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The study of disorder and nanocrystallinity in C–S–H, supplementary cementitious materials and geopolymers using pair distribution function analysis

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ABSTRACT

Significant progress was achieved with the application of Rietveld method to characterize the crystalline phases in portland cement paste. However, to obtain detailed information on the amorphous or poorly crystalline phases, it is necessary to analyze the total scattering data. The pair distribution function (PDF) method has been successfully used in the study of liquids and amorphous solids. The method takes the Sine Fourier transform of the measured structure factor over a wide momentum transfer range, providing a direct measure of the probability of finding an atom surrounding a central atom at a radial distance away. The obtained experimental characteristic distances can be also used to validate the predictions by the theoretical models, such as, molecular dynamics, *ab initio* simulations and density functional theory. The paper summarizes recent results of PDF analysis on silica fume, rice husk ash, fly ash, ASR gel, C–S–H and geopolymers.

Contents

1. Introduction

In this issue of *Cement and Concrete Research*, Bellmann and Stark review the state of the art in the field of cement hydration and microstructure analysis. Our paper presents the fundamentals of total scattering methods and explores how this powerful tool can be used in cement and concrete research to characterize amorphous and poorly crystalline phases. As examples, pair distribution function (PDF) analyses are applied to silica fume, fly ash, rice husk ash, ASR (alkali silica reaction) gel, C–S–H and geopolymers.

In the last century, the ability to determine the atomic structure of complex materials increased exponentially. Study at the atomistic level, which is essential to understanding the basic properties of a material, provides researchers with the tools to create solutions to pressing problems that have previously been dealt with on an *ad hoc* basis because of a fundamental lack of knowledge regarding simple material mechanisms. The periodicity, extended symmetry, and long-range order (LRO) of crystalline materials provided the basis for the development of systematic and quantitative structural analysis methods [1]. Starting from mid-1930 s, x-ray diffraction has been used for quantitative phase analysis of crystalline materials. In the 1970 s, the ground-breaking Rietveld method [2] opened a new, exciting chapter in refinement of crystalline structures. Method uses the whole profile of the powder diffraction pattern, and utilizes the

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