MULTISCALE MODELING FOR HIGH-PERFORMANCE CONCRETE: A REVIEW

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High-performance concrete (HPC) has a complex mechanical performance due to its multiscale and multiphase composite structure. In this review, the various methods of multiscale modeling from different disciplines are summarized and discussed. The conjoint use of multiscale modeling and other methods such as image reconstruction technology for HPC is introduced. The failure mode modeling of HPC using multiscale methods is discussed. Lastly, the multiscale extended finite-element method (XFEM) for high-performance fiber-reinforced concrete (HPFRC) is elaborated. The benefits and perspectives of developing multiscale modeling techniques for HPC are presented.

KEY WORDS: *multiscale modeling, image reconstruction, high-performance concrete, XFEM*

1. INTRODUCTION

Concrete is one of the most commonly used construction materials being applied to infrastructures. Nevertheless, those shortcomings of the conventional concrete, such as low strength, low ductility, and early-age cracking, led to development of high-performance concrete (HPC). Compared with the normal concrete, the HPC has outstanding mechanical properties. However, it is a more complex multiphase composite material, which is composed of coarse/fine aggregates, mineral admixtures and cement paste, chemical additives (superplasticizers), and sometimes polymer fibers etc. Therefore, the mechanical behavior and the damage mechanisms of HPCs are different from normal concretes (Maekawa et al., 2008). To better understand and predict their performances, the development of systematical multiscale modeling of HPC is indispensable.

With the development of the multiscale method and x-ray and image reconstruction methods, the complex physical and chemical properties can be analyzed at various scales. Based on fundamental principles, multiscale modeling provides a framework for constructing mathematical and computational models for the HPC by examining the interaction of multilength scales and the combination between physics and chemistry. Traditionally, conventional macroscale methods, namely, the finite-element method (FEM) and fused deposition modeling (FDM), need more refined meshing to simulate fine scales, and the block element modifier, as a semianalytical method, only needs integration on the boundary of problem domains. However, it is difficult to get an analytical-based solution. Besides, it can cause significant errors when applying a macroconstitutive model to molecular scales. On the other hand, the microscale methods, such as first principles (Bernasconi et al., 1996), density functional theory (DFT), and molecular dynamics (MD) (Alder and Wainwright, 2004), usually require greater time to simulate macroproblems, as it indeed acquires an efficient computation to complete the simulation. To solve the contradiction, coupled methods with different length scales have been attempted in the last two decades, such as the macroscopic, atomistic, ab initio dynamics (MAAD) (Abraham et al., 1998), quality control (QC) method (Knap and Ortiz, 2001), quasicontinuum density functional theory (QC-DFT method) (Woodward et al., 2008), bridging scale method (Fish, 2006; Fish et al., 2007; Li et al., 2008;

Xiao and Belytschko, 2004), and computer-aided architectural design (CAAD) (Shilkrot et al., 2002), etc. Interestingly, similar to biological materials, engineering materials can be regarded as a hierarchical design from macroscale to nanoscale (Yuan and Fish, 2009a,b). Based on this principle and framework of FEM, a method called multiresolution was developed to analyze polycrystalline, porous, and granular materials (McVeigh et al., 2006).

The multiscale method was based on general laws of mechanics, including the constitutive model, the quantum theory, and experimental data as well. In the experimental data, especially for multiphase materials (like HPC), the mechanism of damage and fracture is uncertain. Because of inactions with different length scales and chemical transport, a new experimental technique must be applied to investigate the multiscale structure in the whole field. The x-ray and image reconstruct method (Otani and Obara, 2004) can reconstruct the structure of aggregates, mineral admixtures, etc. The microstructural changes of the HPC subjected to environment load in real time can be observed by 4-D image reconstruction (Hinkle et al., 2012; Tang et al., 2010). Combined with TEM/SEM, the structure at nanoscale can also be reconstructed (Midgley and Weyland, 2003). More complex phenomena such as the growth path of cracks caused by creep and autogenously shrinkage at small scales can also be observed and hence, more accurate multiscale modeling can be established.

In this paper, the development of multiscale modeling and the benefits of using it are introduced in Section 2. In Section 3, the multiscale modeling for high-performance concrete is discussed; the image reconstruction techniques and multiscale failure method for the HPC are reviewed. In Section 4 we discuss the multiscale modeling of high-performance fiber-reinforced concrete.

2. MULTISCALE MODELING

The multiscale modeling method includes multiple models at different scales (from atomic scale to macroscale) (Liu et al., 2004), originating from physical laws of different natures, such as, quantum mechanics, molecular mechanics, and continuum mechanics (shown in Fig. 1).

Available large-scale models, including the FEM, finite difference method (FDM), boundary element method (BEM), and meshfree method, should require constitutive relations, which are almost always obtained from experimental data. The microstructure of materials shows complicated shapes, so mesh refinement is needed at small length scales with FEM, and even smoothing meshing will fail, only when it is replaced by vertex meshes, which reduces the
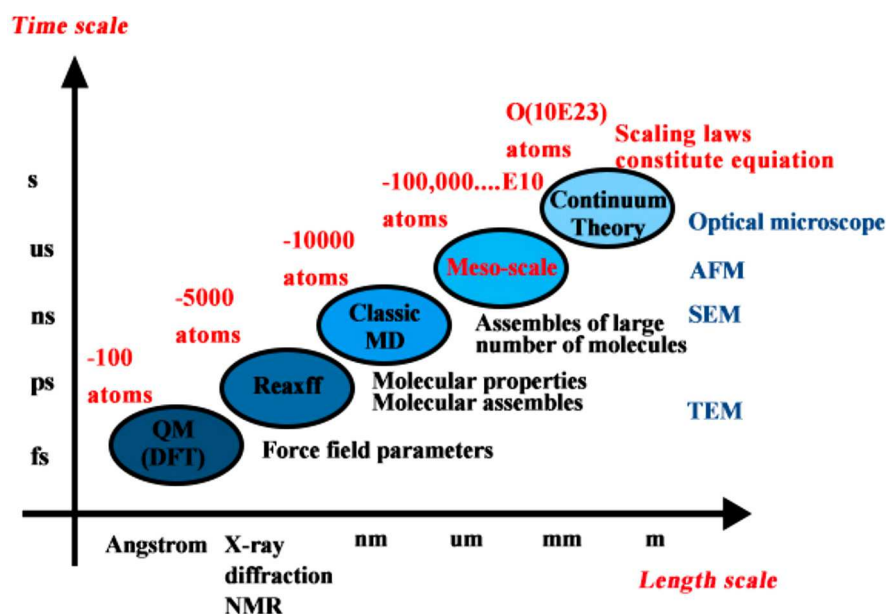

