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A Microstructure-guided Numerical Approach to Evaluate Strain Sensing and Damage Detection Ability of Random Heterogeneous Self-sensing Structural Materials

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Abstract: Heterogeneous self-sensing materials that respond electrically to mechanical strains enable real time health monitoring of structures. To facilitate design and applicability of such smart materials with piezo-resistivity, a finite element-based numerical framework is being proposed in this paper for evaluation of electro-mechanical response and strain-sensing ability. Intrinsic heterogeneous nature of such composites warrants the need for microstructure-based study to have an insight into the effect of microstructural configuration on the macro-scale response. The microstructure-guided simulation framework, presented in this paper, implements interfacial debonding at the matrix-inclusion interface using a coupled interface damage-cohesive zone model and incorporates an isotropic damage model in the matrix under applied strain in the post-peak regime to obtain the deformed/damaged microstructure which is subjected to an electrical potential to simulate change in resistance due to applied strain. The applicability of the simulation framework is confirmed through its successful implementation on a smart structural material containing nano-engineered conductive coating at the inclusion-matrix interfaces. The predicted electro-mechanical responses correspond very well with the experimental observations and thus, the model has the potential to help develop design strategies to tailor the microstructure in these self-sensing materials for efficient performance.

Keywords: Piezo-resistivity; strain sensing; Cohesive zone model; continuum damage; microstructural model

1. INTRODUCTION

Structural Health monitoring (SHM) provides valuable information on the reliability and safety of the structures and it can help develop strategies to save the structures before critical damage threatens the structural integrity [1,2]. Strain- and damage-sensing are integral aspects of SHM. Most of the load-bearing structures are very sensitive to damage and it can cause catastrophic failures leading to immense loss of life and property [1,3]. Therefore costly routine inspections have been used for maintenance of these structures. Traditionally, various non-destructive testing (NDT) techniques such as ultrasound testing, radiographic tests (X-ray) etc. have been used, although they are impractical and expensive for large structures. Thus, there has been a need for a real-time mixed global/local damage-sensing approach. For real-scale industrial structures, use of smart composites is gaining popularity in recent times for strain-sensing in structures [4–6]. In particular, such smart composites achieve damage-sensing capability by utilizing piezoresistivity which is an electromechanical phenomenon that enables certain electrically conductive composites to respond electrically under the influence of strain [7–14]. Electrical resistance methods in these composites have been shown to be sensitive to minor and microscopic changes that include defects or damage [10,14–16]

Design of such smart materials requires a reliable numerical method that can predict electro-mechanical response at different length scales. This paper presents a comprehensive microstructure-guided electro-mechanical response prediction framework for a large class of smart heterogeneous materials using finite element modelling. In particular, the numerical framework is applied towards prediction of strain-sensing efficiencies in smart cementitious composites for infrastructure applications. In cement-based materials self-sensing capability has been achieved using carbon fibers, steel fibers and carbon nanotubes [7,9,14,17]. Although a variety of experimental studies [8–15,18] report on electro-mechanical response of these systems under tension and compression, limited studies exist on prediction of strain-sensing and damage-detection efficiency in such self-sensing cementitious materials which is the primary goal of this research paper. The numerical simulation framework, presented in this paper, is developed for the first time in order to incorporate an applied strain range that encompasses both the elastic and the post-peak constitutive behavior thereby achieving both strain and damage sensing by electrical measurements in these cementitious matrices. The modelling scheme involves: (1) generation of representative microstructure of the heterogeneous composite using a stochastic packing algorithm; (2) application of periodic boundary conditions [19–23] in the representative unit cell to simulate a strain-controlled mechanical test scenario; (3) incorporation of interface damage to simulate interfacial debonding at the

inclusion-matrix interface; (4) incorporation of an isotropic damage theory for damage in the matrix in the post-peak regime; (5) determination of effective constitutive behavior of the heterogeneous material; (6) re-meshing the deformed/damaged geometry corresponding to any specific applied strain and (7) determination of electrical response of the damaged/deformed microstructure. Steps 6 and 7 are performed for strains both in the elastic and the post-peak regime to obtain change in electrical responses for all the applied strains. The versatility of this approach is verified on a smart self-sensing cementitious material enabled by nano-engineered matrix-inclusion interface [24]. This smart material uses thin multi walled carbon nanotube (MWCNT)-based polymeric films at the matrix-inclusion interface [15,16,24]. Thus, this paper intends to demonstrate a numerical framework to evaluate the strain- and damage-sensing efficiency of several heterogeneous materials facilitating microstructure-guided material design.

2. NUMERICAL SIMULATION FRAMEWORK FOR ELECTRO-MECHANICAL RESPONSE EVALUATION AND DAMAGE DETECTION

This section describes the framework which executes numerical simulation to evaluate electro-mechanical response of self-sensing materials using finite element analysis (FEA). Influence of damage and damage-sensing capability of the material is efficiently integrated into the simulation framework. Figure 1 summarizes the numerical simulation framework using a flowchart representation.

