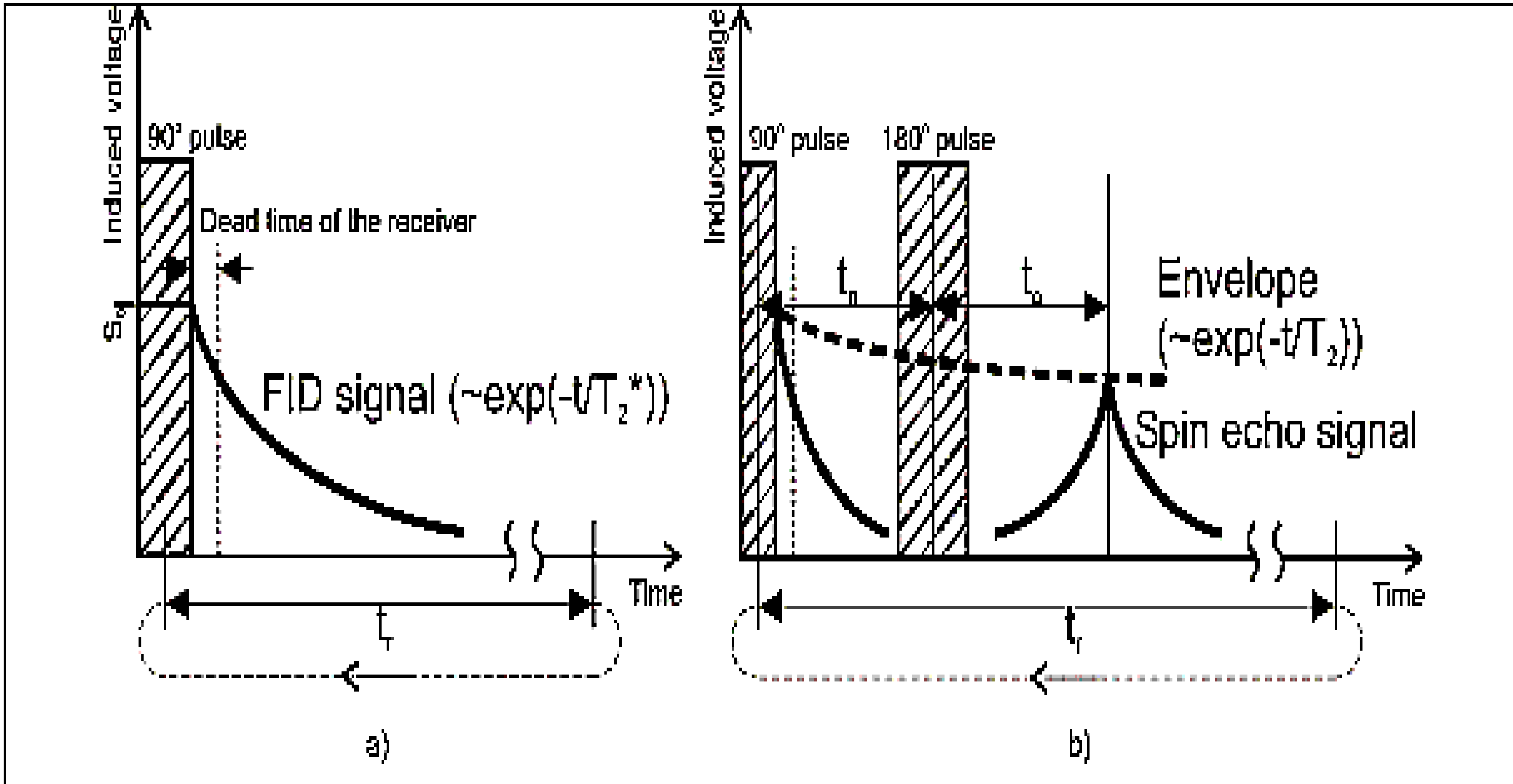
- T_1 – longitudinal relaxation time
- T_2 – transverse relaxation time

Echo formation.

.



Echo formation.

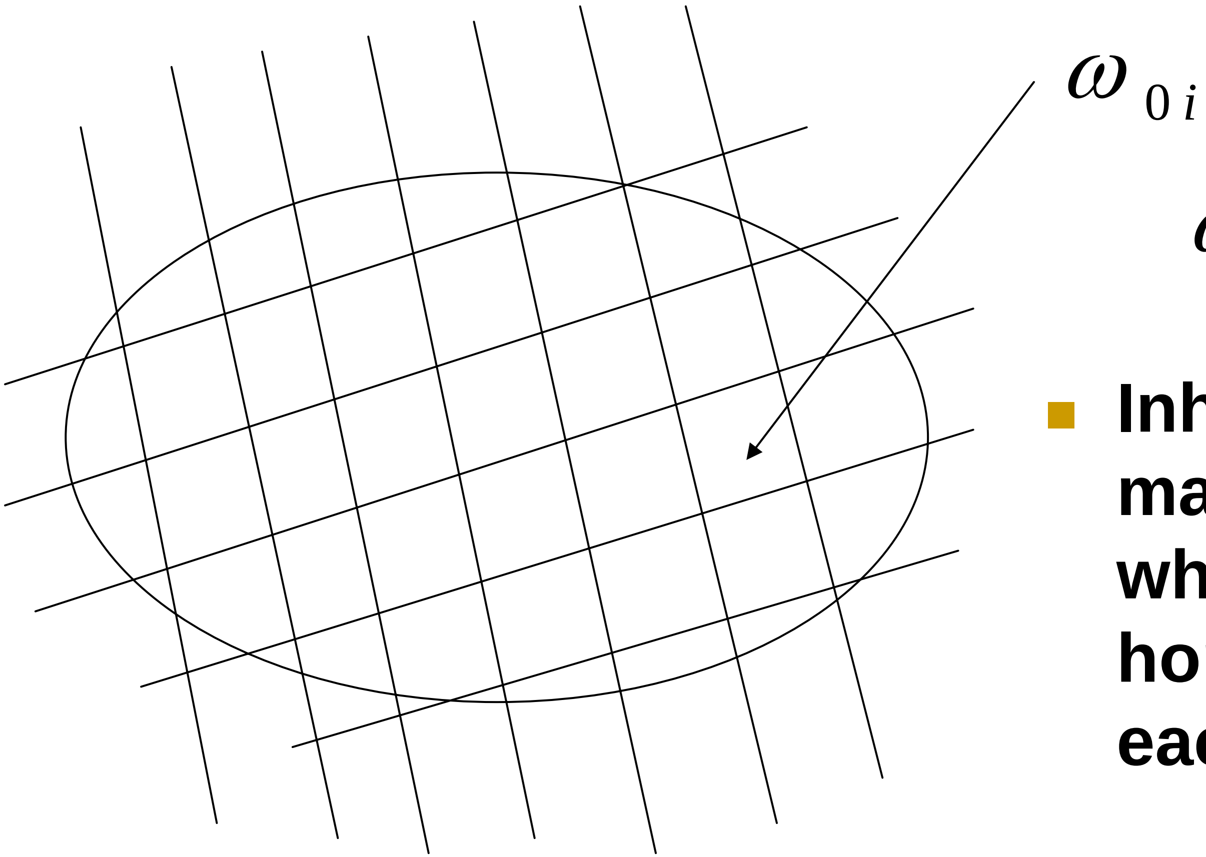


$S = S_0 \cdot [1-\exp(-t_r/T_1)] \cdot \exp(-t/T_2^*)$	$S = S_0 \cdot [1-\exp(-t_r/T_1)] \cdot \exp(-t_e/T_2) \cdot \exp(-t/T_2^*)$

Basics of NMR Imaging

- Phase encoding.
- Frequency encoding
- Slice selection.
- Contrasting.

