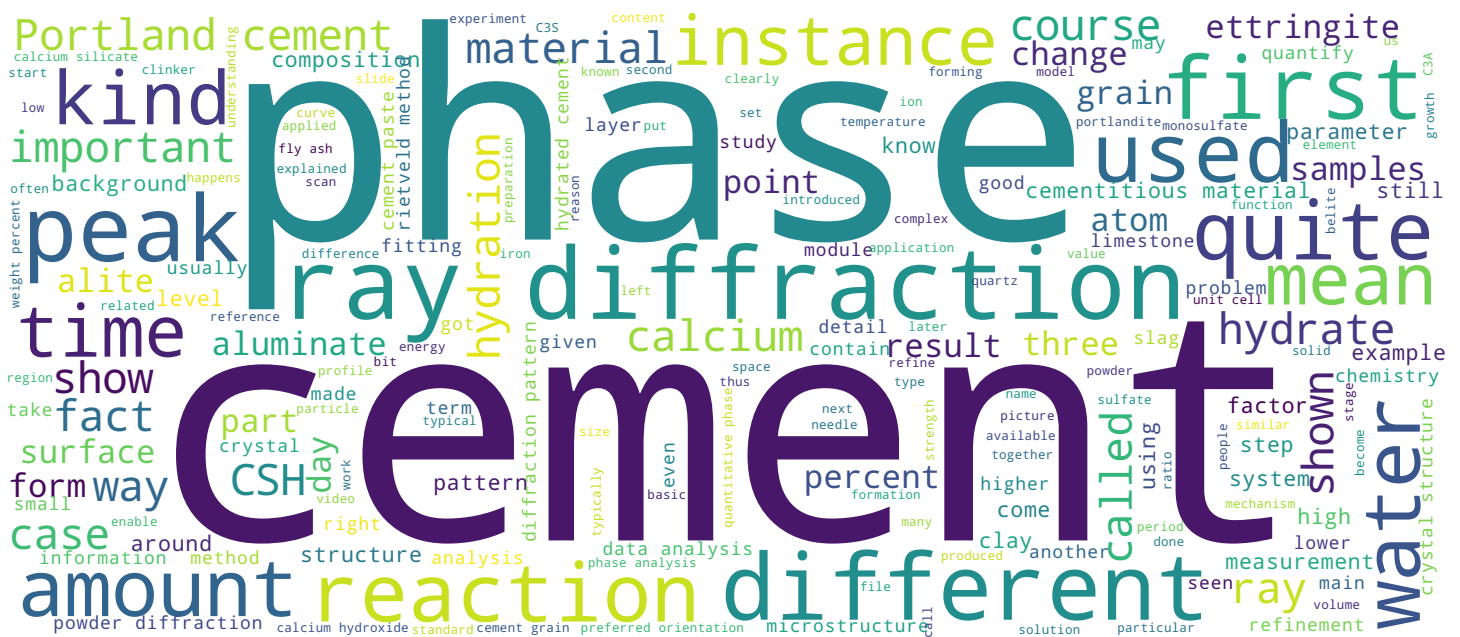


X-ray diffraction applied to cement

Cement Chemistry and Sustainable Cementitious Materials

Dr. Ruben Snellings and Dr. Xuerun Li



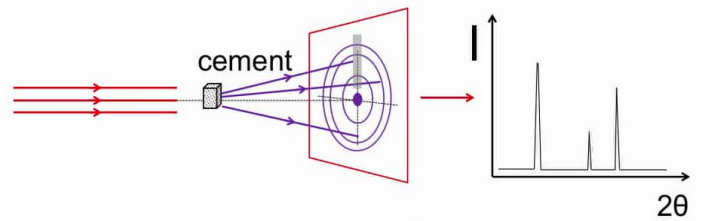
Search MOOC



Video



X-ray diffraction applied to cement



Hi, my name is Ruben Snellings and I have a background in applied mineralogy. In particular I have spend more than 10 years using X-ray diffraction to study cementitious materials. In this lecture series, my fellow team members and me want to introduce you into the basics of X-ray diffraction also called XRD and how you can make use of this powerful technique to study the chemistry of cement. The use of X-ray diffraction as material characterization technique goes back a long time. Major scientific progress was made by applying X-rays and crystals to study how atoms are organized in crystalline materials. In short, X-ray diffraction studies have had an enormous impact on our understanding of how nature works, just by resolving the crystal structures from anything like simple rock salt to very complex molecules such as DNA, penicillin or insulin.