FIG. 1: The scheme of the multiscale models and their corresponding observation techniques

accuracy obviously because of tough element boundaries. The computational cost of the meshfree method increases dramatically, although it is more accurate than FEM. FDM just needs a simple process by Taylor's polynomial, but it has lower accuracy than FEM and requires a strict continuity in the problem region. For BEM, it needs to provide an analytical resolution, which it is very difficult to acquire in an analytical model in multiple scale domains. To seek a more efficient numerical model, Belytschko and colleagues (Belytschko and Black, 1999; Dolbow and Belytschko, 1999) developed an extended finite-element method (XFEM) based on the classical FEM, the partition of unity method (PUM) (Melenk and Babuška, 1996) and level-set method (LSM) (Osher and Sethian, 1988), in which merely a background mesh is needed.

As a common macroscale numerical method, the FEM had been proven strictly by mathematic theories. Based on the framework of FEM, the programing of XFEM is very easily implemented. That is why XFEM has been applied into many fields rapidly, including damage and fracture, composite materials, and microstructure description in the last decades (Afshar et al., 2015; Fish, 1992; Liu et al., 2014; Wu et al., 2010).

Unlike classical FEM, XFEM takes just the enriched function to describe the discontinuous interface based on a physical background mesh and tracks the boundaries on different material regions with LSM, which is very convenient to simulate multiscale problems compared with molecular dynamics and quantum mechanics. For example, XFEM meshes need no extra remeshing on the included regions [Fig. 2(a)]; on the contrary, the FEM needs mesh refinement [Fig. 2(b)].

The formula of XFEM is based on FEM with added enrichment terms (Kumar, 2011):

$$u^h(x) = \sum_{j=1}^{nen} N_j \left[u_j + \sum_{k=1}^{n_0} \varphi_k(x) a_{jk} \right] \tag{1}$$

where φ_k represents the enrichment function, n_0 is the number of inclusions, the additional nodal coefficients a_{jk} are corresponding to the enrichment functions. To separate additional freedoms from normal nodal freedoms, a shifting operation should be applied:

$$u^h(x) = \sum_{j=1}^{nen} N_j \left[u_j + \sum_{k=1}^{n_0} (\varphi_k(x) - \varphi_k(x_j)) a_{jk} \right] \tag{2}$$

(a)   (b)
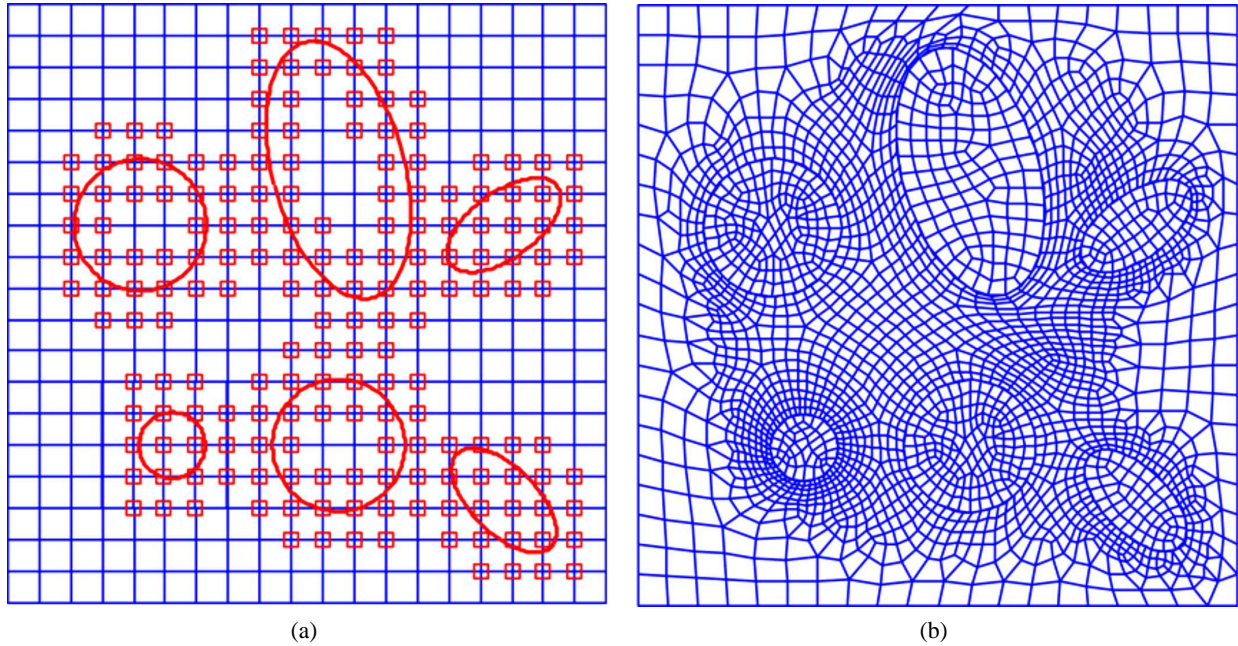
FIG. 2: Comparison with (a) XFEM meshes and (b) FEM meshes redrawn from Kumar (2011)