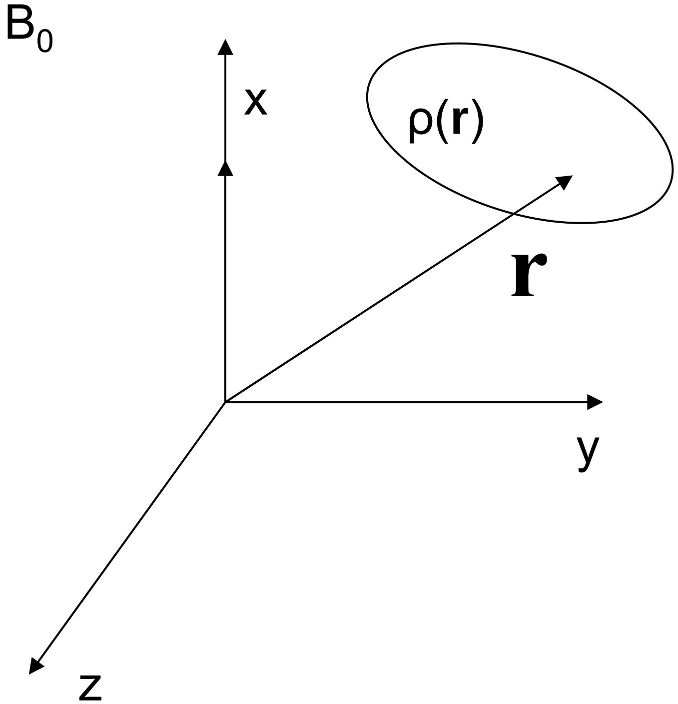
Macroscopic regime.



$$\omega_{0i} = \gamma \cdot B_{0i}$$

- **Inhomogeneous magnetic field for the whole object but homogeneous one for each part**

Fundamentals of NMR Imaging.

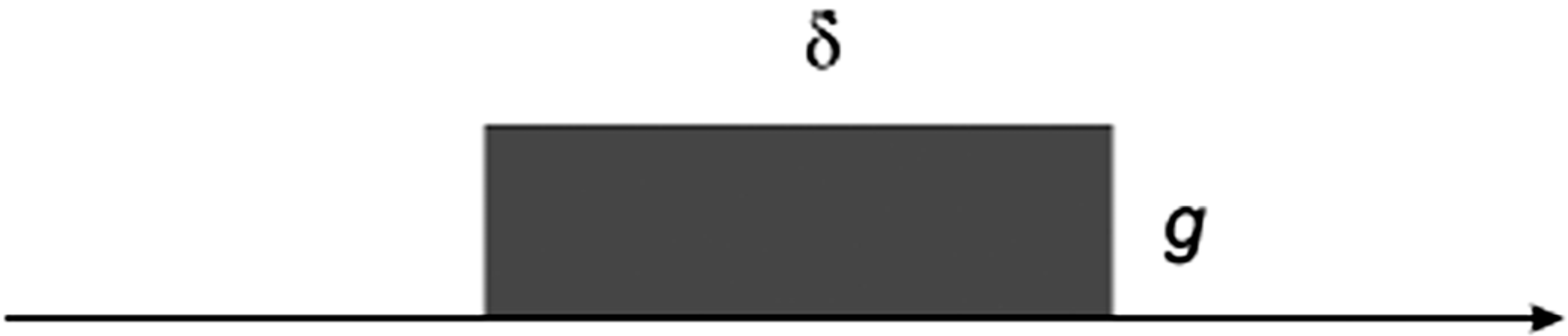


$$\omega(\mathbf{r}) = \gamma\left|\mathbf{B}(\mathbf{r})\right| = \gamma\left(\left|\mathbf{B}_0\right| + \mathbf{g}\cdot\mathbf{r}\right)$$

$$\omega(\mathbf{r}) - \omega_0 = \gamma\mathbf{g}\cdot\mathbf{r}$$

- g – gradient
- B(r) – inhomogeneous field
- ρ(**r**) – spin-density distribution

Pulsed gradient field.



$\omega = \gamma B_0$ $\qquad$ $\omega(r) = \gamma B(r) = \gamma (B_0 + g\, r)$ $\qquad$ $\omega = \gamma B_0$

$\varphi = (\omega - \omega_0)\, t = 0$ $\qquad$ $\varphi(r) = (\omega - \omega_0)\, t = \gamma\, g\, r\, t$ $\qquad$ $\varphi(r) = \gamma\, g\, r\, \delta$

Fundamentals of NMR Imaging.

$$\phi = [\omega(\mathbf{r}) - \omega_0]\delta = \gamma\mathbf{g}\cdot\mathbf{r}\delta$$

$$S(\mathbf{k}) = \int \rho(\mathbf{r})\exp(i\phi(\mathbf{r}))d\mathbf{r} = \int \rho(\mathbf{r})\exp(i2\pi\mathbf{k}\cdot\mathbf{r})d\mathbf{r}$$

$$\mathbf{k} = \frac{1}{2}\pi\gamma\mathbf{g}\delta$$

$$\rho(\mathbf{r}) = \int S(\mathbf{k})\exp(-i2\pi\mathbf{k}\cdot\mathbf{r})d\mathbf{r}$$

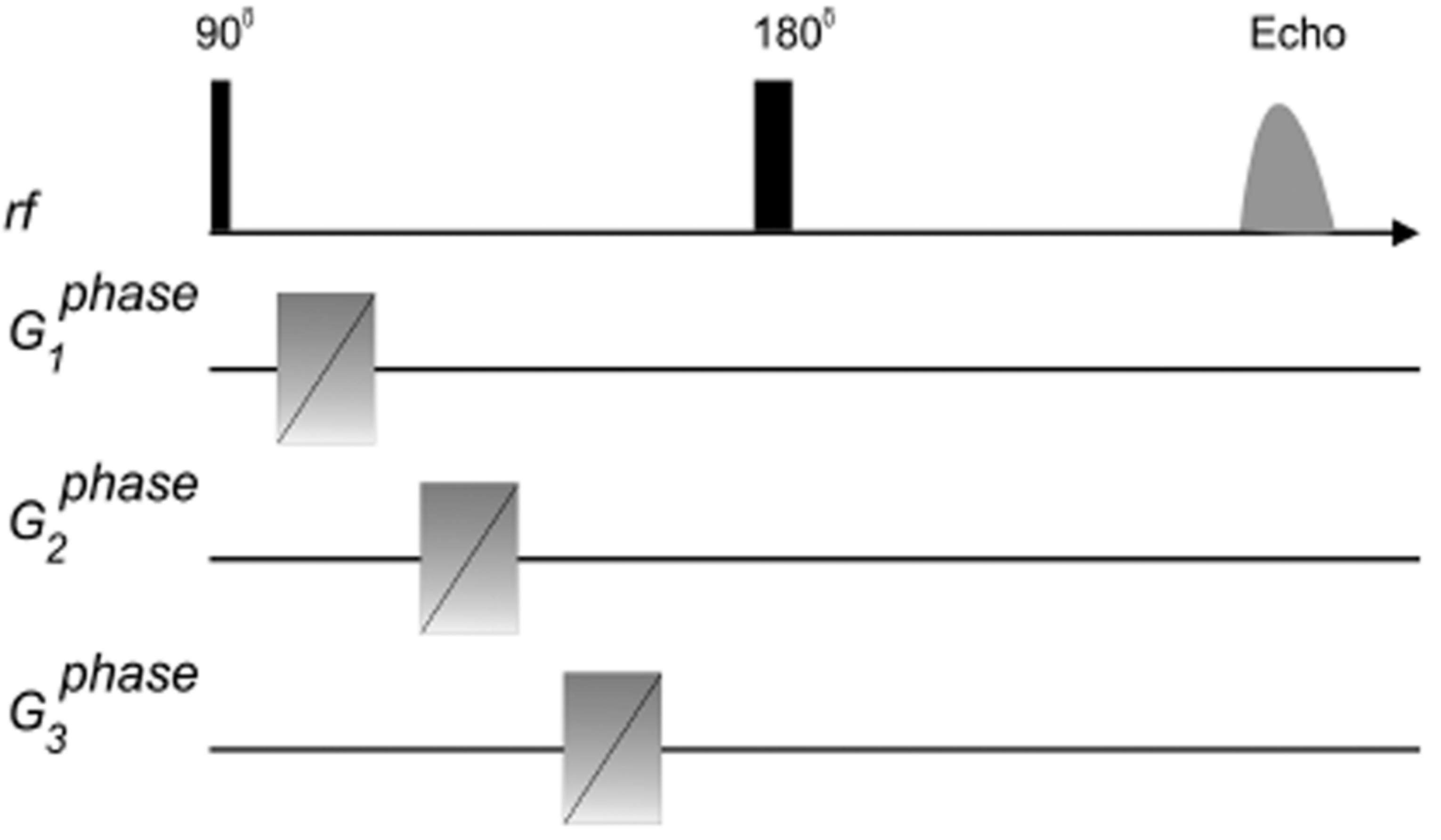
- S(k) – signal
- Φ - phase

Recipe for the phase encoding.

