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Micromechanics constitutive modelling and optimization of strain hardening geopolymer composite

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A B S T R A C T

This paper investigates the micromechanics constitutive modelling and optimization of a fiber-reinforced strain-hardening geopolymer composite (SHGC) recently developed by the authors. Micromechanical parameters of the developed fly ash-based SHGC were independently measured or deduced to compute the analytical crack bridging (σ-δ) relation of the composite. The predicted σ-δ relation was compared with the experimental test results. It was confirmed that the previously developed micromechanics-based model can reasonably predict the σ-δ relation of fly ash-based SHGCs. Using the verified model, a parametric study was then performed to evaluate the effects of fiber length, fiber surface oil-coating, and matrix fracture toughness on critical (minimum) fiber content required to exhibit saturated pseudo strain-hardening (PSH) behavior. The results indicated that the critical fiber content in fly ash-based SHGCs is mainly governed by the energy-based criterion. It was demonstrated that the fiber surface oil coating, the increase of fiber length and the reduction of matrix fracture toughness are effective approaches to reduce the critical fiber content. Using the model, it was demonstrated that fly ash-based SHGCs can be systematically optimized by proper tailoring of the material constituents to achieve saturated PSH behavior with the lowest amount of fiber, and thereby the lowest cost.

1. Introduction

According to European Cement Association (CEMBUREAU) [1], the world cement production has increased drastically over the recent years to 4.3 billion tons in 2014, compared to only about 10 million tons in 1900. It is reported that about 5–7% of total CO_2 emissions worldwide is associated with the cement production [2]. Therefore, the investigation on sustainable alternatives to ordinary Portland cement (OPC) is a rapidly advancing field of research area. Geopolymer is an amorphous aluminosilicate material purported to provide a sustainable alternative to OPC. Geopolymers are synthesized at ambient or elevated temperature by alkali activation of aluminosilicate source materials such as fly ash and slag [3]. Previous studies reported that manufacture of fly ash-based geopolymer requires approximately 60% less energy and emits at least 80% less CO_2, as compared to OPC production [4,5]. Geopolymer concrete exhibits superior mechanical, thermal and chemical properties to “conventional” OPC-based concrete [6]. However, similar to the OPC-based concrete, geopolymer concrete is also inherently brittle and susceptible to cracking, which should be suppressed to promote its widespread application.

To overcome the inherent brittleness of geopolymer, series of investigations have been recently conducted to develop high ductile fiber-reinforced geopolymer composites, demonstrating strain-hardening behavior under direct tension [7–11]. Ohno and Li [7] developed a fly ash-based strain-hardening geopolymer composite (SHGC) reinforced by oil-coated poly vinyl alcohol (PVA) fibers. The developed SHGC demonstrated low to moderate compressive and tensile strengths (of up to 27.6 MPa and 3.4 MPa, respectively), with very high tensile strain capacity (of up to 4.3%). The researchers at Swinburne University of Technology, Australia demonstrated that high compressive and tensile strengths (of up to 63.7 MPa and 5.0 MPa, respectively) can be achieved in fly ash-based PVA-SHGC, while maintaining the high tensile strain capacity (of up to 4.3%) [9,10]. The environmental impact calculation verified that the developed fly ash-based PVA-SHGC is an environmentally friendly and sustainable alternative to “conventional” strain-hardening cementitious composite (SHCC), offering 52% less carbon emission and 17% less energy consumption [11]. Although the developed fly ash-based SHGC has remarkable mechanical properties and environmental advantages, its material cost is relatively higher than that of “conventional” concrete,

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which may limit its widespread application. The higher initial material cost of fly ash-based SHGC over "conventional" concrete is mainly due to use of PVA fibers. Although the cost of PVA fiber is substantially lower than that of high strength and high modulus poly ethylene (PE) fiber [12], the cost of oil-coated PVA fibers is still relatively high compared to other synthetic fibers. Therefore, it is essential and beneficial to understand how fly ash-based SHGCs can be designed to achieve optimal composite performance with the lowest fiber content, and thereby the lowest cost.

Fiber-bridging behavior plays a significant role in the tensile performance of fiber-reinforced brittle matrix composites. Therefore, it is essential to appropriately control the fiber-bridging behavior of the composite to successfully design and optimize fly ash-based SHGCs to exhibit optimal performance, while using minimum fiber content. Some analytical fiber-bridging models have been previously proposed for design and optimization of SHCCs [13–15]. These micromechanics-based models link composite properties to material microstructures, including matrix, fiber and fiber-matrix interface. They are used as powerful analytical tools to tailor the material constituents [12]. The first objective of this study is to ascertain whether the previously developed micromechanics model developed by Yang et al. [15] for SHCC can predict the fiber-bridging behavior of fly ash-based SHGCs. The second objective is to demonstrate how the model can effectively guide towards systematic optimization and component tailoring of fly ash-based SHGC to achieve saturated pseudo strain-hardening (PSH) behavior with the lowest amount of PVA fiber, and thereby the lowest cost.