Similar to the FEM, the strain can be expressed by

$$\epsilon\left(x\right) = \mathbf{B}\left(x\right) \cdot \mathbf{u}^a \tag{3}$$

The strain ϵ at any point x along the direction is written as follows:

$$\epsilon_i\left(x\right) = \sum_{k=1}^{n_0} \mathbf{B}_{ij}\left(x\right)\left[u_j + \sum_{k=1}^{n_0}\left\{\varphi_k\left(x\right) - \varphi_k\left(x_j\right)\right\}a_{jk}\right] + \sum_{j=1}^{nen} N_j\left(x\right)\left[u_j + \sum_{k=1}^{n_0}\frac{\partial\varphi_k\left(x\right)}{\partial x_i}\right] \tag{4}$$

$$\rightarrow \mathbf{B} = [\mathbf{B}^{\text{FEM}}\mathbf{B}_1^{\text{ENR}}\mathbf{B}_2^{\text{ENR}}\ldots\mathbf{B}_{n_0}^{\text{ENR}}] \tag{5}$$

Therefore, the matrix "B" in the XFEM approximation consists of two parts: the classical FEM and virtual part that corresponds to the enriched functions. The stiffness is computed by gauss integration:

$$\mathbf{K}_{ij}^e = \int_{\Omega^e}\mathbf{B}_i\mathbf{D}\mathbf{B}_j d\Omega^e = \sum_{k=1}^{ngp}w_i\mathbf{B}_i\left(x_k\right)\mathbf{D}\left(x_k\right)\mathbf{B}_j(x_k) \tag{6}$$

where $\mathbf{B}_i$ and $\mathbf{B}_j$ are the strain matrixat i-, j-th node, respectively. The interfaces can be easily tracked by LSM. Meanwhile, the boundaries of images can also be tracked (Barman et al., 2011) and applied to image reconstruction (as shown in Fig. 3).

The disadvantage of XFEM analysis is that the freedoms added when using the enrichment functions will consume more computational time. Smoothing the finite-element method (Liu et al., 2007), which is just integrated on boundaries, will reduce the computational time when combined with XFEM.

Recently, a series of multiscale models were developed by combining XFEM with other numerical methods (Zhang et al., 2014). The multiscale methods based on conventional FEM can be transferred into XFEM easily. Coupling XFEM with the multiresolution method and QC method will conventionally implement multiple-scale problems, especially for material failure.

For nanoscale modeling, the molecular dynamics, which is based on classical mechanics and statistic mechanics, is applied in chemical physics, materials science, and biomolecules.

The macroscale models, like FEM models, are of low accuracy to analyze small scales with macroconstitutive relationships, while nanoscale models can accurately capture small-scale chemical and physical essential phenomena. However, they require a high computational cost to deal with large length scales. The multiscale modeling takes advantage of different physical laws at different scales to reduce computational costs, with no compromise on the accuracy. An efficient multiscale modeling system should consist of three closely related components: multiscale analysis, multiscale models, and multiscale algorithms. Firstly, the relation among models at different scales of resolutions and multiscale analysis should be understood. Then, multiscale models help to establish models that couple together at different scales. Lastly, multiscale algorithms are used to solve the multiscale solution efficiently. Meanwhile, to simulate real materials, image processing is applied to remodel structures at different scales. There are many
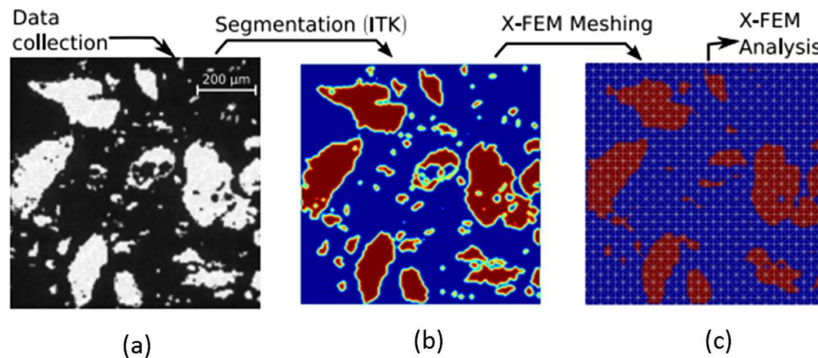
FIG. 3: The framework of XFEM analysis based on image reconstruction, copyright from Legrain et al. (2011)
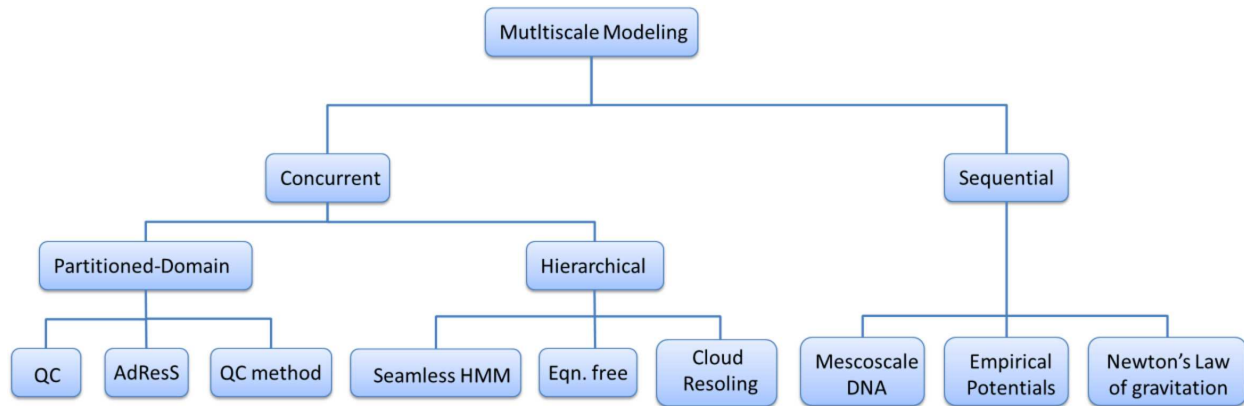
FIG. 4: The system of multiscale modeling (AdResS = adaptive resolution scheme; QM/MM = quantum mechanics/molecular mechanics; HMM = heterogeneous multiscale method)

studies about the multiscale modeling (atomic to continuum). Two main sequential and concurrent multiscale models (Fig. 4) are given as follows.

