


Characterization of Construction Materials
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Lecture -58
Spectroscopy techniques - Principle of NMR spectroscopy

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NMR Principle



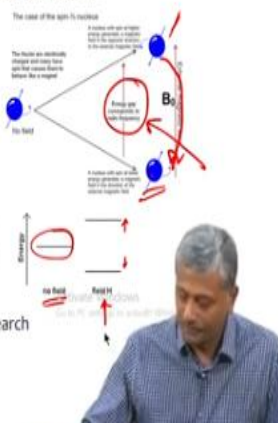
Nuclei with an odd number of protons, neutrons, or both, will have an intrinsic nuclear angular momentum or "nuclear spin".


Spin quantum number for various nuclei

Number of protons	Number of Neutrons	Spin Quantum Number (I)	Examples
Even	Even	0	^{12}C , ^{16}O , ^{18}O
Odd	Even	$\frac{1}{2}$	^1H , ^{13}C , ^{15}N , ^{19}F
Even	Odd	$\frac{1}{2}$	^2H , ^{10}B , ^{11}B , ^{11}Li
Odd	Odd	1	^3H , ^{14}N , ^{14}C

When a nucleus with a non-zero spin is placed in a magnetic field, the nuclear spin can align in either the same direction or in the opposite direction as the external magnetic field. A nucleus that has its spin aligned with the external field will have a lower energy than when it has its spin aligned in the opposite direction to the field. Thus, these two nuclear spin alignments have different energies and application of a magnetic field results in an energy level diagram shown here to the right.

^{29}Si , ^{27}Al common in cement-based materials research



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So, before we proceed further with NMR, I thought, I will again do a brief recap of what we talked about previously. So we know that when there is radio frequency radiation there is certain types of atoms which have odd numbered neutrons or protons in their nuclei which have a finite spin and this finite spin actually can get altered by the absorption of radio frequency radiation. So, the energy state of this atom will increase when it absorbs the radio frequency radiation and of course conversely what can also happen, is that, by emission of the radiation the energy state can come back to its ground state. So, you have energy transitions happening in the nuclei because of the spins and that happens only in specific sets of nuclei which have odd numbered neutrons or protons or both.

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Nuclear spin

- A nucleus with an odd atomic number or an odd mass number has a nuclear spin.
- The spinning charged nucleus generates a magnetic field.

When placed in an external field, spinning protons act like bar magnets.

For more information, https://www.nanochem.org/uploads/Modules/MCMedias/1409057676894/thesis_valor_final.pdf

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Now we also saw the fact that when you place such type of nuclei in an external magnetic field, the spinning protons, which are there in the nuclei act like magnets. So, there are low or high energy configurations possible in this system; the low energy configuration is obviously more stable the higher energy configuration is unstable, in which case you are actually having a system that is not really stable when you have an external magnetic field, that is applied to this spinning nucleus.

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Energy states and shielding

- The magnetic fields of the spinning nuclei will align either *with* the external field, or *against* the field.
- A photon with the right amount of energy can be absorbed and cause the spinning proton to flip.

Circulating electrons create an induced magnetic field that opposes the external magnetic field. Magnetic field strength must be increased for a shielded proton to flip at the same frequency.

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Now we saw that in certain cases the nuclei can be extremely shielded also. Why does the shielding occur? Because you have circulating electrons around the nuclei which are providing

an environment which is separating the nucleus from the applied magnetic field. So, you have this separation or shielding which happens because of the circulating neutrons and obviously elements or atoms which have a larger number of electrons will have greater extent of shielding around them.

So, the magnetic strength must be increased for a shielded proton to flip at the same frequency or for the absorption of the radiation to happen and flipping to happen at the same frequency, you need to then increase the strength of the magnetic field because of the shielding which actually happens.

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NMR Principle (contd.)

The energy (and thus frequency) of an NMR transition depends on the magnetic-field strength and a proportionality factor for each nucleus called the gyromagnetic ratio, γ . The frequency of a transition is given by:

$$\nu = \frac{\gamma H}{2\pi}$$

where ν is the frequency of the resonant radiation and H is the strength of the magnetic field.

