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Multiscale modeling elastic properties of cement-based materials considering imperfect interface effect

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HIGHLIGHTS

- Homogeneous properties of cement pastes were measured by CMS.
- Combined experimental and theoretical methods were used to determine phase volume fraction.
- Multiscale model considering imperfect interface effect was verified at different scales.
- The imperfect interface can be characterized by interface sliding parameter.
- Curing age and material proportion both affect the imperfect interface property.

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ABSTRACT

Imperfect interface between the inclusions and the matrix has a significant influence on the macro properties of the composites. In this study, the effective elastic properties of cement pastes with water/cement (w/c) ratios of 0.3, 0.4, and 0.5 were homogenized from the calcium silicate hydrate (CSH) scale based on a multiscale model. The perfect and imperfect interfaces between inclusions and the matrix were assumed for the prediction. The imperfect interface is characterized by spring-layers of vanishing thickness in the tangential directions, and an interface sliding parameter (π/d) is used to reflect the imperfection of the interfaces. The predicted results were then compared to the measured one by instrumented indentation as well as the existing data from the literature. It is found that the perfect interface condition would overestimate the elastic modulus of cement-based materials. However, the homogenization scheme with imperfect interface can predict the effective elastic properties very well. This indicates that the imperfect interface may exist in cement-based materials and affect the effective elastic properties. The imperfect interface effect appears to be less significant with increasing curing age and vary with the mix proportion of cement-based materials. Therefore, the imperfect interface conditions should be adopted in the homogenization of the elastic properties for cement-based materials.

1. Introduction

Elastic modulus is one of the most important design parameters for concrete structures due to its significant effect on the stress distribution and deformation of the structures. The upscaling technique has received increasing attention in the field of prediction of elastic properties over the last several decades, because this technique can quantify the interplay between the microscopic and macroscopic properties. With the upscaling technique, one is capable of uncovering the underlying mechanism of cementitious materials and optimizing concrete mixture design. Although there are studies on the prediction of elastic modulus for cement-based materials using the upscaling technique [1–5], investigations in this field are still underway due to the multiscale nature and the complex microstructures of cement-based materials.

Analytical homogenization based on continuum micromechanics has become one of the most popular methods to predict the effective properties of composite materials. Recently, various homogenization schemes have been employed to predict the homogeneous properties of cement-based materials [1,3–5]. However, it should be noted that the inclusions are assumed to be perfectly bonded to the matrix in these homogenization schemes. In practice, imperfect interfaces always exist in composite materials and the interface imperfection has a significant influence on the effective properties of the composite materials [6]. Theoretical research efforts have been made to investigate the influence of the imperfect interface on the mechanical properties of composite

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materials. In the models presented in [7–10], the stresses across the matrix-inclusion interface are assumed to be continuous, while the displacements are discontinuous, and the continuous stresses are proportional to the displacement jumps. Such models have been successfully employed to evaluate the effective properties of composite materials including fiber-reinforced composites [7] and asphalt concrete [10]. Recently, several researchers have reported that an imperfect interface does exist between the matrix and the inclusion in cement-based materials [11–13]. Vandamme and Ulm [14] attempted to predict concrete creep by considering the imperfect interface effect. They found that the creep modulus of concrete would be overestimated significantly by the Mori-Tanaka (M-T) scheme with perfect interface between the matrix and the inclusion. However, a modified M-T scheme that allows interface sliding between the matrix and the inclusion can provide a perfect prediction, indicating that imperfect interfaces may exist in cement-based materials. However, theoretical researches of the imperfect interface effect on the elastic properties of cement-based materials are found rare. Therefore, it is of importance to investigate the effect of the imperfect interface on the elastic properties of cement-based materials.

To predict the effective elastic properties of cement-based materials based on a multiscale model considering imperfect interface effect, it is primarily essential to provide the actual mechanical properties of the individual phase at a finer scale. Instrumented indentation is capable of measuring the micromechanical properties of materials. The mechanical properties including indentation modulus and contact hardness can be determined by analyzing the load (P)-depth (h) curve obtained by instrumented indentation. With the introduction of instrumented indentation into cement-based materials, many researchers have successfully measured the elastic properties of cement-based materials at micro scale [5,14–16]. Another indispensable input parameter for the multiscale model considering imperfect interface effect is the volume fraction of different phases. To date, varieties of experimental methods have been adopted to quantify the microstructure and the volume fractions of different phases in cement-based materials [17]. However, none of them can determine the volume fractions of phases at all scales alone due to the very complex microstructures of cement-based materials. Although theoretical models [1,4] could calculate the volume fractions of different phases at all scales, they might deviate from the actual ones due to the complicated hydration reaction of cement-based materials. Up to date, researchers have attempted to combine the experimental methods and the theoretical models to characterize the microstructures of cement-based materials, it has been found a promising way to quantify the microstructures [18–20].

