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# Effect of individual phases on multiscale modeling mechanical properties of hardened cement paste

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## HIGHLIGHTS

- The micro mechanical properties were measured by instrumented indentation.
- The effective pore modulus should be 12 GPa in homogenization modeling.
- The clinker modulus variation has minor effect on effective paste modulus.
- The CSH fraction has major effect on effective paste modulus.

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ABSTRACT

As the input parameters in multiscale modeling the effective elastic modulus of the hardened cement paste, the elastic moduli of individual phases are crucial for assuring the accuracy of the homogenization estimate. In this study, the mechanical properties and the fractions of individual phases are measured by nanoindentation and back scattered electron image analysis, respectively. The mechanical properties of the hardened paste at microscale are measured by microindentation. The effect of individual phases including the CSH, the residual clinker and the capillary pore on the effective modulus of the hardened cement paste is quantified. It is found that the effective modulus of pore needs to be set as 12 GPa rather than 0 GPa as the input for homogenization. As for the solid phases, the variation of the clinker modulus has limited influence on the homogenized modulus of the hardened cement paste. Whereas, the homogenized paste modulus increases significantly with the increasing fraction of high density CSH and the decreasing fraction of low density CSH. The results of this study can help to select appropriate input parameters for multiscale modeling the mechanical properties of cementitious materials.


## 1. Introduction

Cement concrete is a type of multiscale and multiphase material [1–3]. In an effort to effectively characterize the multiscale response, the combination of multiscale experimental techniques and modeling methods is expected. For example, utilizing the moduli and the fractions of individual phases measured at sub-microscale as the input parameters, the effective moduli of the hardened cement pastes with different water to cement ($w/c$) ratios, hydration degrees and curing conditions [3–11] can be homogenized by adopting the finite element methods or the micromechanics-based schemes.

The modulus of the individual phase at the sub-microscale has been viewed as one of the key factors for assuring the accuracy of the homogenized results [9]. Different moduli of individual phases have been measured and adopted for the homogenization estimate [3–11]. For example, the moduli of the residual clinkers were normally set to be 125–145 GPa [3–11]. The values were the average modulus of the four major clinker phases (namely, $C_3S$, $C_2S$, $C_3A$ and $C_4AF$) measured by nanoindentation and resonance frequencies technique [12], or the isotropic elastic modulus of fully dense hot-pressed powder compacts of clinkers [13]. The above experiments were conducted on the pure ordinary Portland cement (OPC) clinkers. In hardened paste, the measured moduli of the residual clinkers by nanoindentation were 95–105 GPa [14], which were much smaller than that of the pure OPC clinkers. When homogenizing the effective modulus of the hardened cement paste, adopting the measured moduli of the residual clinkers is more reasonable compared to that of the pure OPC clinkers, as the residual clinkers in hardened paste are more porous than the pure OPC clinkers. However, the moduli of the residual clinkers have been

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rarely used in the homogenization models [14]. As for the CSH, many literatures have viewed the high density (HD) CSH and the low density (LD) CSH as different phases in the homogenization models [3–7], and the moduli of HD-CSH and LD-CSH were set to be 29 GPa and 22 GPa, respectively. These values were measured by nanoindentation [3]. However, there are some literatures which viewed the moduli of HD-CSH and LD-CSH as quite similar [8–11]. The modulus of the CSH was set to be a single value at the range of 22–25 GPa in their homogenization models [8–11]. As for the capillary pore, it was regarded as a part of hydration product [15] or an individual phase with zero modulus [3,5,8] when modeling the homogenized paste modulus.

Although various values of the moduli of individual phases have been adopted in the homogenization models, the discussion about the effect of the individual phase on the homogenized modulus is not found. Moreover, the volume fractions of individual phases can be quantified by the back scattered electron (BSE) image analysis [16], but they have not been used in modeling the homogenized paste modulus. In this study. The techniques of instrumented indentation are adopted to measure the mechanical properties of the individual phases at sub-microscale and the hardened cement paste at microscale. The technique of BSE image analysis is adopted to measure the fractions of the individual phases at sub-microscale. The effective modulus of the hardened cement paste is homogenized based on the Mori-Tanaka scheme and the self-consistent scheme. Finally, the effect of the different homogenization schemes, different moduli and fractions of the individual phases on the effective modulus of the hardened cement paste is discussed.

## 2. Methodology

### 2.1. Multiscale model

It is generally accepted that the microstructure of concrete can be divided into several elementary levels [1–3], which is displayed in Fig. 1.