Figure 1: Flowchart of numerical simulation framework

The framework involves generation of a representative unit cell and evaluation of electromechanical responses implementing mechanical and electrical modules. The analysis framework is implemented here using a python script for ABAQUS™ solver. The mechanical module simulates a mechanical response of the unit cell under externally applied uniaxial strain and it accounts for interface damage at the matrix-

inclusion interface. In addition, the mechanical module implements constitutive behavior of heterogeneous composites beyond the cracking strain (post-peak response) by implementing an isotropic damage model [25–27] in the matrix through a user-defined subroutine in ABAQUS™ [28–30]. An intermediate remeshing module imports the deformed configuration of the unit cell, obtained from the mechanical module and improves the quality of mesh before exporting the re-meshed unit cell to the electrical module as a starting geometry for the electrical analysis in order to achieve electro-mechanical response of the unit cell under applied strain. The electrical module obtains the deformed configuration of the unit cell from the remeshing module and obtains current distribution in the deformed unit cell under imposed electrical potential. Post processing of the relevant electrical responses in MATLAB© yields a homogenized change in electrical resistivity under different applied strains. Different components of the framework are detailed in the forthcoming sub-sections.

2.1 Generation of Representative Unit Cells

The unit cells are generated here using the Lubachhevsky-Stillinger algorithm [31–33]. This algorithm employs a hard contact model and hence particle overlaps are not allowed. First, the desired inclusions are randomly distributed inside the periodic bounding box with random initial velocities of the particles. The radius of each particle is first initialized as zero. The radius of i^{th} particle (r_i) in the next event is a function of the growth rate (g_i), which is tailored to attain the desired particle size distribution shown in Equation 1.

$$\frac{dr_i}{dt} = g_i \quad (1)$$

Here $i = 1, 2, \dots$ is the number of particles. The growth rate between time t^n and t^{n+1} is computed using a finite difference scheme as follows.

$$g_i = \frac{(r_i^{n+1} - r_i^n)}{\Delta t} \quad (2)$$

Where r_i^{n+1} and r_i^n are radius at time t^n and t^{n+1} respectively and $\Delta t = (t^{n+1} - t^n)$. The particle radii are then updated as follows for time t^{n+1} by employing the growth rate and time increment (Δt) as follows.

$$r_i^{n+1} = r_i^n + g_i \Delta t \quad (3)$$

In addition, the position of particle ' i ' at time t^{n+1} i.e. $\mathbf{x}_i^{n+1}$ is updated considering a constant velocity ($\mathbf{v}_i^n$) between the time nodes.

$$\mathbf{x}_i^{n+1} = \mathbf{x}_i^n + \mathbf{v}_i^n \Delta t \quad (4)$$

The vector that connects the centers of particles 'i' and 'j' is obtained by subtracting the position vectors of the two particles.

$$\mathbf{I}_{ij}^{n+1} = \mathbf{x}_j^{n+1} - \mathbf{x}_i^{n+1} \quad (5)$$

The particles 'i' and 'j' are expected to be in contact if the sum of their radii is equal to the length of the connection vector. The time step size can be calculated as follows and the formulations are adequately detailed in [34].

$$\Delta t = \min \left[\frac{-v \pm \sqrt{v^2 - uw}}{u} \right] \quad (6)$$

where $\Delta t > 0$ and v, u and w are given as

$$v = \mathbf{I}_{ij}^n \cdot [\mathbf{v}_j^n - \mathbf{v}_i^n] - [r_i^n + r_j^n][g_i + g_j] \quad (7a)$$

$$u = [\mathbf{v}_j^n - \mathbf{v}_i^n]^2 - [g_i + g_j]^2 \quad (7b)$$

$$w = \mathbf{I}_{ij}^{n^2} - [r_i^n + r_j^n]^2 \quad (7c)$$

Here, $\mathbf{v}_i^n$ and $\mathbf{v}_j^n$ are the velocities of particles 'i' and 'j' at time t^n . r_i^n and r_j^n are the radius of particles 'i' and 'j' at time t^n . g_i and g_j are growth rates for particle 'i' and 'j' respectively. The vector connecting the position of the two particles at time t^n is given as $\mathbf{I}_{ij}^n = \mathbf{x}_j^n - \mathbf{x}_i^n$. The time step calculation (Equation 6) is performed for each particle pair that are being able to collide and thus minimum time step for all the possible collisions is adopted to move forward for the next event. All the particle positions $\mathbf{x}_i^{n+1}$ are updated using the forward Euler scheme (Equation 4) and new search for the next collision(s) is started. The post-contact velocities are computed as follows.

$$v_{n_i}^{n+1+} = \min\{v_{n_i}^{n+1-}, v_{n_j}^{n+1-}\} - g_i ; v_{n_j}^{n+1+} = \max\{v_{n_i}^{n+1-}, v_{n_j}^{n+1-}\} + g_i \quad (8)$$

Where $v_{n_i}^{n+1+}$ is the velocity after the contact and $v_{n_i}^{n+1-}$ is the velocity before the contact. Thus, all the above-mentioned steps are repeated and in the process of iterations the particles change position in the bounding box, collide and grow in order to obtain desired volume fraction. The algorithm is iterated until the target volume fraction of inclusions is reached. The algorithm is terminated as soon as the volume of the inclusions reaches the target volume fraction implying no further update on the relative positions or velocities of the particles. For the matrix, a homogenous solid section is generated, and the solid cut matrix is obtained by the difference of geometric areas of the solid matrix and the inclusions. Now, the solid cut matrix and inclusions are geometrically stitched at the boundaries to yield an inclusion embedded matrix geometry. Finally, the obtained microstructural information is implemented via a python language script to enable it to be imported to a commercial finite element software.