$$\mathbf{k} = \frac{1}{2}\pi\gamma\,\mathbf{g}\,\delta$$

- apply a phase gradient of effective area k;
- acquire the signal S(k);
- repeat for a number of different equidistant values of k;
- perform the inverse Fourier transformation to reconstruct the spin density function of the sample, ρ(r).

Phase encoding in three dimensions.



Phase encoding: advantages and disadvantages

Advantage:

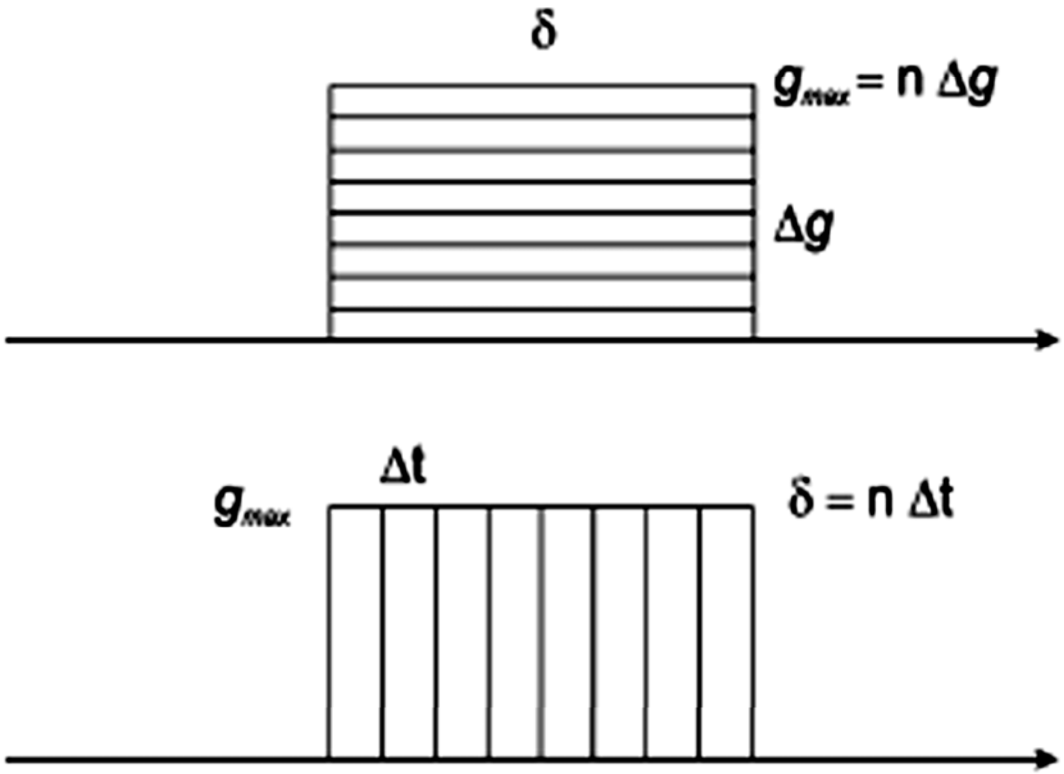
- It contains the full spectroscopic information.

Disadvantage:

- It is very slow.

Frequency encoding.

$$\mathbf{k} = \frac{1}{2}\pi\gamma\mathbf{g}\,\delta$$



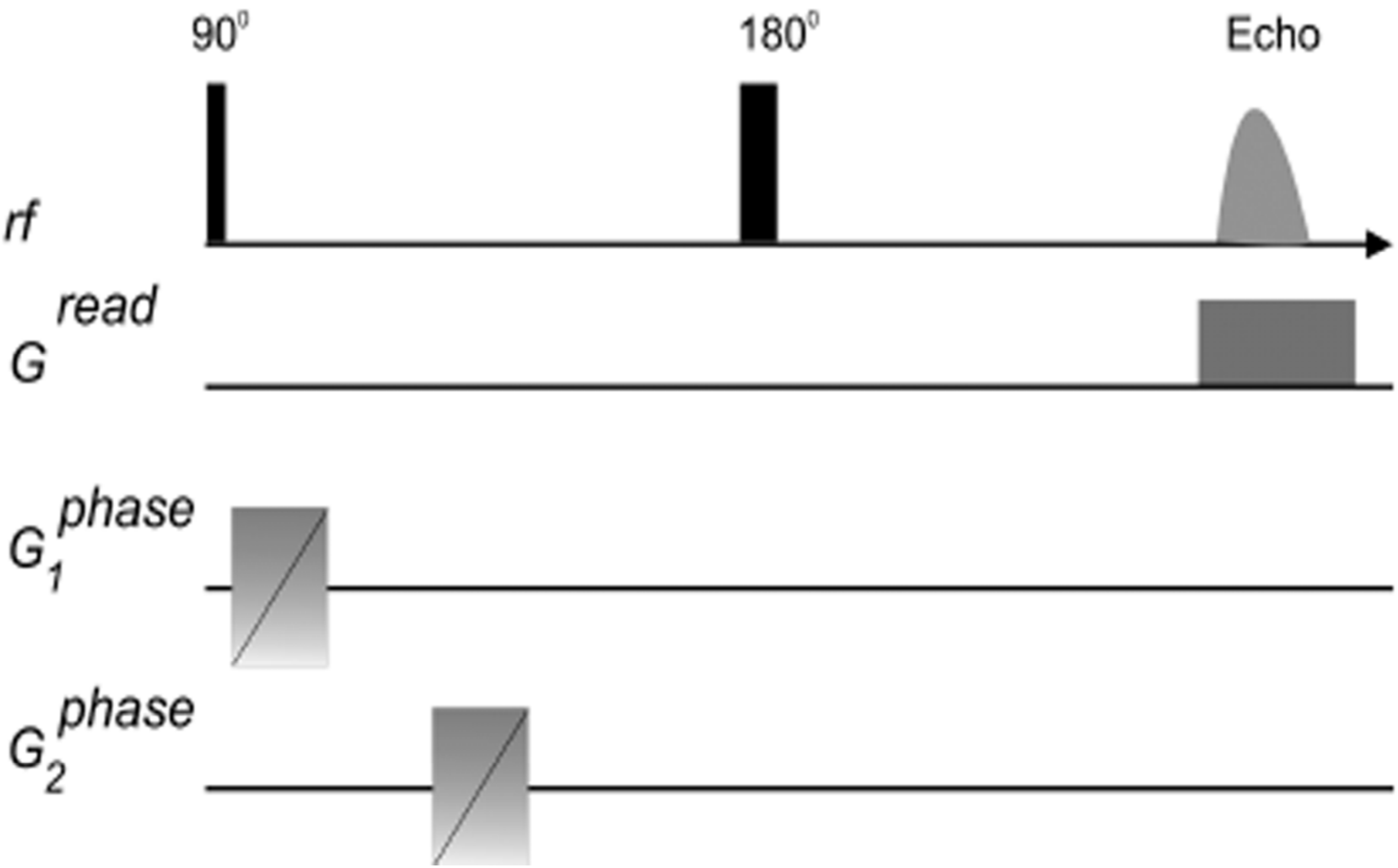
Phase encoding

↓

Frequency encoding

Signal is acquired while the field gradient is present. Read gradient.