Frequency is represented generally in terms of the 'Chemical Shift' in ppm, which is written as:

$$\delta = \left(\frac{\nu_{\text{sample}} - \nu_{\text{ref}}}{\nu_{\text{ref}}} \right) \times 10^6$$

$\delta = 0$ for TMS

The reference is usually taken as TMS (Tetramethyl silane) – unreactive with other organic compounds, volatile, and gives absorption which is mostly shielded

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Now we also saw that the resonance or frequency of the transition (resonant frequency of the transition) is related to a factor called the gyromagnetic ratio (γ) which is unique for every type of atom. So, what you do is when you apply the external magnetic field to the system, the resonant frequency is that at which radio frequencies or radio frequency radiation is getting absorbed, is given by this formula:

$$\nu = \frac{\gamma H}{2\pi}$$

where γ is the gyromagnetic ratio, which is specific to the type of element that is being analyzed, H is the strength of the magnetic field and ν is the frequency. Now when you present data related to NMR it is usually presented in terms of the shift in the radiation or shift in the peak relative to the peak which is offered by a reference material, in this case the reference material used is

tetramethyl silane, which is generally unreactive with other organic compounds and gives absorption which is mostly shielded, so most of the peaks associated with TMS will be towards the location where you have more shielding. Whereas the other atoms that are present which are generating the peaks may be present either to the left or to the right of the TMS peak. So, when you present it in this type of a shift type pattern. So, what would be the δ shift for TMS itself? Since it is a reference material $\delta = 0$ for TMS. So, when you present this information of NMR or absorption of radio frequency radiation by different types of atoms and species, you actually will generate an NMR pattern which will look somewhat in this way.

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The NMR plot

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- More electronegative atoms deshield more and give larger shift values.
- Additional electronegative atoms cause increase in chemical shift.

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Compound	Chemical Shift δ (ppm)	Difference (ppm)
<chem>CH4</chem>	0.2	-
<chem>CH3Cl</chem>	3.0	2.8 ppm
<chem>CH2Cl2</chem>	5.3	2.3 ppm
<chem>CHCl3</chem>	7.3	2.0 ppm
<chem>CCl4</chem>	9.7	-

Note: Each chlorine atom added changes the chemical shift of the remaining methyl protons by about 2.8 ppm.

So, you will be plotting the intensities or the resonant frequencies at which the radiation is getting absorbed with respect to the location. The location is determined by the chemical shift. Now chemical shift (δ) because we are multiplying it by 10^6 , we actually measure the chemical shift in terms of parts per million, ppm. And that is what you will see most NMR patterns being represented as.

Of course, we also had an overview of a typical NMR spectrometer in which you have the sample which is in a liquid state which is actually subjected to this external magnetic field and then you have the radio frequency radiation which is transmitted through the sample. You

have the absorption taking place and then the detector actually detects the RF radiation that comes out of the sample and you will actually be able to figure out at what frequencies did the absorption actually take place?



And this is your diffractogram or your pattern which is obtained as a result of your experiment. So, now of course in this example, the pattern is drawn with respect to the strength of the magnetic field. But you can convert the magnetic field as I showed you earlier into a frequency and the frequency can be converted to the shift.

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NMR experiment

- Keep external magnetic field strength constant and vary the frequency of radiation to see an absorption
- Keep the radio frequency constant and vary the field strength until splitting of spin states corresponds to energy of radio wave
- New instruments use intense RF pulse to excite all nuclei simultaneously and then FT is done


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Now again, you can do this experiment in several ways, one is you keep the external magnetic field strength constant and vary the frequency of radiation to see the absorption. Alternatively, you can keep the radio frequency constant and vary the strength of the magnetic field. So that would be the two ways of actually operating this instrument and modern instruments can actually do multiple frequencies at once and resolve all of them using a Fourier transform, just like we looked at with infrared spectroscopy.


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NMR Signals




- The **number** of signals shows how many different kinds of protons are present.
- The **location** of the signals shows how shielded or deshielded the proton is.
- The **intensity** of the signal shows the number of protons of that type.
- Signal **splitting** shows the number of protons on adjacent atoms

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Handwritten notes on the slide:
- A horizontal axis with '0' in the center. To the left, it says 'Less shielded' with an arrow pointing left. To the right, it says 'More shielded' with an arrow pointing right.
- A red arrow points from the 'More shielded' text down to a peak on a graph.
- A red arrow points from the 'Signal splitting' text to a split peak on a graph.