2.2 Mechanical module

The mechanical module implements periodic boundary conditions [35,36], meshes the unit cell, implements interfacial damage at the inclusion-matrix interface and incorporates isotropic damage in the matrix in the post-peak regime as described in the following sub-sections.

2.2.1 Boundary condition

Once the unit cell is generated, it is imported to the mechanical module. The mechanical module is summarized in Figure 2. The unit cell is first meshed using the python script and Periodic boundary conditions (PBC) [19–21] are applied. PBCs have been applied successfully towards FE analysis of random heterogeneous materials [37]. Periodic boundary conditions are shown to be computationally efficient even with smaller size of unit cells facilitating faster convergence [33]. PBC ensures displacement and traction continuity across the boundaries of neighboring unit cells. In 2D, periodic microstructure the displacement field is given as follows.

$$v_i(x_1, x_2) = \varepsilon_{ij}^0 x_j + v_i^*(x_1, x_2) \quad (9)$$

Here, ε_{ij}^0 is the applied strain tensor, and v_i^* is a periodic function representing the modification of linear displacement field due to the heterogeneous microstructure. On a pair of parallel opposite boundary edges the displacements are given as follows.

$$v_i^{s+} = \varepsilon_{ij}^0 x_j^{s+} + v_i^* \quad (10a)$$

$$v_i^{s-} = \varepsilon_{ij}^0 x_j^{s-} + v_i^* \quad (10b)$$

Here, s^+ and s^- are s^{th} pair of two opposite parallel boundary surfaces of the unit cell. The periodic function v^* is the same at both the parallel opposite edges due to periodicity. Subtracting 10b from 10a the difference in displacements on two parallel edges are obtained as follows.

$$v_i^{s+} - v_i^{s-} = \varepsilon_{ij}^0 (x_j^{s+} - x_j^{s-}) = \varepsilon_{ij}^0 \Delta x_j^s \quad (11)$$

Δx_j^s is constant for an applied ε_{ij}^0 . The strain is applied on the unit cell using the system of equations through a reference point. The general form of system equations can be written as follows.

$$v_i^{s+} - v_i^{s-} + v_i^{\text{dummy}} = 0 \quad (12)$$

Such linear equations are implemented for all parallel face pairs in 3D unit cells. Strain is applied on the unit cell through the constraint equations to simulate a strain-controlled test scenario. More details on the PBC can be found in [34,38].

2.2.2 Incorporation of Interfacial Debonding

The mechanical module incorporates interfacial debonding at the inclusion-matrix interface. The interfacial debonding is implemented here using a continuum damage model coupled with cohesive zone model (CZM) [39–41]. Here, a continuity in displacement is ensured by implementation of zero-thickness interface elements. Such zero-thickness interface elements have been implemented successfully to model relative slip or separation on a predetermined surface in [42,43]. The theoretical framework of CZM involves a phenomenological model of failure where the assumed fictitious micro-cracks in the cohesive zone can exhibit interactive stresses, thereby enabling application of traction-separation law [44,45]. The separation in the traction-separation law is characterized here using an equivalent interface opening (λ). Here, λ consists of positive normal displacement jump $\langle \llbracket u_n \rrbracket \rangle$ and tangential displacement jump $\llbracket u_t \rrbracket$ across the zero-thickness interfacial elements as shown in Equation 13.

$$\lambda = \sqrt{\langle \llbracket u_n \rrbracket \rangle^2 + \llbracket u_t \rrbracket^2} \quad (13)$$

The characteristic value of equivalent interface opening, λ_0 denotes the limit beyond which the traction at any interface element decreases with increasing λ . When $\lambda < \lambda_0$, the equivalent traction σ_c is expressed using a penalty stiffness K_p as follows.

$$\sigma_c = K_p \lambda \quad (14a)$$

when $\lambda \geq \lambda_0$, the following relationship is implemented [43,46].

$$\sigma_c = f_t \exp \frac{-f_t(\lambda - \lambda_0)}{G_F} \quad (14b)$$

Where f_t is the tensile strength and G_F is the total fracture energy. $\lambda_0 = \frac{2G_f}{f_t} = \frac{f_t}{K_p}$ Where initial fracture energy, $G_f = \frac{K_{IC}^2}{E}$, K_{IC} is the mode-I fracture toughness and E is the Young's modulus.