In this study, the effective elastic properties of cement pastes with w/c ratios of 0.3, 0.4, and 0.5 were predicted based on a multiscale model considering the effect of perfect and imperfect interfaces between the matrix and the inclusions. The predicted results were then compared to the measured elastic modulus. In addition, the elastic properties at the mortar and concrete scales from the literature are also used to verify the predicted results from the multiscale model. Finally, comparison of the homogenized results between the perfect vs. imperfect interfaces was also made.

2. Methodology

2.1. Multiscale model of Cement-based materials

It is widely accepted that cement-based materials are multiscale materials and their heterogeneity manifests themselves at different scales [1]. In this study, the microstructure of cement-based materials is broken down into four levels, which is displayed in Fig. 1.

2.1.1. Level I ($10^{-8} \sim 10^{-6}$ m)

Calcium silicate hydrate (CSH) matrix comprises high-density CSH (HD-CSH) and low-density CSH (LD-CSH). The elastic moduli of these two phases can be measured by nanoindentation. At this level, HD-CSH is located in the space confined by LD-CSH. Then, the homogenized CSH is considered as the matrix material at Level II.

2.1.2. Level II ($10^{-6} \sim 10^{-4}$ m)

The homogenized CSH, together with portlandite crystals (CH), unhydrated clinker, and the capillary pore forms the cement paste. At this level, the homogenized CSH serves as the matrix material, while the other phases serve as inclusions. The elastic moduli of cement pastes can be measured by continuous stiffness measurement. Then, the cement paste is considered as the matrix material at level III.

2.1.3. Level III ($10^{-3} \sim 10^{-2}$ m)

The mortar at this scale is a three-phase composite material composed of cement paste, fine aggregate and the interfacial transition zone (ITZ) surrounding the fine aggregate. The cement paste is considered as the matrix material and the sand serves as the inclusion, while the ITZ is represented by spring-layers of vanishing thickness in this study. Then, the mortar is considered as the matrix material at level IV.

2.1.4. Level IV ($10^{-2} \sim 10^{-1}$ m)

This scale refers to the concrete which is also a three-phase composite material. Similar to the mortar, concrete is composed of mortar, coarse aggregate and the ITZ surrounding the coarse aggregate. The mortar is considered as the matrix material and the coarse aggregate serves as the inclusion. The ITZ surrounding the coarse aggregate is also represented by spring-layers of vanishing thickness. Then, the concrete is treated as a continuum.

Obviously, each level described above is separated from the next one by at least one order of length magnitude, which makes it possible to apply the multiscale model to predict the effective elastic properties of cement-based materials [21].

2.2. Perfect vs. Imperfect interface conditions

Recently, homogenization schemes based on continuum micromechanics are very powerful and popular in evaluating the effective elastic properties of composite materials. However, the homogenization schemes based on continuum micromechanics assume that the inclusions are perfectly bonded to the matrix. However, the imperfect interfaces always exist in composite materials, and the effective properties of composite materials will be significantly influenced by the imperfect interface. Therefore, the imperfect interface properties should be taken into consideration when evaluating the effective properties of the composites. In the homogenization scheme considering the effect of the imperfect interface, the interfacial traction is still continuous, but displacement discontinuity may occur at the interface. The interface conditions are given by [22]:

$$\begin{cases} \Delta\sigma_{ij}n_j \equiv \left[\sigma_{ij}(S^+) - \sigma_{ij}(S^-)\right]n_j = 0 \\ \Delta u_i \quad\ \equiv \left[u_i(S^+) - u_i(S^-)\right] = \eta_{ij}\sigma_{jk}n_k \end{cases} \tag{1}$$

where n_j is the unit outward normal vector of the interface S, $\sigma_{ij}(S^+)$ and $\sigma_{ij}(S^-)$ are the values of $\sigma_{ij}(x)$ as $\boldsymbol{x}$ approaches the interface from outside and inside of the inclusion, respectively, so are $u_i(S^+)$ and $u_i(S^-)$; $\boldsymbol{x}$ is the position vector; $\Delta\sigma_{ij}$ and Δu_i are the difference of