Level I ($10^{-8}$–$10^{-6}$ m, the CSH scale): The CSH comprises high density (HD) CSH and low density (LD) CSH. At this level, HD-CSH is located in the space confined by LD-CSH. The LD-CSH is viewed as matrix material, while the HD-CSH is viewed as inclusion.

Level II ($10^{-6}$–$10^{-4}$ m, the cement paste scale): The CSH, together with the portlandite crystals (CH), the residual clinker and the capillary pore constitutes the hardened cement paste. At this level, the CSH is viewed as matrix material, while the other phases are viewed as inclusions. A BSE image of the microstructure of the cement paste is displayed in Fig. 1. In this paper, the CH was not detected by its cluster and platelet morphology in BSE images or by its extreme high Ca content in energy-dispersive X-ray spectroscopy (EDS) analysis. The absence of the large CH crystals may be explained by the nanocomposite of the CH and the HD-CSH in the paste with low water to cement ratio proposed by Chen et al. [17]. Therefore, the CH is not considered as a single phase during the homogenization in this paper.

Level III ($10^{-3}$–$10^{-2}$ m, the mortar scale): The mortar at this scale is composed of the cement paste and the fine aggregate. At this level, the cement paste is viewed as matrix material, while the fine aggregate is viewed as inclusion.

Level IV ($10^{-2}$–$10^{-1}$ m, the concrete scale): The concrete at this scale is composed of the mortar and the coarse aggregate. At this level, the mortar is viewed as matrix material, while the coarse aggregate is viewed as inclusion.

The mechanical properties at higher level can be calculated based on that of the individual phases at lower level by the homogenization model. In this study, the effective modulus of the hardened cement paste at level II is calculated based on the moduli and fractions of individual phases at level I.

### 2.2. Homogenization scheme

Micromechanics is a powerful tool to link the mechanical properties of individual phases and that of the hardened cement paste. Based on the classical Eshelby's solution of the ellipsoidal inclusions embedded in a matrix, the Mori-Tanaka (MT) scheme [18] is suitable for matrix-inclusion morphology by selecting the prevailing phase as the matrix, and the self-consistent (SC) scheme [19] is suitable for the perfect disorder morphology by selecting the homogenized medium as the matrix.

Following the continuum micromechanics, the average stress over the representative volume element (RVE) of the material is defined as:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{D}\int_D \boldsymbol{\sigma} dV = \sum_{i=1}^{N} f_i \bar{\boldsymbol{\sigma}}_i \tag{1}$$

where, $f_i$ is the fraction of the $i$ th inclusion. $\boldsymbol{\sigma}$ is the stress tensor of the $i$ th inclusion, and $\bar{\boldsymbol{\sigma}}_i = \frac{1}{\Omega_i}\int_{\Omega_i} \boldsymbol{\sigma} dV$ is the average stress in the $i$ th inclusion.

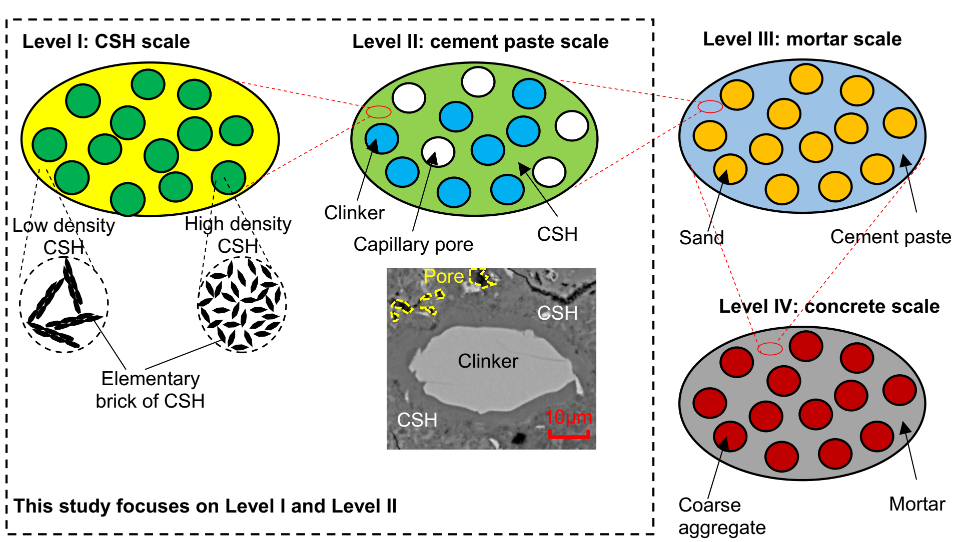


Fig. 1. Multiscale model of concrete.