The equivalent traction is integrated over the volume to obtain the potential ϕ , the partial derivatives of which with respect to normal and tangential components of the displacement jump yield the normal traction t_{cn} and tangential traction t_{ct} respectively as shown in Equation 15.

$$\mathbf{t}_c = \begin{pmatrix} t_{cn} \\ t_{ct} \end{pmatrix} = \begin{pmatrix} \frac{\partial \Phi}{\partial \llbracket u_n \rrbracket} \\ \frac{\partial \Phi}{\partial \llbracket u_t \rrbracket} \end{pmatrix} \quad (15)$$

The mechanical tangent material matrix C_c^u can be expressed as partial derivatives of the resulting traction with respect to displacement jump as shown in Equation 16.

$$C_c^u = \begin{bmatrix} \frac{\partial t_{cn}}{\partial \llbracket u_n \rrbracket} & \frac{\partial t_{cn}}{\partial \llbracket u_t \rrbracket} \\ \frac{\partial t_{ct}}{\partial \llbracket u_n \rrbracket} & \frac{\partial t_{ct}}{\partial \llbracket u_t \rrbracket} \end{bmatrix} \quad (16)$$

It should be noted here that the above formulations are applied for tension, when the interface opening in the normal direction is positive. In case of compression the normal interface compressive pressure is given as follows.

$$t_{cn} = K_p \llbracket u_n \rrbracket \quad (17)$$

Therefore, the mechanical tangent material matrix can be expressed as follows.

$$C_c^u = \begin{bmatrix} K_p & 0 \\ 0 & \frac{\partial t_{ct}}{\partial \llbracket u_t \rrbracket} \end{bmatrix} \quad (18)$$

The tangent material matrix C_c^u is transformed to the local co-ordinate system to obtain stiffness matrix of each cohesive element. While the penalty stiffness governs the traction-separation law with increase in λ when $\lambda < \lambda_0$, the mechanical stiffness matrix is modified at every iteration with increasing λ based on phenomenological damage model when $\lambda \geq \lambda_0$. Damaged mechanical stiffness matrix for interface elements obtained is used as the initial stiffness of the cohesive elements in the next step with increment in λ . Here, progressive debonding has been characterized with increasing λ using a scalar interface damage parameter D_c which is defined as follows.

$$D_c = \frac{\lambda}{\lambda_{cr}} \quad (19)$$

Where λ_{cr} corresponds to equivalent interface opening at very low traction values in the post-peak regime of the traction-separation behavior, generally computed at $0.1 f_t$ in the post-peak regime [43]. The numerical simulation of the CZM extended damage model, as explained above, is implemented here using user-defined subroutine in ABAQUSTM and it requires initial fracture energy (G_f), total fracture energy (G_F) and tensile strength of matrix (f_t) as input [47].

2.2.3 Damage in the matrix

In order to incorporate damage in the matrix in the post-peak regime, a damage module is incorporated inside the mechanical module. A continuum damage model is implemented here in the matrix once the applied strain exceeds the elastic limit (ε_{EL}). Assuming isotropic stiffness degradation, the damage variable, D is given as [25–27,48] follows.

$$\sigma = (1 - D)C:\varepsilon \quad (20)$$

Where the effective stress tensor is denoted by σ , C denotes fourth order tensor of elasticity and ε is the strain tensor. The value of damage, D ranges from 0 (undamaged) to 1 (completely damaged). The damage rate denoted by $\dot{D}$ assumes only zero or positive values which can be explained by its proportionality with the damage energy release rate [25]. The overall damage D is a weighted sum of its tensile and compressive parts (D_t and D_c) that addresses the difference in tensile and compressive behavior of heterogeneous materials as shown in Equation 21 [25,26].

$$D = \alpha_t D_t + \alpha_c D_c \quad (21)$$

For uniaxial tension value, of the parameter α_t becomes 1 and the parameter α_c becomes zero whereas the values of the parameters α_t and α_c are taken as zero and 1 respectively for uniaxial compression [25]. A non-local equivalent strain $\tilde{\varepsilon}$ is used to obtain the tensile and compressive damage, D_t and D_c respectively which is defined as follows [25,48].

$$\tilde{\varepsilon} = \sqrt{\sum_i <\varepsilon_i>_+^2} \quad (22)$$

Where $<\varepsilon_i>_+$ is the positive part of the principal strain. The damage D_t and D_c evolve as a function of $\tilde{\varepsilon}$ as per the Equation 23-a and 23-b follows [25–27,48,49].

$$D_t(\tilde{\varepsilon}) = 1 - \frac{\varepsilon_{D_0}(1 - A_t)}{\tilde{\varepsilon}} - \frac{A_t}{\exp[B_t(\tilde{\varepsilon} - \varepsilon_{D_0})]} \quad (23-a)$$

$$D_c(\tilde{\varepsilon}) = 1 - \frac{\varepsilon_{D_0}(1 - A_c)}{\tilde{\varepsilon}} - \frac{A_c}{\exp[B_c(\tilde{\varepsilon} - \varepsilon_{D_0})]} \quad (23-b)$$

Where ε_{D_0} is damage initiation threshold (the ratio of tensile strength to the Young's modulus for quasi-brittle materials). The model can be fitted to experimentally obtained uniaxial tensile and compressive constitutive response of various matrices to obtain corresponding values for the parameters ε_{D_0} , A_t , B_t , A_c and B_c . The material continuum damage is implemented here using user defined subroutine in

ABAQUS™ [30]. The mechanically deformed/damaged geometry thus obtained is exported to re-meshing module to improve the quality of mesh as explained in the forthcoming section.