So now the NMR signals or the peaks that you get at different locations that means with respect to different chemical shift (δ):

- The number of signals shows how many different types or kinds of protons are present. You may have different kinds of protons within the same sample like: silicon, aluminium and so on and so forth.
- The location of the signals shows how shielded or de-shielded the proton is. Now more the shielding, where will the δ value go when higher shielding is there? Towards 0 or even to the right of 0, that means in the negative regime. So, we plot the δ , 0 here, negative is in this direction (right) and the positive is in this direction (left), so this is less shielded (+ve) and this is more shielded (-ve).
- The intensity of the signal shows the number of protons of that type, for example, if you are getting silica which is in the dual state that means there are 2 silica tetrahedra joined together. So that is called a disilicate. So that will have a specific location of the peak or specific chemical shift at which you detect that peak and the intensity of that peak will tell you how much of the disilicates are present in your system.
- Signal splitting shows the number of protons on adjacent atoms. In a molecule, if you have protons on adjacent atoms that are both being subjected to this nuclear transition, then the peak itself may show a splitting type of a behavior and that indicates the number of protons on adjacent atoms that are creating these interactions next to each other.

So of course, the NMR plot, as I said you plot against the δ or the shift, the closer to 0 you are, the more shielded the material is, that is, closer to 0 means you are in the increased shielding direction. You can also go towards negative direction, negative means what, if you look at this formula once again:

$$\delta = \left(\frac{\nu_{sample} - \nu_{ref}}{\nu_{ref}} \right) 1 * 10^6$$

So, here a negative value simply means the frequency of the sample is lesser than the frequency of the reference; positive implies frequency of sample is more than frequency of reference. So generally, in a sample, if you have more electronegative atoms, there is a lot more de-shielding and that generates a greater shift.

Just an example was given here previously of methane and as you increase the level of substitution of hydrogen by chlorine inside methane, you get increasing shift to the left that means the electrons or the compound gets more and more de-shielded. So, you increase the chemical shift, that means you are going towards the left from 0, as you are getting more and more de-shielding because of electronegative atoms that are present in your material.


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Magic Angle Spinning (MAS)


- By spinning the sample (usually at a frequency of 1 to 130 kHz) at the magic angle θ_m (ca. 54.74°, where $\cos^2\theta_m = 1/3$) with respect to the direction of the magnetic field, the normally broad lines become narrower, increasing the resolution for better identification and analysis of the spectrum
- Used in solid state NMR

Wikipedia

Activate Windows
Go to Settings to activate Windows.

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MAS-NMR



Now in some cases when we want to use solid samples, you can actually use a technique called Magic Angle Spinning (MAS). There we actually spin the sample at a range of frequencies between 1 and 130 kHz at the magic angle θ_m which is about 54.74°, which corresponds to


$\cos^2\theta_m = (1/3)$, with respect to the direction of magnetic field, what we essentially do by doing so is we make the broad lines of radiation much narrower and we are able to identify much better and analyze the spectrum in solid state NMR. So typically, when we do silicon or aluminium type of detection in nuclear magnetic resonance typically for identification of the types of C-S-H that are present in your cementitious systems, we opt for solid state NMR with MAS experiments.

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C-S-H's NMR Spectra

- Frequency of 59.59 MHz for ^{29}Si (magnetic field of 11.72 T) and a frequency of 130.4 MHz for ^{27}Al
- Software enables several NMR spectra to be decomposed simultaneously using the same spectral parameters for each individual component across the collected data.
- Relative intensity of some components can be fixed to agree with the proportion of the corresponding sites in the structural model of the material.
- For ^{29}Si spectra, choosing each component as a mixture of a Gaussian (bell curve) and a Lorentzian (sharp peak) function is an acceptable method