3-dimensional frequency encoding



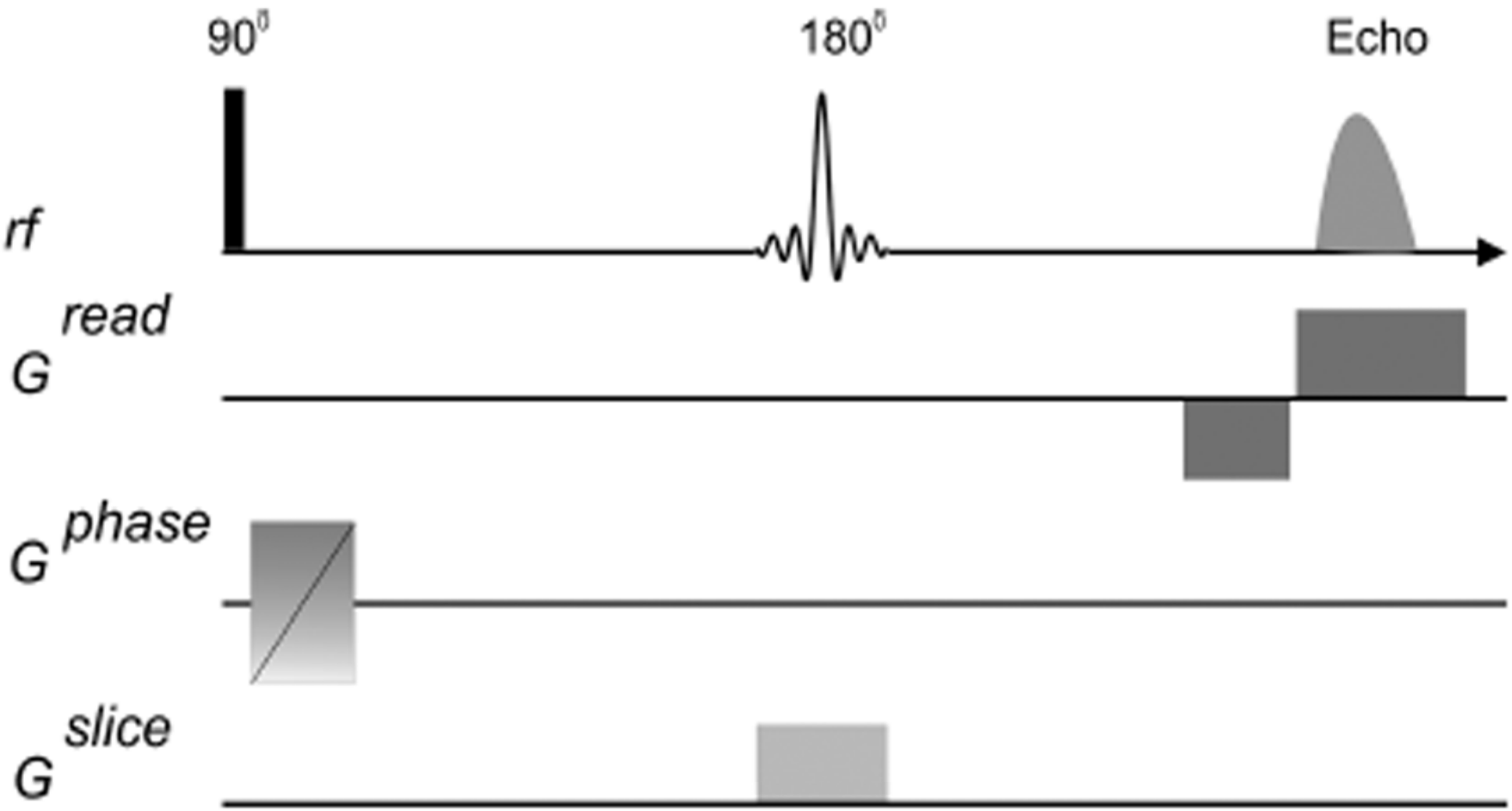
Features of frequency encoding.

- In FE spectral information of the spin system is masked by the spatial encoding; the result will be a superposition of chemical shifts and position information.
- Two lines spectrum will render a double image.

Slice detection.

- We have implicitly assumed above that all rf pulses in the imaging sequence affect the whole number of spin in the same way. But this is strictly true for a “hard pulse”, i.e., a pulse with a bandwidth greatly exceeding the range of Larmor frequencies in the sample.
- We have to define the shape of the slice we want to excite, and perform inverse Fourier transform to find out what the equivalent pulse should look like.

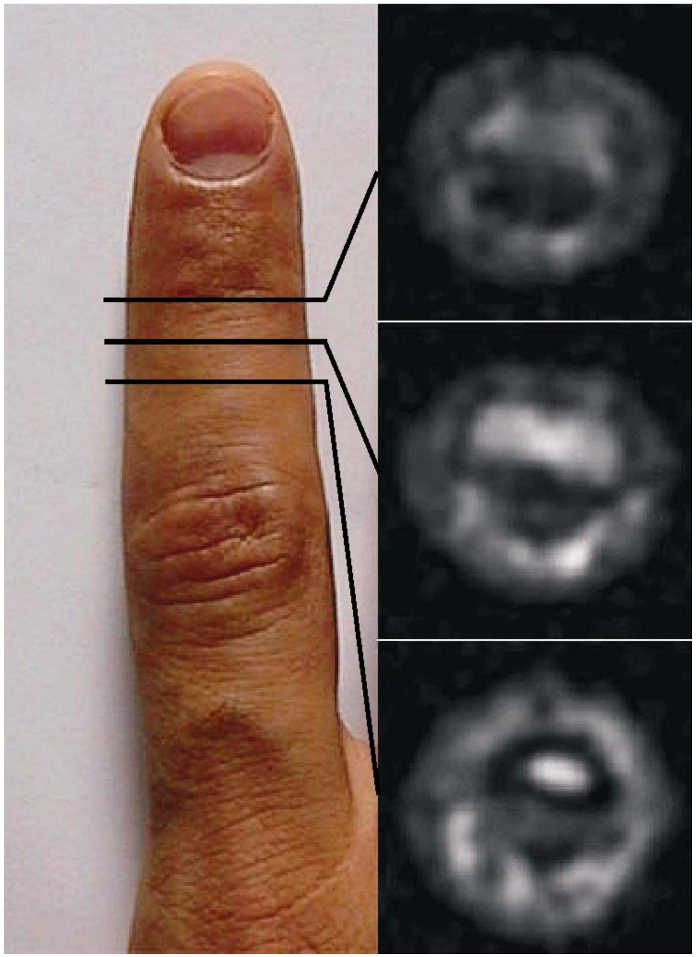
Example.



Contrasting.

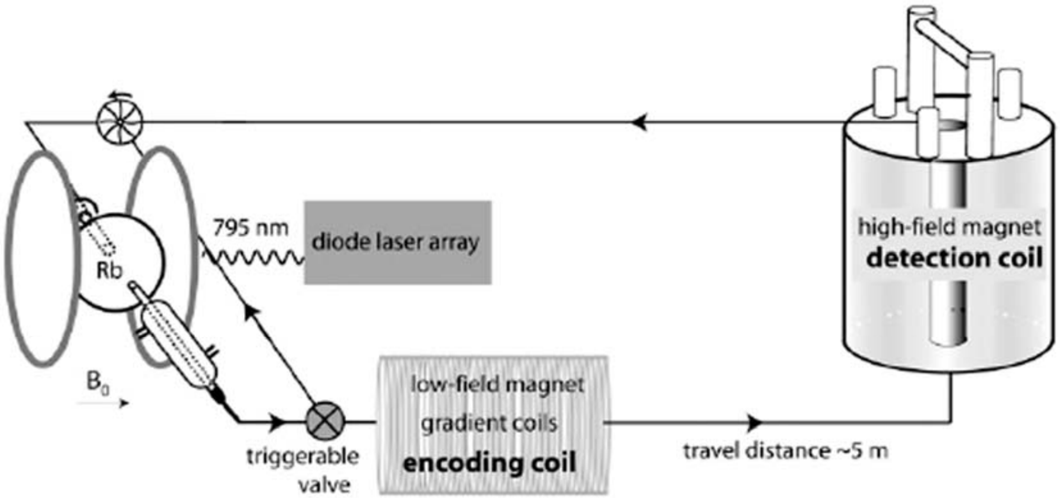
- Relaxation contrast. Take advantage of different T_1 and T_2 relaxation times.
- They alter when a liquid interact with a surface (application for porous media).
- Set repetition time of a sequence to an intermediate value between those of the different components of the heterogeneous sample.
- Pixels of short T_1 will appear with full brightness, while those for long T_1 will be darker.