2.1 Sequential Multiscale Modeling

In sequential multiscale modeling, lower scale simulation is applied to describe the details of constitutive relations for microscale models (Kouznetsova and Geers, 2008). For example, based on the elastic theory, the macro model for linear elastic problems can be described as Hooke's law:

$$\sigma_{ij} = c_{ijkl} \epsilon_{kl} \tag{7}$$

where σ_{ij}, ϵ_{kl} are the stress tensor and strain tensor, respectively, and c_{ijkl} is the elastic tensor. In conventional large-scale models, the c_{ijkl} is normally determined from the experiment, while the elastic constant c_{ijkl} is deduced by evaluating the interaction of atoms with a fine model in a sequential multiscale approach. Another example is performing MD simulation by using empirical potentials, where the parameters in the potential are precomputed using quantum mechanics (Legrain et al., 2011).

2.2 Concurrent Multiscale Modeling

Unlike sequential multiscale modeling, different scale solutions are solved by different scale models in concurrent multiscale modeling (Tinsley Oden et al., 2006). In large domains, macroscale models are computed, and then microscale models are applied as the computation proceeds for areas subjected to extreme loads. In the adjacent domains, the macro- and microscale models are used concurrently. Concurrent multiple-scale modeling can be classified into two categories: "partitioned-domain" and "hierarchical" methods (Oosterlee, 1995).

Partitioned-domain concurrent approaches are implemented by dividing the physical problem into two or more contiguous domains, which are solved by a different physical model for each. An example to analyze dynamic fracture with coupling MD with XFEM is shown in Fig. 5(a). To acquire a high accuracy for the stress intensity factor, a fine-scale model, MD, is used at the vicinity of the crack tip. On the other hand, the XFEM is applied to other regions to improve the computational efficiency. The compatibility with the boundary of two methods is ensured by a coupled domain and Lagrangian multiplier method or penalty method (Aubertin et al., 2010). Similarly, Gracie and Belytschko (2009) analyzed multiscale dislocations and fracture problems by combining XFEM with the bridging domain method (BDM) (Xiao and Belytschko, 2004).

Hierarchical methods [shown in Fig. 5(b)], on the other hand, take advantage of both scales. The macroscale model makes regular appeals to the microscale model to determine a constitutive law and, conversely, the microscale model assists the large-scale model for its boundary conditions.
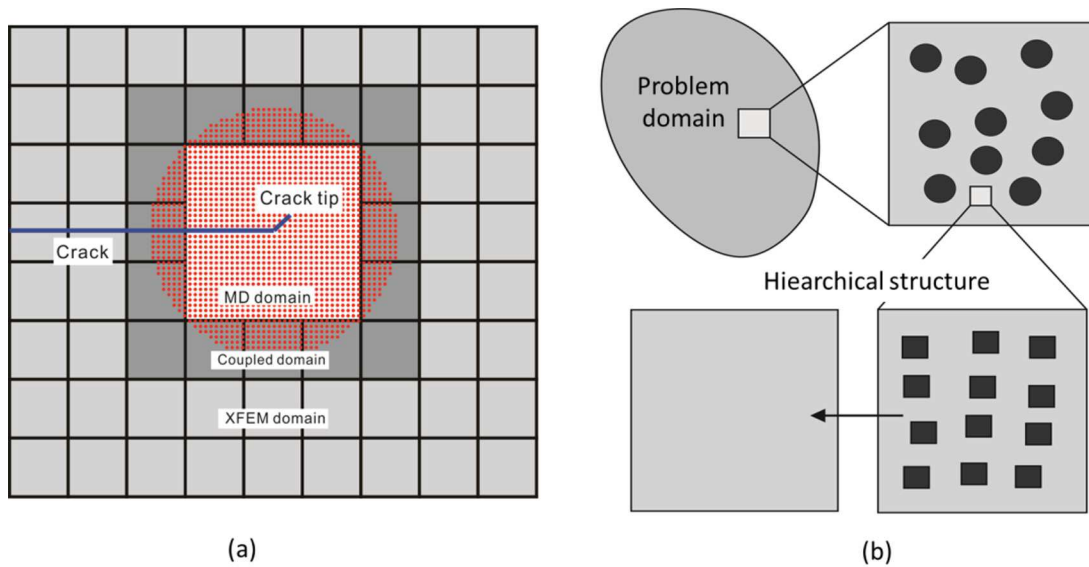
FIG. 5: (a) The coupled MD and XFEM and (b) the multiresolution framework

3. MULTISCALE MODELING FOR HIGH-PERFORMANCE CONCRETE

3.1 The Framework of Multiscale Model for HPC

The high-performance concrete, characterized by its high performance in terms of workability, mechanical properties, and durability, is a complex system that involves different scales of materials. Concurrent use of supplementary cementitious materials, superplasticizers, as well as other chemical additives leads to complex effects of each additive on others and on the properties of the HPC. For example, the water reducing admixture has expansive behavior, while the thermal expansion causes evaporation of water, and then a shrinkage crack happens. Therefore, new multiscale and multifield models should be developed with the ability to describe the physicochemical mechanisms integrated with structural analysis and materials science (Ahmed et al., 2013).