Neithalath, 2018 State Window



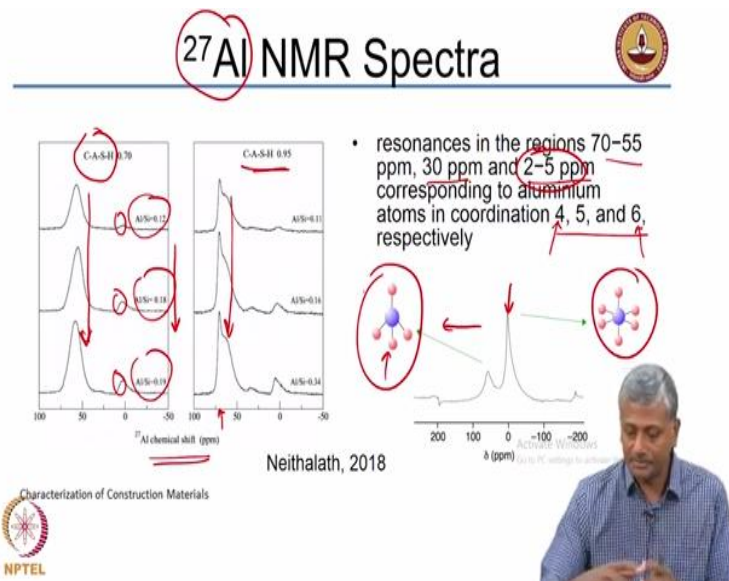
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Now just to give you an example of how relevant NMR is to identify the state of the C-S-H present in our cementitious systems. So generally, for silicon we have a frequency of 59.59 MHz which corresponds to a magnetic field of 11.72 Tesla and for aluminum it is 130.4 MHz, which is typically used because, why do we want to detect silicon and aluminium is because, these are principal components that are present in your C-S-H.

Now when you use software associated with the NMR spectrometer it allows several NMR spectra to be decomposed simultaneously, using the same spectral parameters. So, you actually get an analysis of each individual component across the entire collected data. And what we want to do is fix the relative intensity to agree with the proportion of the corresponding sites. So, what we have to come up with first is a structural model of the material that we are trying to analyze and based on that structural model, we fix the maximum limits for certain components, or fix maximum relative intensities for the components.

For ^{29}Si spectra, what we can do is choose each component, for example, if you get a peak like this, each of these peaks can be deconvoluted or broken down into a mixture of wider peaks and sharper peaks. So each peak is broken down into a combination of wide peaks and sharper peaks, wide peaks are basically your bell curves - Gaussian peaks, the sharper peaks are the Lorentzian curves which produce the patterns which are looking much sharper and less broader as compared to the others.

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So, this is NMR spectra of calcium aluminosilicate hydrate, C-A-S-H, at different water-cement ratios, so this is the aluminium NMR spectra ^{27}Al . So here what you see are different states of the bonding in alumina. For instance, resonances in the region 70 - 55 ppm, 30 ppm and 2-5 ppm correspond to aluminum atoms and coordination of 4, 5 and 6 respectively.

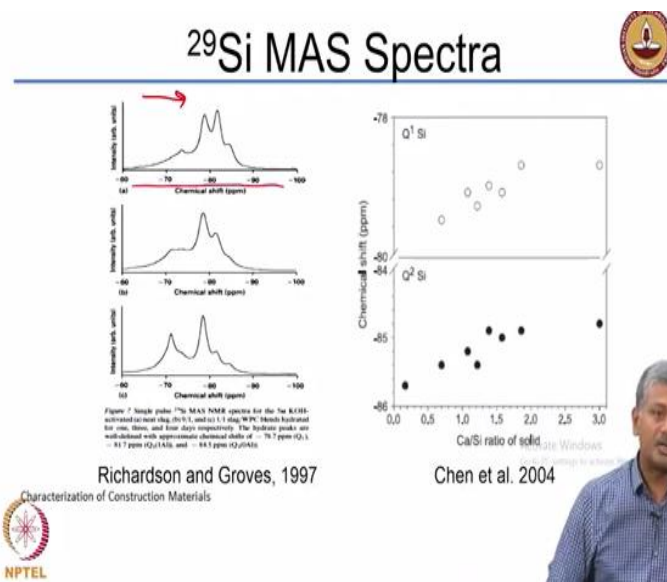
What do you mean by the coordination number of an atom? The number of atoms that are right next to it, or that are bonded right next to it. So, the coordination state of 4 implies the aluminum is in tetrahedral state, 6 means octahedral state, and that is what we associate with commonly with alumina is that alumina should be octahedral state. So, at octahedral state you expect the shielding to be more or less? There will be greater shielding for higher coordination number. When you have a coordination number that is higher, you will have greater shielding. And when that happens, your location of the aluminium peak is very close to 0 (2-5 ppm). So, this peak here in this Al NMR spectra, corresponds to the octahedral state of aluminum, whereas

the peaks to the left of this which are showing a greater shift or more de-shielded values, you are getting alumina in other coordination forms.