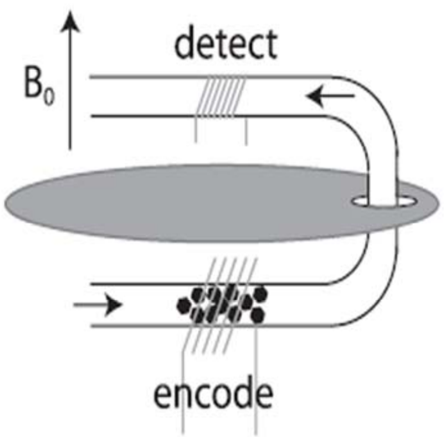
in vivo imaging of a human finger



- **The most important target of this project is to use the open tomograph to image biological tissues.**
- **In the images the dimension and shape of the bone can be identified as well as the positions of vessels, arteries, and the tendon.**

Incredible technique.





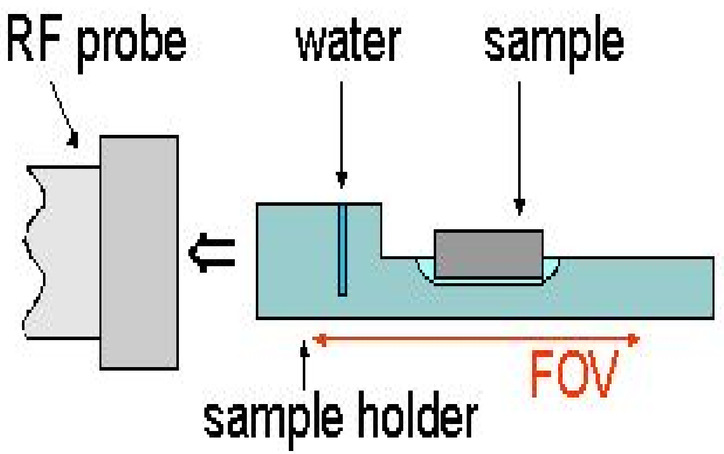
The xenon is optically hyperpolarized, then introduced into the encoding chamber, where it flows through the voids in the sample. Because the sample is surrounded by a large radiofrequency coil, the filling factor is poor. Bearing the encoded information, the gas flows on to the detection chamber. Since xenon has a long spin-relaxation time, no spin-polarization or pulse-timing information is lost during transport.

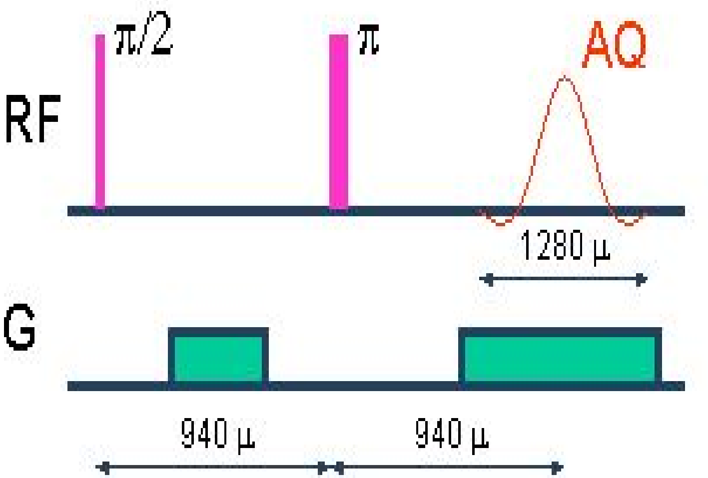
Application of NMR Imaging to porous media.

- Water transport in porous media.
- Aerogel study.
- Concrete study.
- Tires and air springs.
- Food industry.
- Tires and air springs.
- Porosity of bones.

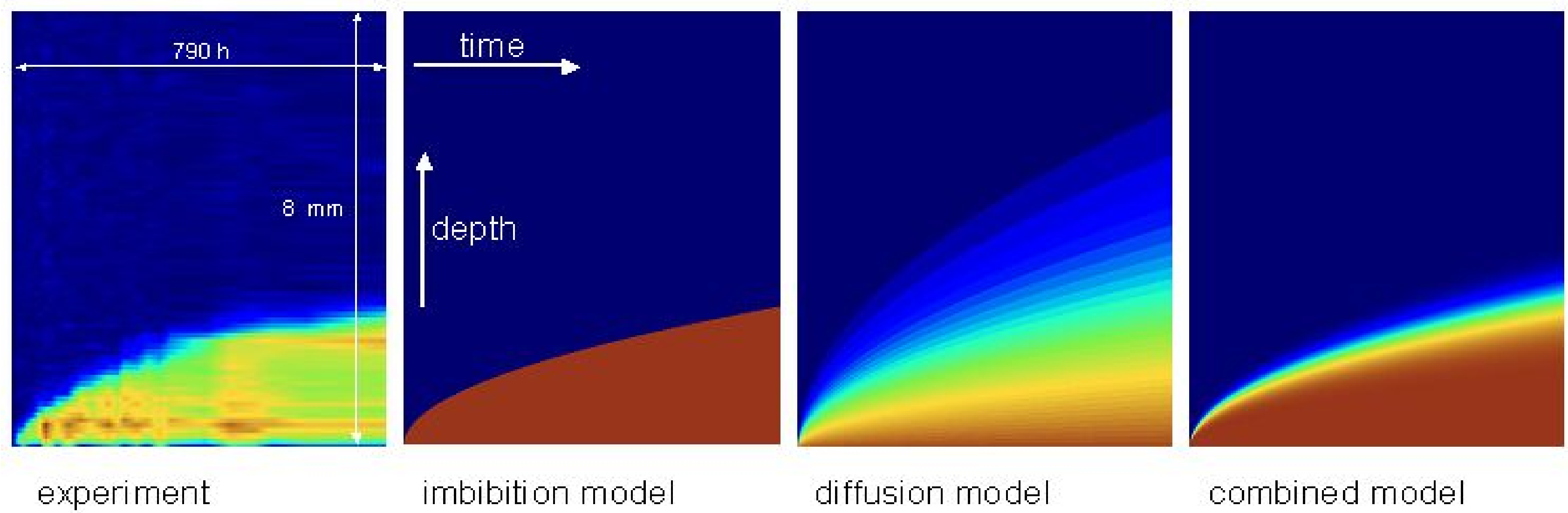
Water migration in porous materials.

Water in pores of many materials is often unwanted since it may reduce their durability and lifetime. From that perspective it is important to understand how water migrates into these materials. Water migration can be accurately monitored via high-resolution magnetic resonance imaging in non-magnetic and non-conductive materials. We were particularly interested in situations where at the beginning of migration the material was completely dry and at the end was saturated with water. Water migration was monitored by 1D profiles of water concentration along the direction of migration.





Water migration in porous materials.