Figure 2. Schematic representation of the mechanical module

2.3 Intermediate Re-meshing Module

The deformed or damaged geometry of the unit cell, obtained from mechanical module, is re-meshed using this intermediate module. This module implements remeshing using a MATLAB subroutine. The subroutine operates on the deformed geometry and performs re-meshing/ mesh-refinements wherever

the aspect ratio of the elements exceeds 3. The remeshing module, thus improve the quality of mesh in the deformed/damaged unit cell. The re-meshed deformed or damaged unit cell is then exported to the electrical module for electrical analysis.

2.4 Electrical module

The electrical module imports the deformed and re-meshed unit cell and assigns electrical properties to the component phases. In order to characterize the electrical response of the damaged unit cell, the damaged elements in the matrix are modeled with an electrical conductivity that decreases proportionally with the mechanical damage variable D . The electrical conductivity of the damaged elements (σ_i) can be expressed in terms of the initial conductivity (σ_{i-1}) as follows.

$$\sigma_i = (1 - D)\sigma_{i-1} \quad (24)$$

Similar relationships have been successfully implemented for thermal analyses coupled with mechanical damage elsewhere [43,50]. At every state of progressive damage, the conductivity is reduced proportional to the damage variable D . As the material damages fully, the simulation framework theoretically assumes an infinite resistance. In order to characterize the electrical behavior of the mechanical damage on the inclusion-matrix interface, the interface elements where the interface damage variable (D_c) reaches 1, are considered a perfect resistor with infinitely high electrical resistance.

After assignment of material properties, boundary conditions are incorporated. All other faces except the ones perpendicular to Y axis are insulated as can be seen in Figure 3. A unit potential is applied across the microstructure in the Y direction as shown in Figure 3. The electrical module computes current density ($\bar{J}$) from the input electrical conductivity(σ) of component phases and the applied electric field ($\bar{E}$) using Ohm's Law ($\bar{J} = \sigma \bar{E}$). The simulation yields the electric field and current density distribution in the unit cell which when volumetrically averaged by a post-processing module yields the average electrical conductivity as per Equation 25 [51,52].

$$\sigma = \frac{\bar{J}}{\bar{E}} \quad (25)$$

For a comparative representation, the average electrical conductivities (σ) are expressed in terms of the fractional change in resistance (FCR) which is the ratio of the change in resistance (ΔR) and the bulk resistance of mechanically undeformed microstructure (R_0) as shown in Equation 26 [51].

$$FCR = \frac{\Delta R}{R_0} = \frac{\sigma_0}{\sigma} - 1 \quad (26)$$

Where σ_0 is the conductivity response of the mechanically undeformed microstructure. In order to characterize the electrical response of the damaged microstructure, the damaged elements are modeled as insulators as explained earlier. The additional resistivity thus imparted to the overall microstructure leads to a different trend in FCR plotted with strain beyond the elastic limit.

Figure 3. Schematic representation of the electrical module

The microstructure guided electro-mechanical simulation can be performed at different length scales so as to obtain macro-scale electro-mechanical response of heterogeneous smart materials. The numerical simulation framework, presented herein, can be used towards prediction of macroscopic electro-mechanical response of several random heterogeneous smart materials facilitating microstructure-guided material-design. In the forthcoming section, the numerical prediction scheme is applied to a smart cementitious material enabled by a nano-engineered matrix-inclusion interface to evaluate the effectiveness of the modelling framework.

3. APPLICATION OF THE MODEL TO A SMART STRUCTURAL MATERIAL CONTAINING NANO-ENGINEERED INCLUSION-MATRIX INTERFACES

This section describes the application of the aforementioned framework to a smart self-sensing cementitious material enabled through a nano-engineered cement-aggregate interface [16,24]. Such

conductive coatings contain carbon nanotube (CNT) based thin latex films, the synthesis and application procedure of which is discussed in detail in [15,53]. These films are deposited on sand via airbrushing thus enabling a higher degree of dispersion in the composite matrix of the composite with a lesser carbon content than conventional CNT dispersion techniques [24,54]. Such conductive coatings are experimentally shown to be extremely effective in self-sensing applications [16,24]. The forthcoming subsections apply the electro-mechanical simulation framework to elucidate the influence of interfacial debonding, electrical conductivity and thickness of coating for a compressive understanding. In addition, this section also compares the numerical simulation results, obtained from the simulation framework for the smart self-sensing cementitious material with the experimental results reported in [16] with a view to validate the simulation framework.