In Section 2, the multiscale modeling was briefly introduced. This method was widely applied to analyze the durability, toughness, and damage of infrastructure materials, concrete and HPC.

Conventionally, fine meshes are used to capture the discontinue features and the coarse meshes to describe the physical problems, albeit all meshes are based on macroconstitutive relationships (Chaudhuri, 2013). These two or more scale models consider concrete as homogenous in representative elements. However, concrete or HPC is a complex multiphase material, and its components always depend on the time scale because of physicochemical interactions (shown in Fig. 6). The multiscale (from nanosize to macrosize) mechanism of HPC is described not only by physics but coupling between hygral-, thermal-, chemical-, and mechanical processes. According to the geometrical size (see Fig. 7), four scales as follows were used to model the multiscale properties of HPC:

a. Macro- (m): In this structural scale, concrete is regarded as a homogeneous material with different mechanical behaviors: elastoplastic or viscoelastic. FEM, BEM, or XFEM can be used to simulate concrete at this scale.

b. Meso- (mm): The size of coarse aggregates up to mesoscale can be visible by human eyes. So, concrete can be seen as a two-phase heterogeneous material: a matrix made of mortar and coarse aggregates as inclusions. In high-performance fiber-reinforced concrete, the micrometer-scale fibers should be considered.

c. Micro- (μm): The mortar-forming matrix of concrete can be regarded as a random and heterogeneous material made of cement paste, fine aggregates, and water. In addition, cement paste, made of different type of components, including unhydrated and hydrated cement particles, pores, and capillary water, can be described at the microscale.
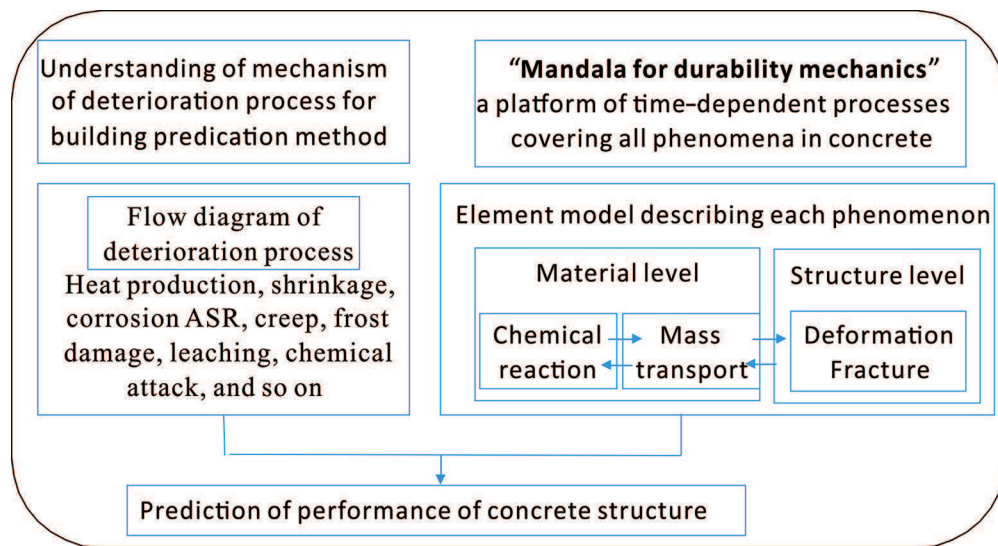
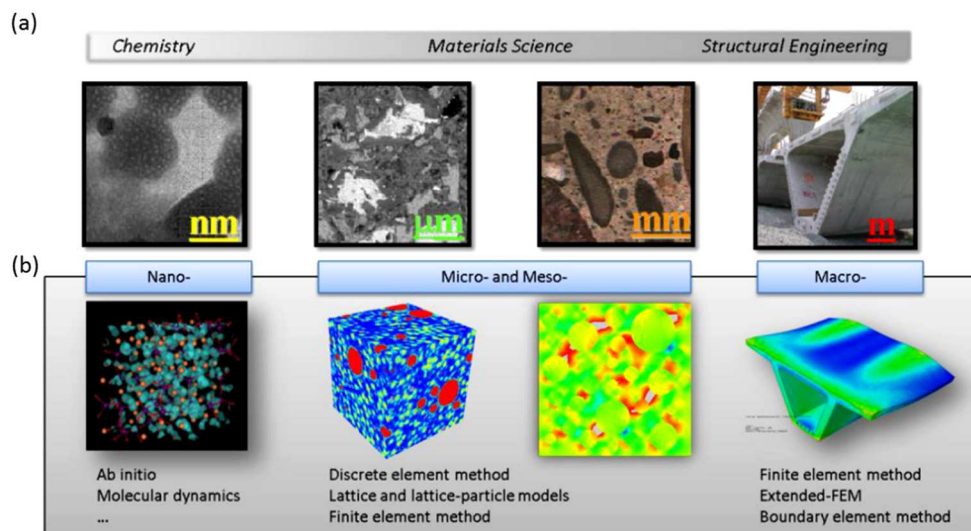**FIG. 6:** The framework of durability mechanics

FIG. 7: Concrete as a multiscale and multidisciplinary material

Meso- and microscale can be simulated by FEM lattice (Gates et al., 2005) to describe different mechanical behaviors at macroscales.

d. Nano- (nm): The molecular structure of cement (e.g., C-S-H gel) is analyzed by MD, *ab initio* or DFT at this scale. The capillary molecular water can also be analyzed.

Concurrent multiscale modeling is mostly used because the C-S-H gel, cement paste, fine or coarse aggregates have different performances in terms of mechanical behavior. In nanoscale, MD combined with *ab initio* or DFT provides important information about the interaction of calcium and silicates, and water molecules and their position within C-S-H chain. Moreover, like the hydration, transport of chemicals within the matrix plays an important role affecting the macromechanical behavior, which needs to be considered.