So that is what is being represented in this picture here with respect to the change in the Al/Si ratio of the C-A-S-H, you do get this octahedral coordination, which seems to increase with higher levels of alumina incorporated in the C-A-S-H. What does that mean with respect to cement chemistry? What does that mean? When will you increase the alumina content in the C-A-S-H? When you have more pozzolans in the system like fly ash or slag, which bring in their own alumina, which are reactive alumina you actually will incorporate that into the structure of C-A-S-H. So, with that you will actually increase this octahedral coordination of your aluminum, which is present in this system.

You also see that you are actually changing the coordination, which is in the other region, that is 55 - 70 region, which is the tetrahedral aluminum. So you see that, that is also increasing as you increase the Al/Si ratio. So, with this you can actually track the growth of your C-A-S-H or the change in characteristic of the C-A-S-H with respect to firstly, time and then secondly, with respect to the increasing degree of substitution of cement with pozzolanic additives. So, this NMR is actually a very strong technique which helps you determine these kinds of structural changes that are happening in your C-A-S-H.

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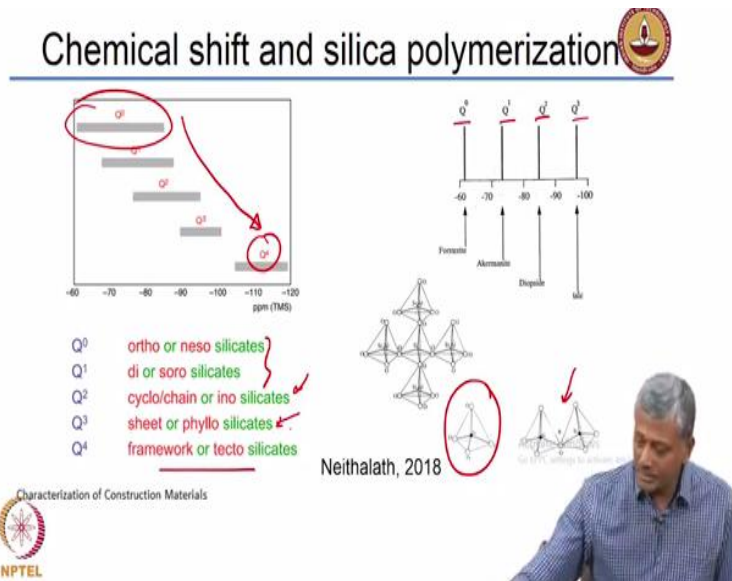


Now, this is a Silicon MAS spectra. So, in silicon spectra the shift is to the negative side, you see here the axis is plotted to the negative side. So, just to come back once again (in NMR Plot slide) to this representation of the shift here. So, the instrument typically has a specific frequency of operation 300 MHz NMR instrument. So, in which case, the frequency of TMS will be exactly 300 MHz. The, resonant frequency for TMS will be exactly 300 MHz that means the shift will be 0. So, corresponding to that shift location, you now have de-shielded atoms which are representing a shift which is on the positive side. Whereas more shielded, highly shielded atoms are to the negative side.

In the case of silica, you will see that, the shift is towards the negative side. Now interestingly with silica you get different types of bonded states of silica. Now in the, Simplest form, how does silica exist? In tetrahedral state - you have SiO_4 , tetrahedral silica that is a stable silica form on its own. You know that in quartz, you have this tetrahedral silica which are arranged in a regular pattern. In glass you have the same tetrahedral silica, but they are arranged in a very disordered pattern which makes quartz to be unreactive and glass to be reactive.

So now what happens is with increasing degree of reaction in a cementitious system, your tetrahedral silicate will start getting converted into other forms of silicates. For example, we know that structure of C-S-H is often told to be chain like or sheet like, in which case you start forming a greater degree of coordination for the silica tetrahedra. So, there are different states in which silica systems exist within the cement paste and because of which you get multiple peaks given by NMR with respect to the type of silica that you are trying to observe. Now, it will be shown in much more clarity in the next slide.