3.1 Influence of conductive coating on the strain sensing and damage detection capability

As explained earlier, the mechanical module is first initiated which generates the unit cell using Lubachhevsky-Stillinger algorithm [31,32,55], meshes the unit cell, applies periodic boundary conditions and implements a displacement-controlled simulation to obtain the deformed unit cell. Here, the volume fraction of sand is 45% [16]. The generated unit cell is shown in Figure 4(a). Sand particles (d_{50} is 600 μm [56]) are dispersed in the unit cell of edge length 3 mm. Based on a sensitivity study, the edge length of unit cell is adopted here as five times the mean diameter of sand particles beyond which any increase in the size of the unit cell results in insignificant change in the results. Similar relative size of unit cell with respect to size of inclusion has been successfully applied to evaluate micromechanical responses of cementitious composites in [33,37]. An absolute thickness of 10 μm of the conductive coating is adopted in this study unless varied to evaluate the influence of coating thickness. A thickness of 10 μm has been shown to yield an electrically conducting composite in [15]. This study also considers interfacial transition zone (ITZ) around the sand particles. The thickness of ITZ is considered to be 20 μm [57–59]. In order to implement interfacial debonding zero-thickness interfacial elements are implemented at the conductive coating-ITZ interface (refer to section 2.2.2). The unit cell is finely meshed using CPE4R elements in ABAQUS™. A mesh-sensitivity study was performed and a mesh containing 362137 CPE4R elements (in ABAQUS™) yielded converged solution. The converged mesh is shown in Figure 4(b). Here 2D unit cells are considered instead of 3D as a tradeoff between computational efficiency and demand. Similar 2D unit cells are successfully adopted for cementitious materials in [33,56].

Figure 4. (a) generated microstructure with the coated sand particles dispersed in hardened cement paste (HCP) matrix and (b) meshed microstructure

The mechanically deformed configuration, obtained from mechanical module, is imported to the remeshing module where the deformed geometry is re-meshed ensuring a good quality (aspect ratio ≤ 3) of elements [60–62]. The re-meshed unit cell is imported to electrical module for electrical analysis. The electrical module implements insulation at the edges parallel to y axis and applies a unit potential difference to obtain electric current distribution (ECD) and electric field in the unit cell. The post processing module computes the fractional change in resistance as explained earlier. The input material properties, shown in Table 1, are adopted from [15,51,56,59,63–67].

Table 1. The input material properties: Young's modulus (E), Poisson's ratio (ν) and electrical conductivity (σ)

Phases	E (GPa) [56,65,68]	ν [56,65,68]	σ (S/m) [51,63,64,67,69,70]
HCP	20	0.2	0.002
Sand	70	0.17	1.00E-08
Coating	3.4	0.4	1000
ITZ	10	0.2	0.002

3.1.1 Consideration of interfacial debonding

The mechanical module implements a continuum damage model coupled with cohesive zone model (CZM) at the zero-thickness interfacial elements in between the conductive coating and the ITZ, as explained earlier, to simulate debonding at the cement paste-coated aggregate interface under tensile strains. The traction-separation law is defined by tensile strength (f_t), total fracture energy (G_F) and initial fracture energy (G_f) as explained earlier in section 2.2.2. Values of these parameters, adopted in this simulation are 2.7 MPa, 25 N/m and 19 N/m respectively as reported in [71–73]. It should be noted that values of these parameters for the interface elements are considered same as the HCP matrix in this study due to lack of data. Debonding subroutine is implemented as explained in section 2.2.2 and values of scalar interface damage parameter (D_c) are obtained for the zero-thickness cohesive interface elements. The electrical module assigns insulation behavior at the interface elements where the value of D_c reaches 1.

Figures 5(a-1), (a-2) and (a-3) plot the interface damage parameter, D_c (Equation 19) in the zero-thickness interfacial elements under applied strain of 0%, 0.00075% and 0.0161% respectively whereas Figures 5(b-1), (b-2) and (b-3) show the corresponding electric current densities under applied unit electrical potential. The figures suggest that the debonding areas increase progressively with increase in strain. Consequently, the electric current densities at the conductive coating gets altered resulting in change in the characteristics of the electrical response in the unit cell. Figures 5(b-1), (b-2) and (b-3) show overall reduction in the current density with progressive debonding and deformation due to increase in applied strain. Enlarged views of a sand particle under these strains also reveal alteration of ECD in the conductive coating with progressive interfacial debonding resulting in change in resistance and thereby change in FCR.

Figure 5. Influence of interfacial debonding on the electro-mechanical response: (a-1) interface damage parameter in the unit cell without any externally applied strain; interface damage parameter corresponding to applied strain of (a-2) 0.0075% and (a-3) 0.0161%; (b-1) ECD along Y direction for applied unit electrical potential corresponding to: (b-1) undeformed unit cell, (b-2) unit cell under applied strain of 0.0075% and (b-3) unit cell under applied strain of 0.0161%

In order to evaluate the influence of debonding on the FCR, a dimensionless scalar parameter, fractional interface debonding is introduced which can be defined as the fraction of the total perimeter of inclusions that has de-bonded completely ($D_c=1$). Figure 6 shows the fractional interface debonding and FCR with

variation of applied strain. The fractional interface debonding increases progressively with increase in tensile strain. Consequently, the FCR also increases due to additional resistance in the unit cell imparted by the de-bonded interface which makes the associated fraction of conductive coating ineffective. With progressive interfacial debonding, the stress in the matrix increases due to lack of stress-transfer from the matrix to the stiffer inclusions. Finally, the stress in the matrix reaches its strength when the strain is increased beyond 0.0161% and the damage in the matrix is initiated. Beyond this point, fractional interface debonding remains almost constant and the progressive damage in the matrix becomes dominant. The influence of progressive matrix-damage on the FCR is elucidated in the forthcoming section with a view to evaluate the damage-sensing capability of this smart cementitious material.