- **Images above depict water concentration (image intensity in color coded scale) as a function of depth (vertical axis) and time (horizontal axis) as measured in the experiment on dental cement. The experimental results were analysed by three different mathematical models: an imbibition model, a diffusion model, and a combination of both models. From the results it can be clearly seen that depth of the region saturated with water increases as the square root function of time.**

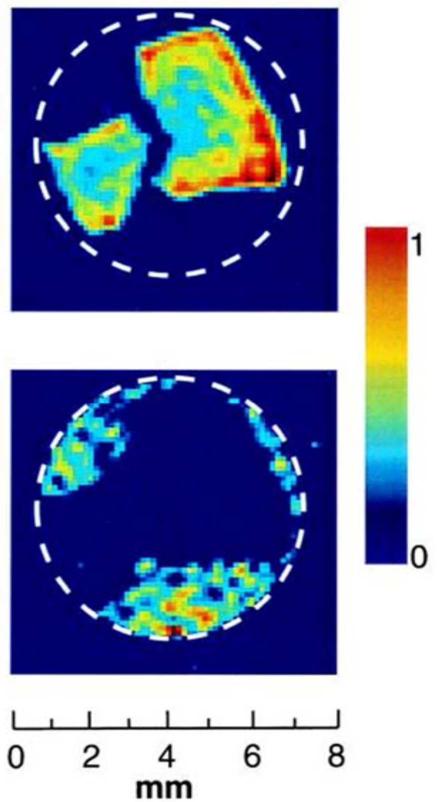
Aerogel properties.

- **Aerogel** is a solid-state substance similar to gel where the liquid component is replaced with gas. The result is an extremely low density solid.
- Remarkable thermal, conductive, radiative insulator.
- Strong desiccant.

Uses.

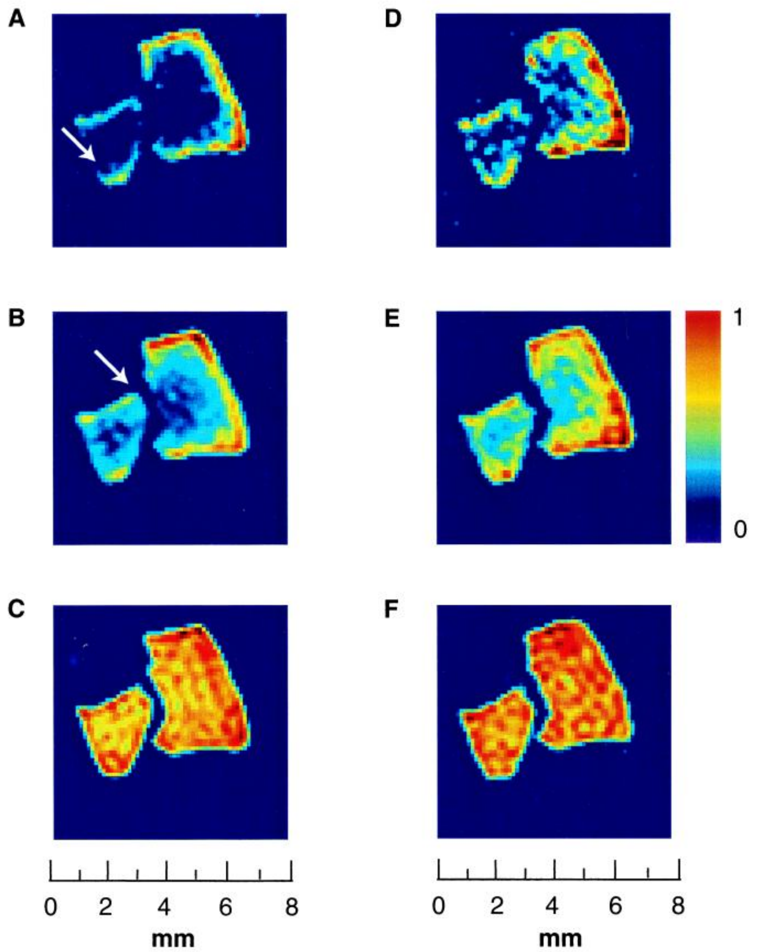
- Chemical absorber for cleaning up spills. Great catalyst.
- Thermal insulation material for windows.
- Reinforcing structures, and hybridizing compounds.
- Particle trap and detectors.
- Insulators for skylights.
- Thickening agent.

Aerogel study.



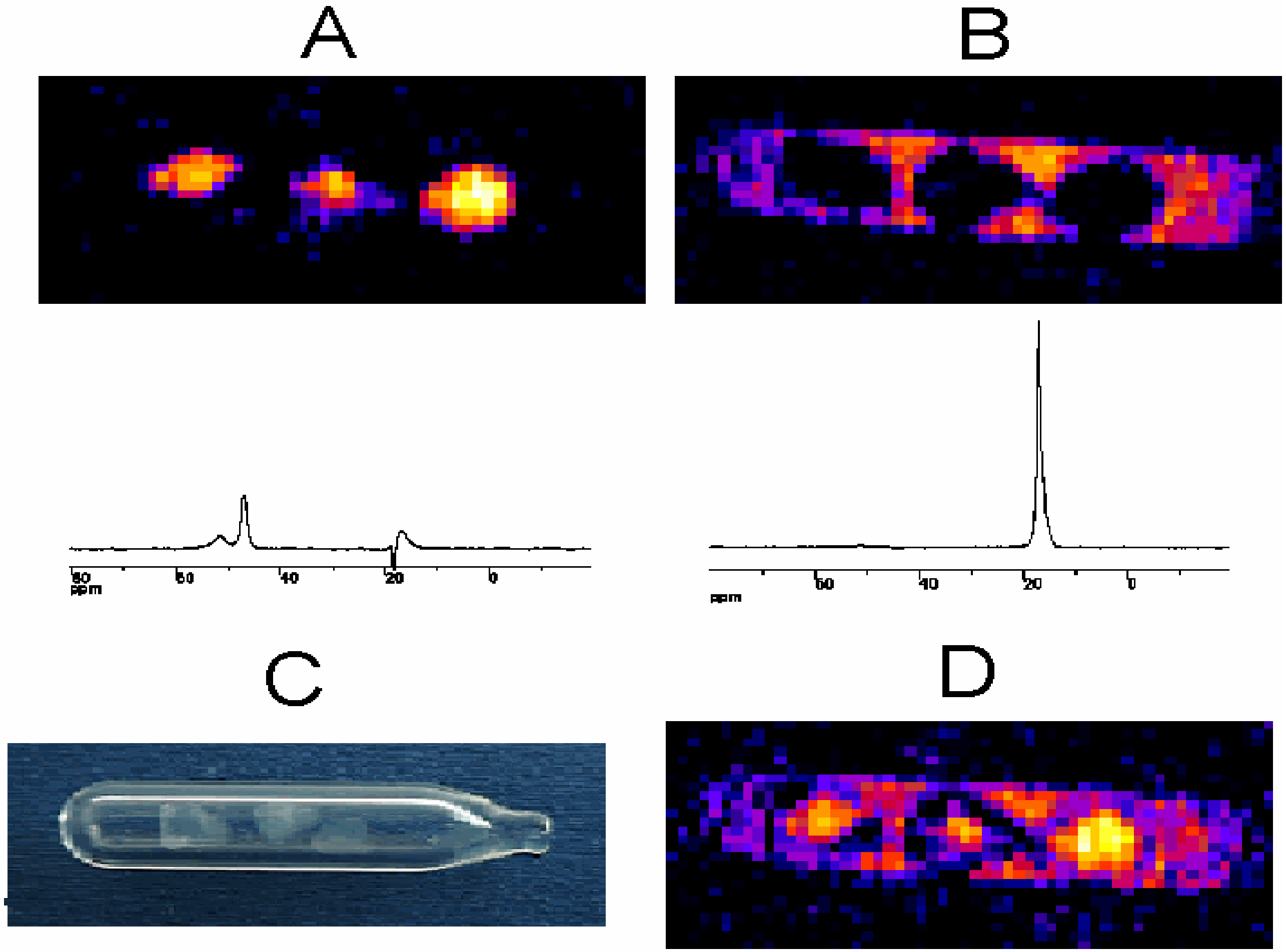
- **Images of xenon diffusing through aerogel fragments can be separated from those of the bulk phase xenon gas. The gas diffusion around and into the material can be visualized by spin density images encoded with varying time delays between excitation pulses.**

Aerogel study



The penetration of xenon into aerogel fragments as a function of the ‘‘transport time’’ (the time delay between excitation pulses) and the total gas pressure. NMR images of a higher pressure gas mixture (total pressure 4 atm) penetrating aerogel fragments via diffusion are shown in Fig. *A–C*, and a lower pressure gas mixture (total pressure 1 atm) is shown in Fig. *D–F*. For short time delays between the pulses, the images show xenon signal at the outer regions of the aerogel fragments (Fig. *A* and *D*).