In concrete, the cementitious materials act a time-dependent behavior, caused by chemical reaction, environmental actions, and external load. This behavior can be described at a materials level (physiochemistry reaction and transport), a structural level (facture), and their combination (Basheer et al., 1996). The hydration process between cement paste and water, and the degree of hydration determined by water to cement ratio (w/c), play an essential role in concrete performance (Narayanan and Ramamurthy, 2000). In the last decades, several micromodels have been developed, namely, CEMHYD3D (Manzano et al., 2009), DuCOM (Bentz, 2006), HYMOSTRUC (Kishi and Maekawa, 1996), Navi's model Pignat (Navi and Pignat, 1996), and CCBM (Maruyama et al., 2007). The HPC produces lower hydration heat than conventional concrete because of low w/c. Besides, factors such as the transport of moisture and CO_2, Ca^{2+} leaching, Cl^- ingression, corrosion, and the effect of admixtures (such as a water reducer) should be considered in multiscale models (Cheung et al., 2011).

In general, concrete is regarded as a heterogeneous material at the meso level, but the properties of concrete vary in different specimens because of various sizes, shapes, and spatial distribution of aggregates. Some stochastically designed multiscale models (SMM), which are based on the asymptotic homogenization method (Guedes and Kikuchi, 1990) and stochastically FEM/XFEM (Fish and Wu, 2011; Nouy and Clément, 2010; Wu and Fish, 2010), have been developed in the last few years and can be used to process the random properties of aggregates (Duddu et al., 2008; Rahman, 2009). In addition, a so-called interfacial transition zone (ITZ) between the aggregates and the matrix can be captured by SMM.

The numerical methods, such as FEM, XFEM BEM, and the meshless method, are often applied to simulate the macrostructural behavior, durability, damage, fracture, dynamic response, etc. for concrete, as well as coupling the fine scales to describe the properties of microstructure. However, it is a challenge to simulate the time-scale behavior of concrete (Wu et al., 2016). The macroconstitutive models, especially for damage constitutive relationships, should be built to be coupled with mechanical, thermal, and transport properties of concrete (Cervera et al., 1999). The concurrent multiscale method, used in multiphase at different scales, is more efficient.

3.2 Combining Image Reconstruction with Multiscale Modeling

In the most mesoscale models, the random structure of aggregates is often generated by 2D or 3D stochastic computational algorithms or determines the spatial structure by destructing the concrete. On the contrary, the micro-x-ray computed tomography (μCT) which is widely applied in medical examination and geometric engineering, when coupled with image reconstruction algorithms, such as fast Fourier transform (FFT) and LSM, can provide a nondestructive technique to reconstruct the distribution of aggregate, and even the multi-interface will be captured. Based on image reconstruction, efficient multiscale models can be established (see Fig. 8).

In a common image reconstruction model, a coarse boundary often is captured because of low resolution of CT based on x-ray. Furthermore, voxel meshes are used in the multiscale model. However, the image reconstruction based on LSM can track the smooth boundary and be simulated accurately by XFEM (Lian et al., 2013). It is worth noting that the image reconstruction can be assembled with an image resolution of the x-ray, the multiresolution image technique, or microscopy scanning tools (SEM/TEM or AFM). The framework of multiscale image reconstruction is given here (see Fig. 9).

The micromodel of concrete can be reconstructed by combining with SEM/TEM or AFM with x-ray tomography (Liu et al., 2013). Through adding a time scale, the 4D image reconstruction can be used to describe the multiscale structure of concrete in real time. The multiscale model based on multiscale resolution image reconstruction can then be built. The displacement and strain of the 3D field for concrete can be determined by coupling with digital volume correlation (DVC) (Bay et al., 1999), which is widely applied in biological, geometrical, and aerospace research.