Figure 6: Fractional interface damage and FCR with varying tensile strain

3.1.2 Influence of conductive coating on damage-sensing capability

This section implements a continuum damage model, explained earlier (refer to section 2.2.3), in the HCP matrix of the mortar microstructure to evaluate the damage-sensing capability of the smart material in the post-peak regime. The model assumes isotropic stiffness degradation and it requires the parameters ε_{D_0} , A_t , B_t , A_c and B_c for HCP matrix as input (Equation 23). In the context of tensile damage, the values of the parameters ε_{D_0} , A_t and B_t for HCP matrix are 0.0001, 1 and 10000 respectively which are adopted from the literature [43]. The damage model parameters in ITZ are considered to be same as the HCP matrix due to lack of data. The continuum damage model is implemented using user defined subroutine in ABAQUS™ and the scalar damage variable, D (Equation 23) in the matrix is obtained.

To obtain the electrical responses, the damaged microstructure is re-meshed and imported to the electrical module where the electrical conductivity of damaged elements was modified proportional to

the damage variable D (Equation 24). Figures 7(a-1), (a-2) and (a-3) plot the values of the damage variable (D) under applied tensile strain of 161, 170 and 210 $\mu\epsilon$ respectively. While Figure 7 (a-1) doesn't show any damage in the matrix, Figures 7 (a-2), (a-3) show progressive damage in the matrix with increase in the applied strain in the post-peak regime. The extent of interfacial damage (debonding) remains almost same beyond applied strain of 161 $\mu\epsilon$. Figures 7(b-1), (b-2) and (b-3) show the influence of progressive matrix-damage (under applied tensile strain of 161, 170 and 210 $\mu\epsilon$ respectively) on the electrical response. The general trend in the electrical responses suggest a decrease in the ECD with progressive damage.

Figure 7: Progressive damage in HCP matrix corresponding to applied strain of (a-1)161 $\mu\epsilon$, (a-2) 170 $\mu\epsilon$ and (a-3) 210 $\mu\epsilon$; ECD (A/m^2) in Y direction in the unit cells corresponding to applied strain of: (b-1)161 $\mu\epsilon$, (b-2) 170 $\mu\epsilon$ and (b-3) 210 $\mu\epsilon$

In order to shed more light on the relationship between damage and electrical response, Figure 8 plots the overall variation of FCR and stress with increasing tensile strain. It can be observed clearly from Figure 8 that, the FCR increases almost linearly with increase in strain initially up to a tensile strain of approximately 25-30 $\mu\epsilon$ beyond which the relationship becomes non-linear due to onset of interfacial debonding. As the damage in matrix initiates (beyond the peak stress), the rate of increase in FCR with respect to increase in strain increases rapidly and the sudden jump represents the onset of damage in the matrix. Thus, the relationship, shown in Figure 8, substantiates the strain-sensing capability of the smart

cementitious material in the pre-peak regime as well as damage sensing capability in the post-peak regime.

Figure 8. Progressive damage and FCR with increasing tensile strain

3.1.3 Influence of thickness and electrical conductivity of the coating

While the previous section highlighted the strain/damage sensing capability of the smart material, this section elucidates the influence of the electrical conductivity and thickness of the coating on the overall sensing efficiency. Figure 9(a) shows the influence of thickness of coating on the FCR while considering a constant electrical conductivity of 1000 S/m for the coating [63,64]. The general trend suggests that the FCR increases with increase in coating thickness for all the applied strains although the rate of increase in FCR with respect to coating thickness decreases beyond a thickness of 12 microns, a phenomenon often observed in non-conductive matrices with conductive phases [17,74]. Almost insignificant amount of increase in FCR is observed when the thickness increased from 18 microns to 30 microns. From the simulations, it is clear that a thin conductive film of around 10-20 microns thickness is enough to obtain the efficiency required for strain-sensing in these materials. Figure 9(b) shows the influence of electrical conductivity of the coating of thickness 10 microns on the overall FCR of the smart material. Variation of CNT loading in the latex matrix leads to a change in overall conductivity of the MWCNT-latex film deposited on the sand. A wide range of values of conductivity have been reported in literature[63,74,75], the maximum being 1000 S/m[63,64]. An almost linearly increasing trend of FCR is observed with the increase in the coating conductivity which can be attributed to the increasing overall conductivity of the system due to increase in the volume fraction of conductive coating. Trends in both Figures 9(a) and (b) suggest a significant increase in FCR when the strain is increased from 27 $\mu\epsilon$ to 81 $\mu\epsilon$. This is attributed to the onset of interfacial debonding beyond 27 $\mu\epsilon$ which results in additional resistance and thereby

increase in FCR as explainer earlier in this paper. The parametric variations indicate that the FCR is more sensitive to change in coating thickness as compared to change in conductivity of coating within bounds. FCR increased more than four-folds when the thickness of coating increased from 8 microns to 20 microns whereas a relatively smaller increase (about 60%) in FCR was observed when the conductivity increased from 200 to 1000 S/m. Its significance lies in the fact that the experimental limitations of achieving higher coating conductivity with CNT loading [64] can be offset with the variation of thickness of such coatings to obtain a more sensitive overall system.

