

Conclusions and perspectives

XRD has become a quantitative characterisation tool in cementitious materials

+ Assets

- + 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)

X-ray diffraction has become a standard characterization tool in cement material science. If properly used, a wealth of information and cement phase composition can be retrieved, both qualitatively and quantitatively. The solids in cement can be quantitatively characterized and sample preparation is rather straightforward. Another advantage is that measurement times are quite short and that XRD equipment is found in most material science labs. Even more so it has found application of quality control of cement production. However, one should realize that cement and hydrated cements are particularly complex multicomponent materials.

Notes

Summary



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Conclusions and perspectives

- **Latest developments**
 1. Spread of Rietveld quantitative phase analysis (software developments – spread of expertise)
 2. New, performant detector systems enable in situ studies, acquisition of large, systematic sets of data
- **Outlook**
 - New and further improved crystal structures
 - Built-in cross-checks/combined analysis with other characterisation techniques
 - Further developments in automation
 - New methods, such as PONKCS to be further developed and adopted

This leads to inherent limitations such as an accuracy which is limited to about 2 to 3 weight percent for major phases such as alite and 1 to 2 weight percent for minor phases. Also, as in many techniques, when one is going beyond the state-of-the-art or the standard practice, it is necessary to develop to some extent some expert knowledge. Definitely X-ray diffraction analysis will find an even broader use and acceptance in the cement science community of the future as many more researchers will have access to the equipment and the supporting data analysis software will definitely become even more performant and user friendly. This will however not mean that the cement inherent challenges and practical problems will disappear. On the contrary, even more attention will need to be given to education and training to safeguard the quality of the results and to realize the full potential of XRD. As an outlook, major changes in XRD analysis and cements are of course difficult to anticipate. However the predictable future path of XRD data analysis will likely involve improvements of current methods and databases to facilitate broader applicability, more automatization and improved reliability, accuracy and precision of the methods.

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In this respect, it is also a new and further improved crystal structure that will be introduced. And this will enable to further enhance the accuracy of the results and widen the scope of samples and problems that can be addressed. It is also to be expected that cross checks of the XRD results, with other independent techniques will become implemented. It will become used more and more and automated in the analysis software packages. On a more methodological level, every quantification methods such as PONKCS, the Rietveld will be developed further and adopted to confront the most challenging systems that remain today out of reach: quantitative phase analysis by X-ray diffraction.

Notes

Summary



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Further reading

- Aranda, M. A. G., Á. G. De la Torre, and L. León-Reina (2012). "Rietveld Quantitative Phase Analysis of OPC Clinkers, Cements and Hydration Products." *Reviews in Mineralogy & Geochemistry* **74**:169–209.
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It is clear that the XRD analysis of cement still has not reached its full potential and that future developments and breakthroughs are still lying ahead.

Notes

Summary



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