3.3 Multiscale Analysis for Material Failure of HPC

Indeed, HPC performs with outstanding mechanical properties compared with conventional concrete. However, the different damage mechanisms (e.g., crack growth, interface debonding, and chemical erosion) also can decrease the strength and toughness of HPC.
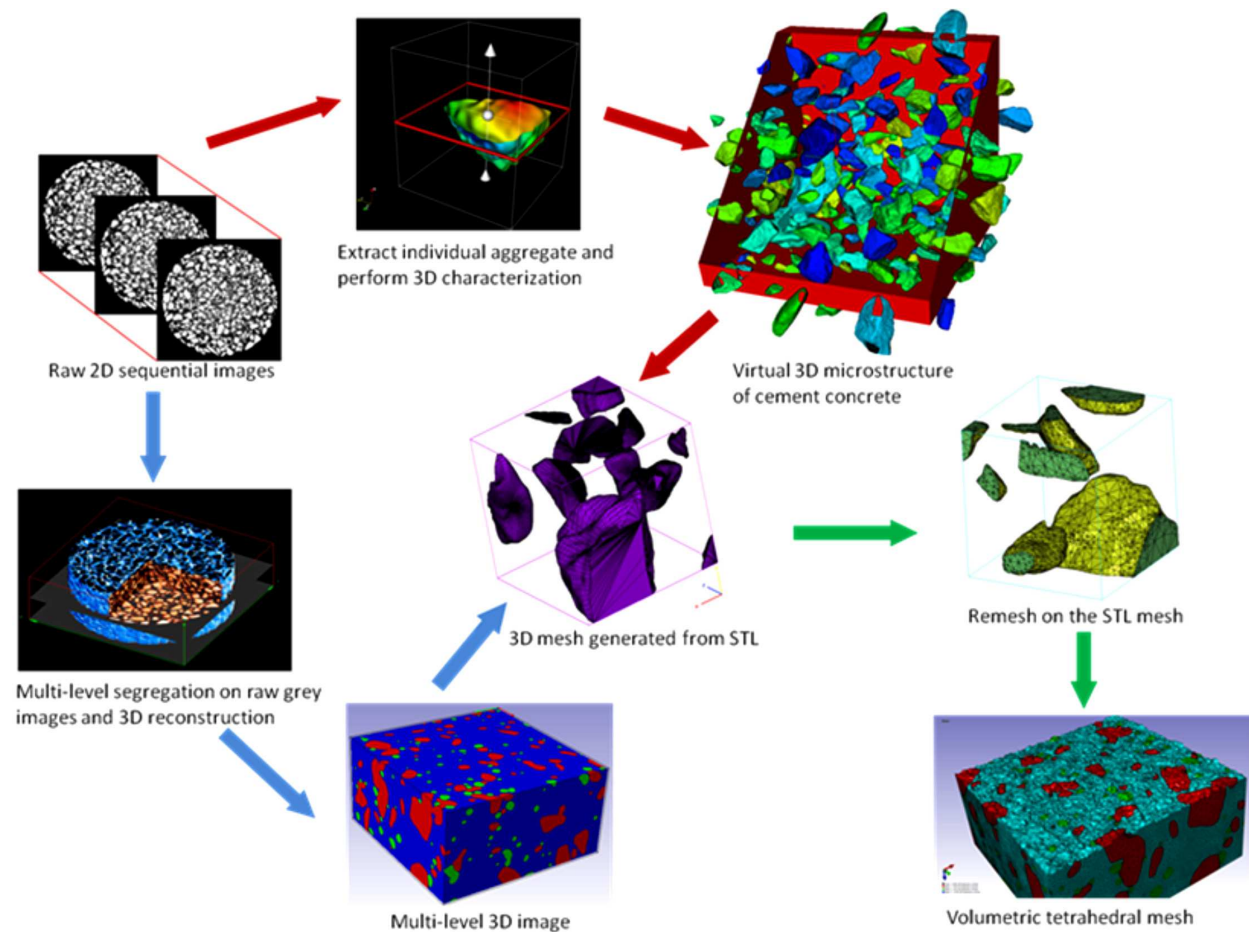
FIG. 8: The scheme of multiscale analysis for HPC (Lian et al., 2013)

Nonstructural cracks are one cause of failure, which is formed by heat conduction and shrinkage and adversely affect the early-age strength of HPC. The heat from hydration or freeze and thawing causes thermal stress within the matrix due to thermal gradients by which thermal cracking forms. The chemo-mechanical-thermal model is often applied to analyze the damage of concrete using a constitutive relationship based on the free energy in thermodynamics (Cervera et al., 1999). The frost damage of concrete was studied by combining the XFEM and cohesive models based on the mechanism that crystallization of ice exerts pressure on the capillary pores and causes the crack initiation and propagation (Ng, 2012).

On the other hand, the mechanism of shrinkage cracking (autogenous shrinkage cracking and drying shrinkage cracking) is primary attributed to three factors: capillary tension, disjoining pressure, and surface tension of colloidal cement hydrate (Hua et al., 1995). However, temperature difference and water contents produced by hydration can affect the shrinkage cracking. Therefore, the multiscale and multifield models are mostly used to simulate the shrinkage or shrinkage cracking. There is a two-phase multiscale model, similar to a composite material model, to analyze the shrinkage which suggests that chemical shrinkage contributes clearly to the autogenous shrinkage at early stages (Wu et al., 2017). However, the drying shrinkage and longtime autogenous shrinkage occur due to capillary tension and disjoining pressure (Schröfl et al., 2012). The volume ratio of the mixture (cement paste to aggregate and water-to-binder ratios) was optimized by an atom-continuum approach with reduced deformation caused by autogenous shrinkage (Pichler et al., 2007). In common multiscale models, the aggregate shrinkage was ignored. A new multiscale model base DuCOM showed that the shrinkage of concrete increased significantly when the shrinkage of a
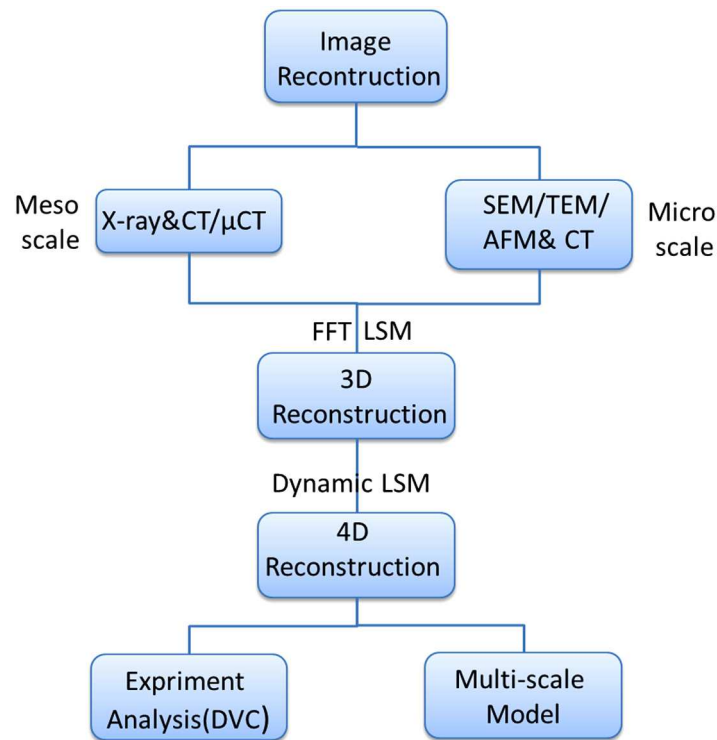
FIG. 9: The multiscale image reconstruction

low modulus aggregate was taken account (Asamoto et al., 2008). Also, a chemo-, porous-, viscoelastic modeling was proposed, which suggested that pore pressure is crucial to estimate the capillary tension (Pittman, 1992). Porosity was considered in this model as the chemical dilation or water evaporation are affected by the pore structure in concrete.