Pore Structure Investigations by MRI



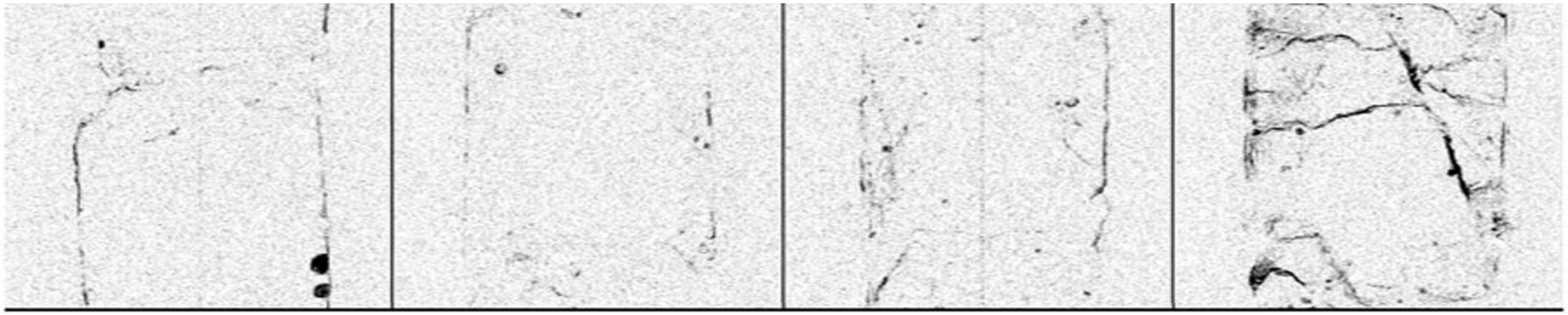
Aerogel study

- **Aerogels are ultralight porous materials, typically based on silica,with densities ranging from 0.003 to 0.25 gycm3. The aerogel chemical composition, microstructure, and physical properties can be controlled at the nanometer scale, giving rise to unique optical, thermal, acoustic, mechanical, and electrical properties**.

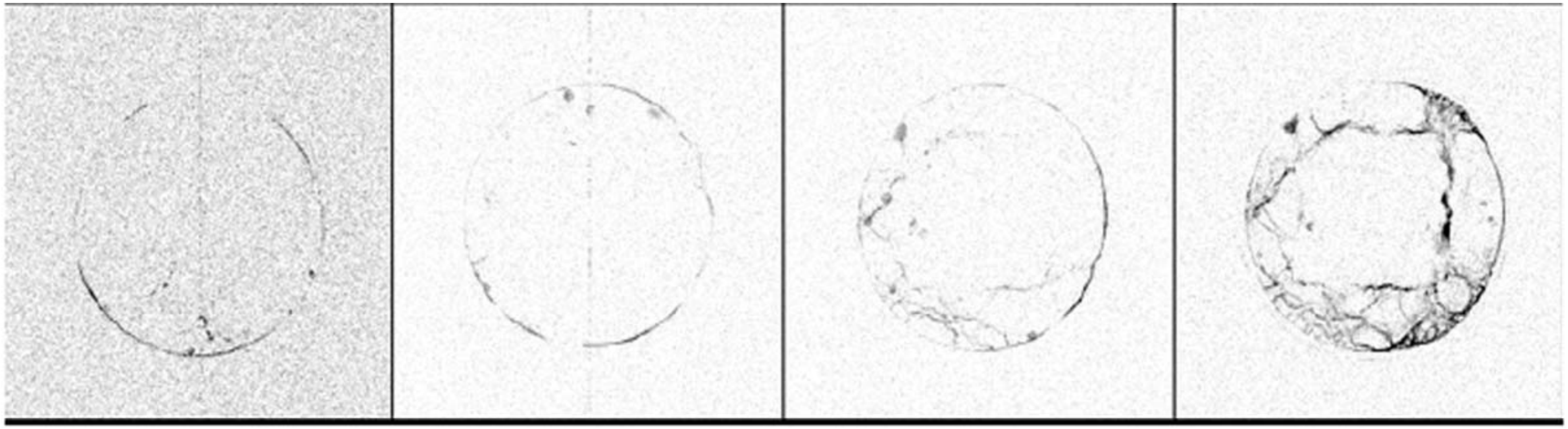
Concrete study

- Concrete is a conglomerate made by mixing aggregates, sand, cement and water in suitable proportions.
- Porosity, permeability, durability and fracture propagation are all aspects that require study.
- More recently, single-point imaging (SPI) has been used to study shrinkage and drying of concrete and mortar. Freeze/thaw effects have also been studied.

Concrete study.