This paper at first briefly reviews the micromechanics-based design framework for strain-hardening behavior, along with fiber-bridging constitutive law and micromechanics-based modelling in randomly oriented short fiber-reinforced brittle matrix composites. A micromechanical investigation was conducted to achieve the first objective of the study. The investigation involved determination of fiber-matrix interface properties and matrix fracture properties using single-fiber pullout tests and matrix fracture toughness tests, respectively. The micromechanical properties inferred from the experimental tests were then used as input parameters in the statistical scale-linking model [15] to analytically compute the fiber-bridging constitutive law (σ-δ relation) of fly ash-based SHGC. To verify the model, the computed σ-δ relation of the composite was compared with the experimentally observed uniaxial tension test results. Using the verified model, a parametric study was performed to achieve the second objective of the study. The effects of fiber length, fiber surface oil-coating, and matrix fracture toughness on the critical volume fraction of fiber were investigated via the parametric study.

2. Micromechanics-based design framework for strain-hardening behavior

The PSH behavior in short fiber-reinforced brittle matrix composite is a consequence of multiple cracking of the matrix, which can be achieved if steady-state flat crack extension governs the cracking behavior under tension [15]. The steady-state cracking requires crack tip toughness to be less than the complementary energy. This condition presented in Eq. (1) is often known as energy-based condition for the PSH behavior.

$$J_{tip} \le \sigma_0\delta_0 - \int_0^{\delta_0} \sigma(\delta)d\delta \;\equiv\; J_b' \tag{1}$$

where J_b' is the complementary energy calculated from the bridging stress-crack opening σ(δ) curve and J_{tip} is the crack tip toughness, which can be approximately determined from the following equation for small fiber content:

$$J_{tip} = \frac{K_m^2}{E_m} \tag{2}$$

where E_m is the matrix elastic modulus and K_m is the matrix fracture toughness [16].

The second condition for the PSH behavior, often known as the strength-based condition, requires that a micro-crack starts from a defect site when the load is less than the bridging capacity of the fibers. This condition is presented in Eq. (3).

$$\sigma_{fc} \le \sigma_0 \tag{3}$$

where σ_0 is the maximum fiber bridging stress and σ_{fc} is the first cracking strength of the composite under direct tension. Satisfaction of both conditions is compulsory to achieve the PSH behavior.

Kanda and Li [17] recommended two PSH performance indices, viz. strength-performance index (PSH strength=σ_0/σ_{fc}) and energy-performance index (PSH energy=J_b'/J_{tip}) to quantitatively evaluate the margin between σ_0 and σ_{fc}, as well as J_b' and J_{tip}. In theory, both performance indices must be greater than one to achieve the PSH behavior. Higher values of the performance indices indicate greater possibility of saturated PSH behavior, resulting in higher tensile strain capacity [17].

3. Fiber-bridging constitutive law and micromechanics-based modelling of randomly oriented short fiber-reinforced brittle matrix composite

The relationship between the fiber bridging stress (σ) transferred across a matrix crack and the opening of that crack (δ) can be expressed in terms of the fiber-bridging constitutive law (σ-δ relation) of the composite [18]. Understanding the σ-δ relation is of primary importance in development of strain-hardening composites. It is because on the one hand, the σ-δ relation relates to material microstructure (micro-scale), and on the other hand it governs the composite tensile performance (macro-scale) [18]. The σ-δ relation of a composite is expressed as a function of matrix, fiber and interface related micromechanical parameters.

The micromechanical parameters related to the fiber include fiber length (L_f), diameter (d_f), elastic modulus (E_f), tensile strength (σ_{fu}) and volume fraction (V_f). Matrix fracture toughness (K_m) and elastic modulus (E_m) are considered as the matrix-related micromechanical parameters. The fiber-matrix interface is characterized in terms of frictional bond strength (τ_0), chemical bond strength (G_d), slip-hardening coefficient (β), snubbing coefficient (f) and fiber strength reduction factor (f′). τ_0 quantifies the interface friction force at the onset of fiber slippage. G_d describes the fracture energy required for chemical debonding of the fiber from surrounding matrix [18]. β is to characterize the fiber sliding behavior, which can be either slip-hardening, constant friction or slip-softening [19]. f is introduced to account for fiber orientation effect on the fiber pullout load [16]. The load needed to pull out an inclined fiber from a matrix crack can be higher than that of a straight fiber (with zero inclination). The increase in pullout load is attributed to the additional frictional snubbing force and the bending of the fiber at the corner of exit from the matrix [20]. f′ is introduced to account for reduction of fiber strength when pulled out at an inclined angle, which can be attributed to fiber surface abrasion, spalling of the matrix foundation and fiber bending, all of which are intensified with higher inclination angles [21]. It has been reported that hydrophilic fibers (such as PVA fiber), even with no inclination, exhibit lower tensile strength in a pulled-to-rupture test when embedded in a matrix than in the standard fiber strength test (i.e. the fixed-end strength test). In other words, the in-situ tensile strength of a fiber embedded in a matrix (apparent fiber strength) is lower than the nominal strength of the fiber reported by the manufacturer [21].

The σ-δ relation of a composite can be computed via analytical fiber-bridging models. Yang et al. [15] developed an analytical model on the basis of fracture mechanics, micromechanics, and probabilistics