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The degree of silica polymerization is represented by these terms Q⁰, Q¹, Q² and Q³. Q⁰ corresponds to the simple tetrahedral state of silica and that has a peak in this range of about -60 ppm to about -80 ppm. As you move more and more from Q⁰ to Q⁴, as expected, the amount of shielding increases. So, it becomes more and more negative with respect to TMS and you get the Q⁴ type of silica which is basically a framework of tecto silicates. When you form a framework that means you have a three-dimensional coordination of the silica tetrahedra, those are tectosilicates and you see here Q⁴ type of a system. At the smaller end you have the orthosilicates Q⁰ which is simple tetrahedra or you have a disilicate where you have two tetrahedra combined together. And then you start forming cyclic or chain or sheet silicates or phyllo silicates. So, phyllo silicates are often common in C-S-H, but C-S-H is not entirely all sheet like, it may also contain some lower forms of silica like disilicates or cyclic silicates. So, because of this, when you actually evaluate C-S-H, for silicon signals using NMR, you will actually get a combination of different peaks. So, you need to identify which one corresponds to which type of silicate polymerization.

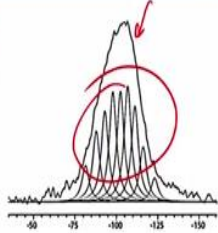
And more interestingly you can actually use this instrument to find out how does a pozzolanic cementitious mixture change with respect to time? Because the initial pozzolanic state which brings in the amorphous silica will mostly have the Q⁰ type of peaks, amorphous

silica will mostly have Q^0 or Q^1 type of peaks. As it becomes more and more organized in the C-S-H structure, it will start creating the higher forms of the silica, like Q^2 or Q^3 for instance.



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^{29}Si NMR Spectrum of fly ash and deconvolution 

- The peaks at -82, -93, -97, -102 and -107 ppm (± 1 ppm) can be attributed to the starting vitreous material in the fly ash ✓
- The peak at -87.8 ppm can be attributed to the crystalline mullite present in the fly ash, and the peaks beyond -109 ppm represent the different crystalline silica phases in fly ash



[Cement and Concrete Composites](#), Volume 57, March 2015, 34-43

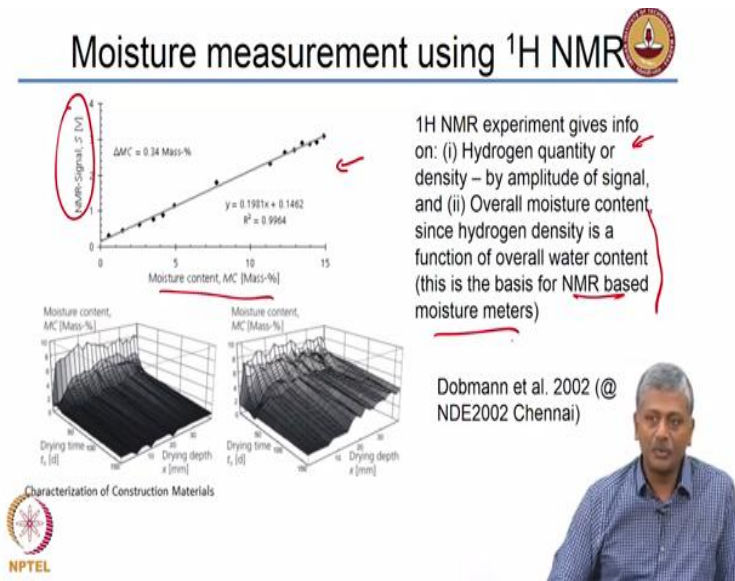
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So, there is an example given here of the ^{29}Si NMR spectrum of fly ash and how it is actually deconvoluted. So here, this is the actual signal that you are obtaining from your NMR spectroscopy. Now, why is this happening? Because all these peaks that are here are converging. So, there is interference from all the peaks and ultimately it gives a summation which is given as one peak. So, what you need to do is now break this down into the individual peaks that you have in your system.

So again, the peaks at all these locations (-82, -93, -97, -102, -107) are attributed to the starting vitreous material, that means the glassy material in the fly ash.