Figure 9. (a) Variation of FCR with varying coating-thickness; (b) relationship between FCR and the conductivity of the coating for different applied strains.

3.2 Comparison of simulation results with experimental observations

This section applies the numerical simulation framework to predict strain-sensing behavior of the smart cementitious material containing nano-engineered cement-aggregate interface under compression and compares the numerical simulation results with the experimental results reported in [16]. The mortar consists of 45% coated sand and the binder contains 25% ground granulated blast furnace slag (GGBFS) by weight as cement-replacement. The thickness of the conductive coating is 10 microns [15]. The material properties of sand, conductive coating and ITZ are reported in Table 1 [15,51,56,59,63–67]. The conductivity of the matrix is reduced by 20% owing to the presence of 25% GGBFS by weight [76,77] whereas the values of Young's modulus and Poisson's ratio of the binder matrix are considered same as that of HCP [78]. Interfacial debonding is incorporated using traction-separation law defined by the parameters initial fracture energy (G_f), total fracture energy (G_F) and tensile strength of matrix (f_t). Values of these parameters adopted in this simulation are considered same as the HCP matrix as reported earlier in the section 3.1.1. Here in case of compression, the tangent material matrix, shown in Equation

18, is used and the scalar interface damage parameter, D_c is obtained in the matrix as well as in the ITZ. Isotropic damage under compression is incorporated using the parameters ε_{D_0} , A_c and B_c . The values of these parameters used in this simulation are 0.0001, 1 and 10000 respectively [43]. The deformed/damaged unit cell is re-meshed and imported to the electrical module which computes electrical responses for varying strains as explained earlier in this paper.

Figure 10 compares the FCR values obtained from the simulation framework to the ones reported in an experimental study [16]. Figure 10(a) plots the simulation results considering only interfacial debonding without considering damage in the matrix. The simulated FCR values correspond well with the experimental measurements when the applied compressive strain is lower than approximately 0.16% whereas the simulated values diverge from the experimental observations at higher compressive strains. This can be attributed to the damage in the matrix which is not captured by the model. Figure 10(b) shows the simulated FCR values when isotropic damage model in the matrix is incorporated in addition to interface damage. Upon implementation of continuum damage in the matrix, the high strain FCRs also match closely with the experimental measurements as can be seen in Figure 10(b). Incorporation of the isotropic damage enables significantly improved prediction of FCR in the post-peak regime thus verifying applicability of the current simulation framework towards prediction of strain-sensing and damage-sensing capabilities of smart cementitious materials.

Figure 10. The simulated and experimental FCR with varying compressive strain: (a) The simulation does not consider damage in the matrix; (b) simulation incorporates isotropic damage in HCP matrix

4. CONCLUSIONS

This paper presents a comprehensive numerical approach towards prediction of electro-mechanical response and strain-sensing capability of smart random heterogeneous materials. The framework first generates representative unit cell using Lubachevsky–Stillinger algorithm and the generated unit cell is imported into the mechanical module. The mechanical module applies periodic boundary conditions, meshes the unit cell, implements interfacial damage at the inclusion-matrix interface and incorporates isotropic damage in the matrix in the post-peak regime to obtain the deformed/damaged microstructure for any applied tensile or compressive strain. The deformed/damaged microstructure, obtained from the mechanical module, is imported into a remeshing subroutine that meshes the deformed/damaged unit cell and improves the quality of mesh for a better solution. The re-meshed unit cell is imported into the electrical module to obtain the electrical responses for the applied strain.

The applicability of the simulation framework is confirmed here through its successful implementation on a smart cementitious material containing nano-engineered conductive coating at the cement-aggregate interface. Representative microstructures of the smart cementitious material were first generated and the electro-mechanical responses were simulated using combined use of a mechanical module, remeshing module and electrical module. In the pre-peak regime, progressive interfacial debonding with increasing tensile strain resulted in significant progressive increase in FCR, signifying efficient strain-sensing capability of the material. With progressive interfacial debonding, the stress in the matrix kept on increasing and damage in the matrix was initiated in the matrix when the stress in the matrix exceeded the tensile strength. The onset of damage in the matrix was reflected in the form of significant jump in FCR, substantiating damage-sensing capability of the smart mortar. Parametric study with variations in thickness and conductivity of the coating revealed that limitations of achieving higher coating conductivity with increased CNT loadings [74] can be offset with the variation of thickness of such coatings to obtain a more sensitive overall system. The validation of the simulation approach presented here provides confidence on its capability to be implemented for various smart heterogeneous composites and it can help develop design strategies to tailor the microstructure for efficient performance.

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5. DATA AVAILABILITY

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study

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