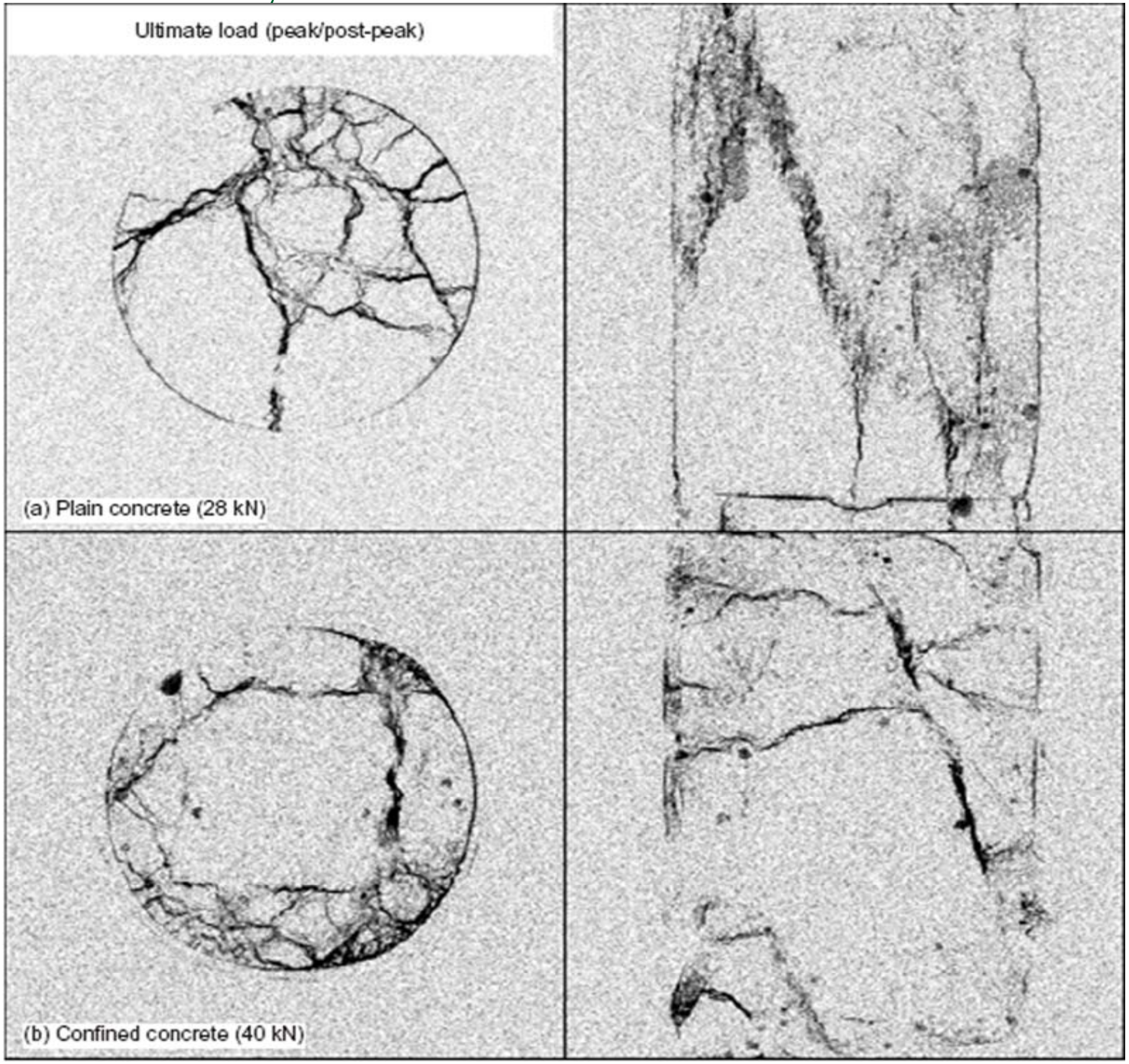


.. *Progression of fracture for confined samples (slices parallel to the loading direction)*

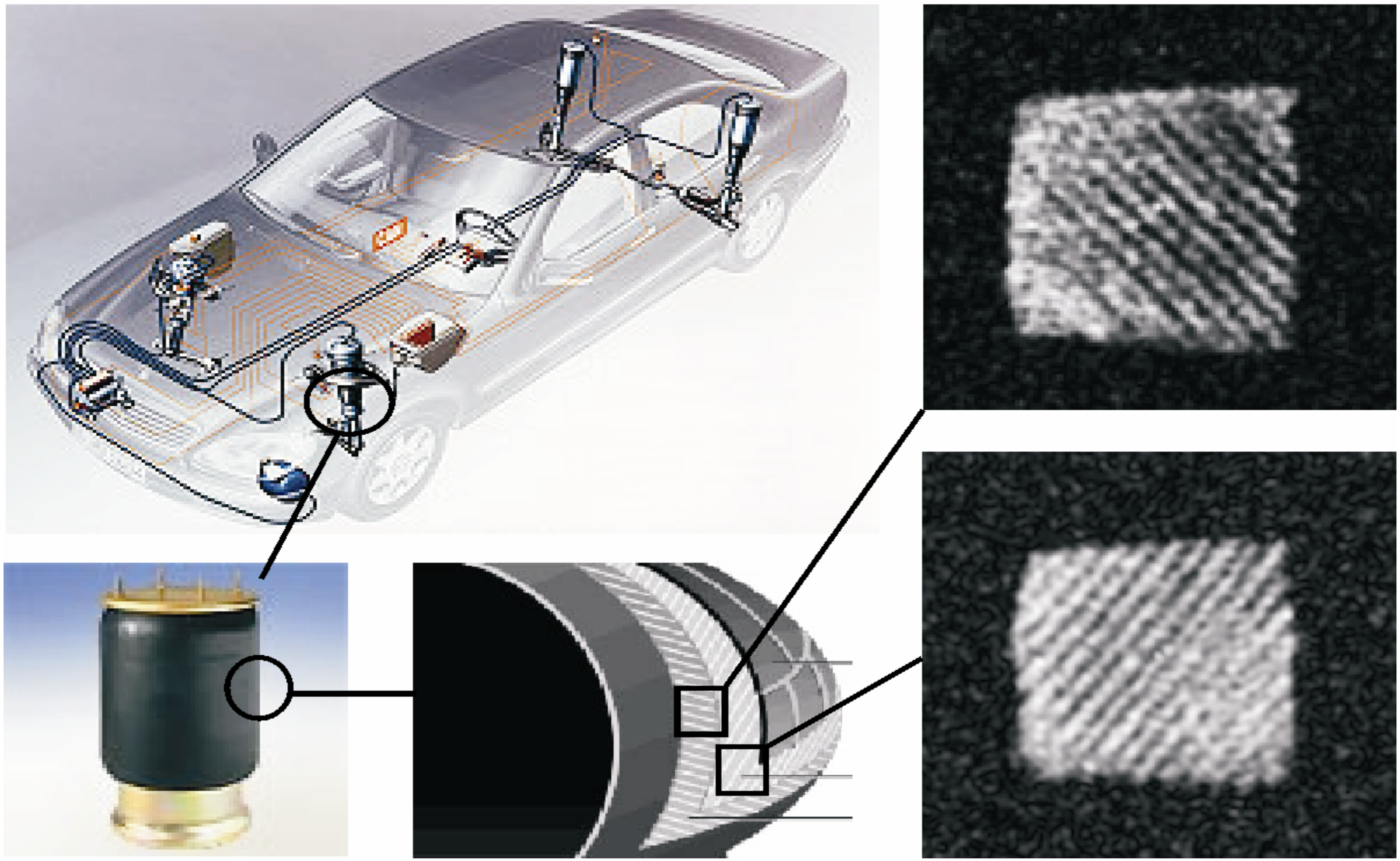


Progression of fracture for confined samples (slices transverse to the loading direction)

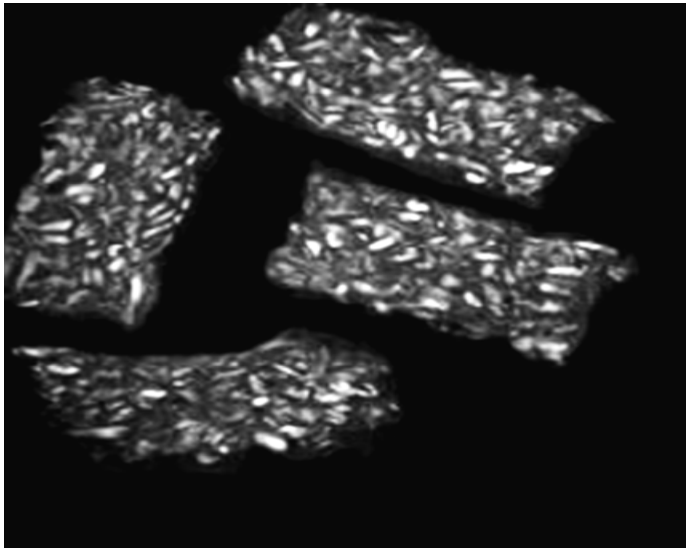
Concrete study.

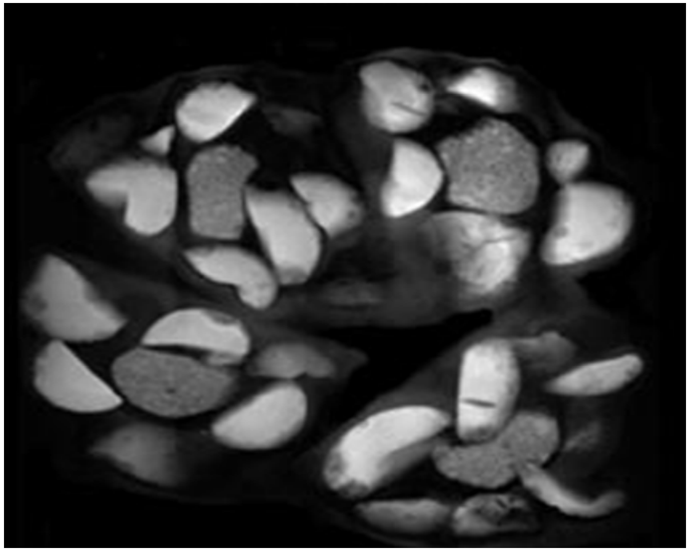


Imaging fibers in an air spring



Porous materials in food production.





- [1]H NMR image of a chocolate-caramel-nut candy bar. The H spin density is uniform throughout the candy. Contrasts from the differences in relaxation times of free and bound water and oil.
- [1]H NMR image of four coconut-chocolate candy bars. The contrast is due to relaxation time variations within the candy bar.