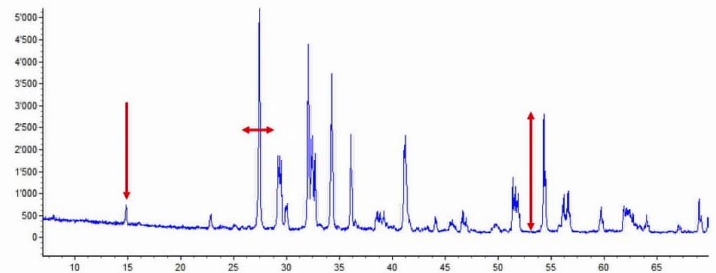
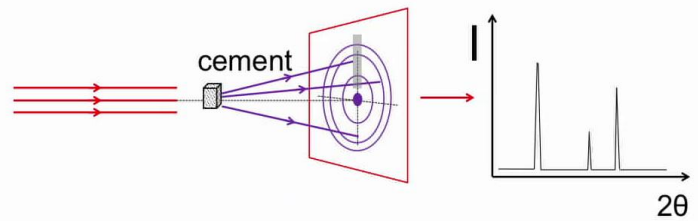
Notes

Summary



0m 04s

X-ray diffraction applied to cement



Similarly X-ray diffraction was applied to study the main phases present in cement such as C3S, C2S, C3A and C4AF. It enables to describe differences in atomic arrangements that underlie large changes in chemical reactivity. One of the most striking examples of this is C2S that changes from very reactive in the alpha form to largely unreactive in the gamma form. A large spectacle impact is that X-ray diffraction data can be used to quantify the composition of complex materials such as cement. This capability has led to widespread application of the powder diffraction technique in research labs. Even more so, its ease of application has led to its introduction as a quality control system in clinker production plants. This course aims to show you how X-ray diffraction really works, how you can properly carry out the measurements and then how you should read, interpret and analyse the collected data to obtain your desired results. This course is aimed at the level of master students, graduate students or professionals that are planning to embark on X-ray diffraction studies to study cement. Preferably, the student has followed introductory courses in chemistry or materials science. Having followed the basic course in crystallography is helpful as well.

Notes

Summary



1m 02s

X-ray diffraction applied to cement



- X-ray diffraction basics and measurements
- Basics on scattering, diffraction and X-rays
- XRD experiments – (demo)
- Qualitative data analysis – (demo)
- Advanced data analysis and applications to cement
- The Rietveld method
- Quantitative phase analysis – (demos)
- Practical guidelines

This lecture series consists of two main parts. In part one the basics of X-ray diffraction are introduced and it is shown how powder diffraction patterns are collected and how one should read and interpret the data. In part two more advanced data analysis methods are explained and demonstrated. In particular, it is shown how X-ray diffraction can be used to quantify the cement phase composition.

Notes

Summary



2m 32s

X-ray diffraction basics and measurements



Introduction and history

Diffraction basics

Inside the diffraction pattern

XRD equipment and measurements

(Sample preparation demo)

Qualitative XRD data analysis

(Phase identification demo)

In part one, X-ray diffraction basics and measurements - this part consists of four sections. First a brief history of X-ray diffraction gives an overview of the underlying principles. Next, the basic features of the powder diffraction pattern are described and it is shown how these features can be related to material properties. Then the third section explains and demonstrates how a laboratory powder diffractometer works and how one should best prepare samples. This will be illustrated with demonstration videos. Finally the principles of qualitative XRD data analysis, or phase identification, are explained and there will be example videos on how to do this in practice.

Notes

Summary



2m 59s



The Rietveld method

(Simple data fitting demo)

Quantitative phase analysis - standard

(Anhydrous Portland cement)

Quantification of amorphous content

(Hydrated and blended cements)

Practical guidelines

Part 2, advanced data analysis and applications to cement, consists of four sections as well. In the first section the principles of quantitative phase analysis by the rietveld method are described and a straightforward demonstration of data fitting is given. In the second section we apply this rietveld method to analyze the phase composition of a Portland cement. Then, even increasing the level of complexity, in the third section we are going to look at how we can cope with samples that contain X-ray amorphous materials such as blast furnace slag or calcium silicate hydrates. This way we can analyze blended cements and even hydrated cements. Several approaches are introduced and practical advantages and disadvantages are discussed. Concrete examples on real samples will be given. Finally, the last section collects and summarizes practical guidelines for data analysis. This will enable you to develop the appropriate measurement and data treatment strategy for your problem.

Notes

Summary



3m 51s

X-ray diffraction applied to cement

XRD is a standard quantitative characterisation tool in the study of cementitious materials

- + Phase assemblage characterisation: quantification of individual phases
- + Straightforward sample preparation
- + Short measurement times
- + Accessible in most material science labs
- + Automated analysis possible (e.g. cement production)
- Accuracy: 2-3 wt.% for major phases, 1-2 wt.% for minor phases (can be better)
- Expert knowledge needed for non-routine analyses

As a wrap up of this introduction, we would like to give you a clear view of what are the main advantages and limitations of X-ray diffraction to study cements. On the one hand, XRD has become a standard material characterization tool because one can characterize the phase assemblage in detail. For instance, one can quantify what happens to individual phases during cement hydration. Further, sample preparation is straightforward and measurement times are short, making the collection of data inexpensive and accessible. And in fact most material science departments or universities have XRD equipment available. Finally, significant progress in software development has made data treatment less tedious and in some case semi-automatic routines can be easily implemented. On the other hand, one should be aware that there are limitations as well. First of all, the accuracy in terms of phase quantification is limited to about two to three weight percent for major phases and around one weight percent for minor phases. Also, one should realize that for non-routine types of analysis, considerable expertise and understanding of the underlying theory is needed. This course really aims to get you started in XRD measurements and also to transfer many practical tips and tricks that usually do not find their way through to the specialized scientific literature, or handbooks on this subject.

Notes

Summary



4m 58s