Chapter 21
A Method of 3-D Microstructure Reconstruction in the Simulation Model of Cement Hydration

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ABSTRACT
An accurate and reliable computer simulation system can help practical experiments greatly. In a cement hydration simulation system, the basic requirement is to reconstruct the 3-D microstructure of the cement particles in the initial state while mixed with water. A 2-D SEM/X-ray image is certainly achievable; however, it is not easy to obtain parallel images due to the small scale of the cement particles. In this regard, a method is proposed to reconstruct the 3-D structure from a single microstructure image. In this method, micro-particles are regenerated in a growing trees mode, which by modifying the generating probability of the leaves, the irregularity and the surface fraction of particles can be controlled. This method can fulfill the requirement for the parameters of the 3-D image while assuring that the 2-D image is in full accord.

INTRODUCTION
Today, rapid developing computing technology provides incredible aids in various fields, CAD, CAM, computer simulation etc. An accurate and reliable simulation system can help laboratorial experiments greatly, while replacing practical experiments. The simulation of cement hydration is a novel and reliable approach in studying the properties of cement. Based on scanning electron microscopy (SEM), X-ray technology and powerful computing ability, a digital computer simulation of cement hydration is proposed to represent the procedure of cement hydration in microscope and predict the properties of the concrete to a rather accurate degree. Based on the simulation, a favorable proportion and
maintaining method can be found. While, 2-D images which SEM/X-ray technology mostly offered cannot satisfy the requirement of researching on the relationship between microstructure and properties of cement, the requirement of the researching on the transforming mechanism in physical and chemical procedure. So reconstructing the 3-D microstructure is inevitable. Based on SEM/X-ray technology and digital image processing, we begin with a 2-D SEM/X-ray image, combining with the characteristic of cement particles, label the pixels then reconstruct the 3-D structure ensuring all the parameters in accord with that of the 3-D structure.

In this paper, a method of 3-D reconstruction is introduced, and a tree structure is used to model the structure of cement particles. For each particle, the tree will generate from a root, by choosing the probability of the leaves’ growing condition different shapes of the trees can be achieved. Thus, the shape of particles can be simulated in proper surface fraction, which is most important in the hydration procedure. The probability of the leaves’ growing are discussed and formulated through an experiment, and the relationship between shape and the parameter probability will be found.

The rest of this paper is organized as follows: In the next section, basic knowledge of our research are described, including the application on SEM and X-ray technology on cement microstructure research and the procedure of achieving the 2-D image. Following, the method on 3-D reconstruction and result of the method are being revealed. At last, experimental result will be presented.

**RELATED WORK AND TECHNOLOGY**

**Application of Scanning Electron Microscopy (SEM) and X-Ray Images**

In recent years, the applications of SEM and X-ray images in describing the properties of cement materials have made a great progress (Dale & Paul, 1994; Li, 2000; Bentz, 1993; Wittmann, Roelfstra, & Sadouki, 1984). The SEM and X-ray microscope analyzing technology have been used in recognizing the main phases in Portland cement (Dale & Paul, 1994; Bentz, 1997). In addition to a standard SEM, backscatter electron imaging (BSE) capabilities provide the technicians with a unique advantage in evaluating particle structures. BSE images are used to distinguish between particles based on atomic weight (the brighter the particle image, the heavier the atomic weight) (Dale & Paul, 1994; Li, 2000). X-ray is used to detect and recognize different chemical elements. Combining the BSE and X-ray images of the same sample digital image can be achieved in which different compositions are classified and colored.

**2-D Digital Images of Cement Particles**

Bentz and Stutzman prepared the specimen (Dale & Paul, 1994; Bentz, 1993), using SEM and X-ray technology, as described above, mapping each pixel of a 2-D image into a certain phase in the specimen. First about 25 grams of the cement powder of interest are blended with an epoxy resin to form almost dry paste. The paste is pressed into a sample mold and cured at 60 °C for 24 hours. The cured specimen is cut using a low-speed diamond-wafering saw. Second, sawing marks are easily removed by sandpaper. Finally polishing is done on a lap wheel for about 30 seconds each. The specimen is cleaned after each polishing stage by gently wiping on a clean cloth. The specimen is then coated with carbon to provide a conductive surface for viewing in the SEM. In the BE images, brightness is proportional to the average atomic number of a phase. For the major phases presented in portland cement, the phases from brightest to darkest are tetracalcium aluminoferrite (C₄AF), tricalcium silicate (C₃S), tricalcium aluminate (C₃A) and dicalcium silicate (C₂S), gypsum, and the resin-filled voids. To supplement the information content of the BE image, X-ray