And peak at -87.8 is attributed to crystalline mullite and for -109 and beyond it, is different crystalline silica phases in the fly ash. The more the crystalline phases, the greater the degree of coordination, so you are shifting to higher negative values in the case of silicon. So, there are a lot of ways in which such data can be interpreted and because of this NMR remains a very powerful tool as far as cement paste analysis is concerned.

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One more aspect of NMR is the capability to measure moisture, because again water has hydrogen and by doing a proton NMR, you can actually determine the moisture states inside materials. And most of your moisture meters that are used in practice are either electrical based because electrical properties are sensitive to the moisture content of porous materials or they are NMR based. NMR happens to be a very useful technique for determining the amount of moisture present inside material.

So generally proton NMR experiments can give information on hydrogen quantity or density by analyzing the amplitude of the signal. For instance, here on this picture, the amplitude of the NMR signal is plotted against the moisture content in wood, this is actually for wood, and you see here that with increasing moisture content you get a relatively good increase in the signal intensity. So more the moisture content is, the greater is the amount of hydrogen protons that is present in the system, and so you get a greater intensity in the signal. Hydrogen density is a function of overall water content, most NMR based moisture meters are measuring moisture in the systems by estimation of the hydrogen density in the system.

Now one more method of using NMR is actually to look at what happens when the atom starts relaxing. So, I told you that atom absorbs energy and becomes more unstable, but over time what will happen is, it will take time to come back to its ground state. So, the time it takes

for that relaxation to happen, for it to come back to the ground state is another characteristic experiment that is used with NMR spectra. So, I am not covering that in our lecture here, but you may come across several research studies which have actually used the relaxation time for atoms to come back to their ground state and that can also be used to actually characterize and quantify the type of species that are present inside your sample.

So NMR is a highly powerful technique to look at the coordination states of different atoms that are present in the system and it primarily from a cementitious materials viewpoint, it gives us an idea about what is the structure of the calcium silicate hydrate that is forming in the system.

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References



- The Chemistry Hypermedia Project:
<http://www.chem.vt.edu/chem-ed/index.html>
- Wikipedia!
- <http://www.fc.up.pt/pessoas/peter.eaton/tutorial/webCT/index.html>
- http://chemwiki.ucdavis.edu/Wikitexts/UCD_Chem_205/%3A_Larsen/ChemWiki_Module_Topics/How_an_FTIR_Spectrometer_Operates



So, with that we finish this chapter on spectroscopy techniques. There are tons of references available for spectroscopy techniques on the web and there are several textbooks. What I have done is listed a few references, which could be useful for you to actually look at more details of these techniques.

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Further reading



- Overview About The Use Of Fourier Transform Infrared Spectroscopy To Study Cementitious Materials, M. Horgnies, J. J. Chen & C. Bouillon, <https://www.witpress.com/elibrary/wit-transactions-on-engineering-sciences/77/247/12>
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- ^{29}Si NMR in Cement: A Theoretical Study on Calcium Silicate Hydrates, Journal of Physical Chemistry C, 2012, 116 (17), pp 9755–9761



And there are a lot of papers that you can read further to get an assessment of how these spectroscopy techniques can be applied for analysis of cementitious specimens. So again here, this is a very good paper: Use of FTIR To Study Cementitious Materials, and this one here by a Grimmer and Zanni and Sozzani, that is actually a good book for NMR of cement-based materials. If you want to look at a paper, this paper by Jørgen Skibsted is very commonly cited paper with respect to use of NMR for characterization of cementitious materials.

So again, there are a lot of papers that you can actually look at with NMR. The more you read the more confusing it becomes, because this technique is quite complicated. So, although I have tried to simplify it in the best way possible, I am sure that there is a lot of questions in your mind. Some of those questions may get answered by reading some of these papers.

But please remember the principle of spectroscopy techniques was quite similar. Across the range of techniques that we talked about, the techniques were based on the absorption of electromagnetic radiation at a given wavelength, which is characteristic of the type of phase or atom or molecule that is present in the system. While some radiations are at very low frequencies like radio frequency and so on, there are other radiations which are absorbed at higher frequencies like ultraviolet or even greater than that obviously is X-ray and so on, which introduce some transitions within your phases which can be governed by identifying the

locations of the transitions and that leads you to analysis of the type of material that you are looking at. So, spectroscopy has a common background but the way in which the instrumentation is set up and the interpretation of the data is done is quite different, so with that we finish this chapter.