In contrast to a nonstructural crack, structural cracks may cause catastrophic destruction of concrete when subjected to external loads. For structural cracks, the damage of concrete is simulated by coupled thermo-hygro-chemo-mechanical models. Under fire loading, for instance, spalling of concrete takes place attributed to two principal mechanisms: thermohygral and thermomechanical interactions. In recent research (Gawin et al., 2006), it shows that in the thermohygral process the pore pressure increases as the pore water vaporizes, and then the tensile stress in the concrete matrix increases drastically. In thermomechanical processes, compressive stresses parallel to the heated surface increase; in contrast, the tensile strength perpendicular to the heated surface drops down, which causes delamination of concrete mainly at the surface. The meshfree model proves to be efficient to model large displacements (blast impact, explosion) without mesh generation, although it increases the computational time compared to FEM. A multiscale meshfree modeling, based on a semi-Lagrangian reproducing the kernel particle method (Wang and Lin, 2011) and energy bridging theory (Li and Ren, 2010), is applied to simulate the damage of high-strength concrete under explosion penetration. As the extreme material separation and number of fragments are formed, the LSM is used to determine the surface normal given a contact surface. Therefore, the damage evolution model based on a continuum-damage link to microscale failure was developed (Krajcinovic, 2000).

In multiscale modeling, which considers moisture transport, the porosity described at different scale is shown in Fig. 10.

4. MULTISCALE MODELING FOR HIGH-PERFORMANCE FIBER-REINFORCED CONCRETE

Different contents and types of fibers are used to enhance the toughness of high-performance concrete. The multiscale modeling for high-performance fiber-reinforced concrete (HPFRC) should be considered differently, with the addition
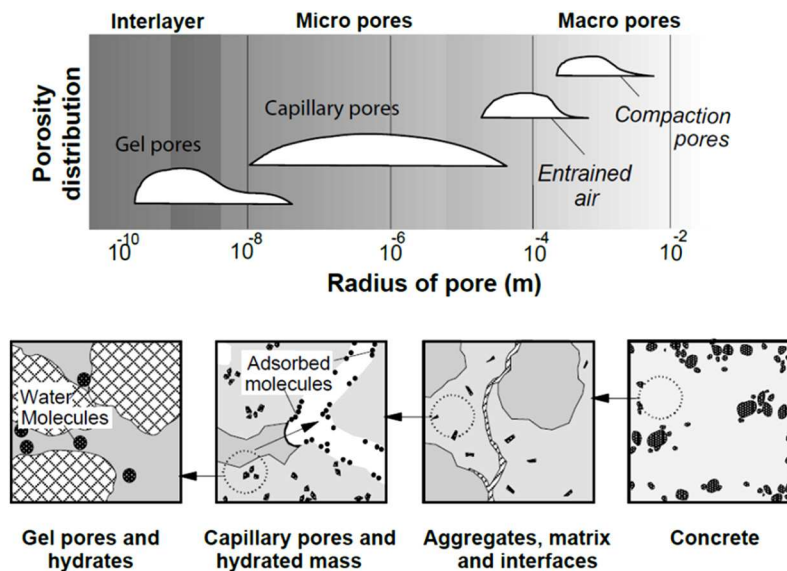
FIG. 10: The multiscale structure of porosity (Maekawa et al., 2008)

of fibers, from the multiscale modeling for HPC. The corresponding models can be classified into three categories: (a) multiscale continuum models, in which equivalent stiffness and modulus are acquired by regarding the fibers and the matrix as a homogenous composite material; (b) embedded models that define the matrix element by taking the fiber stiffness and considers the rotation of fibers (Monti and Spacone, 2000); and (c) multiscale structure models that consider the fibers and matrix as separate constituents.

Multiscale continuum models are the most common model in which the fiber-reiforced concrete can be regarded as an isotropic or anisitropic composite material due to the different oritention of the fibers. In this model, the homogneous method is mostly used as well as the continumm damage or nonlocal damage models (Han et al., 2014; Karihaloo and Wang, 2000). As for the second category, an embedded rebar model is applied to analyze the fracture of high-performance fiber-reinforced cementitious composites (HPFRCC) combined with XFEM, although as multiple cracks are simulated, there are some errors between simulation and expriemental results in four-point bending expeiments; and the interface of the fiber and matrix is igonored (Padmarajaiah and Ramaswamy, 2002). In another embedded model using micromorphic approach, the slipping of the fiber-matrix interface is considered in mesoscale, albeit the slippage does not occur (Huespe et al., 2013). In multiscale structural models, a 3D modeling for carbon nanotube/polymer composites has been proposed and the CNT networks and polymer interphase regions were described clearly. The results proved that the polymer interphase region predominantly attribute to reinforcement (Han et al., 2014). Another multiscale structure model was based on XFEM, in which the fibers are regarded as 1D "inclusion," an enrichment function to describe the discontinous interface of the fiber and the matrix (as shown in Fig. 11). The translation and rotation of fibers were considered by a rigid constraint equation, but bending and stretching were ignored because of the low stiffness of fibers. This approach successfully avioded the complex mesh generation in FEM and accurately characterized the elastic behavior of multiple short fiber-reinforced composites without complex mesh refinment at the interface (Thostenson and Chou, 2003). However, the failure model of fiber was not taken into account.

The pullout of fiber is important to evaluate the fiber-matrix interface strength (Thouiess et al., 1989). But few multiscale models considered both fracture and deboning of fiber, even though the fiber-matrix interface had been described accurately by LSM (Sonon and Massart, 2013). In the fiber-reinforced concrete, except for fracture, the pullout and delamination of fibers can cause the premature failure of reinforced concrete.

The interface between fibers and the bulk paste can activate the growth of microcracks when the concrete is subjected to external loads. Some literature has proposed analytical and empirical models to evaluate the interfacial
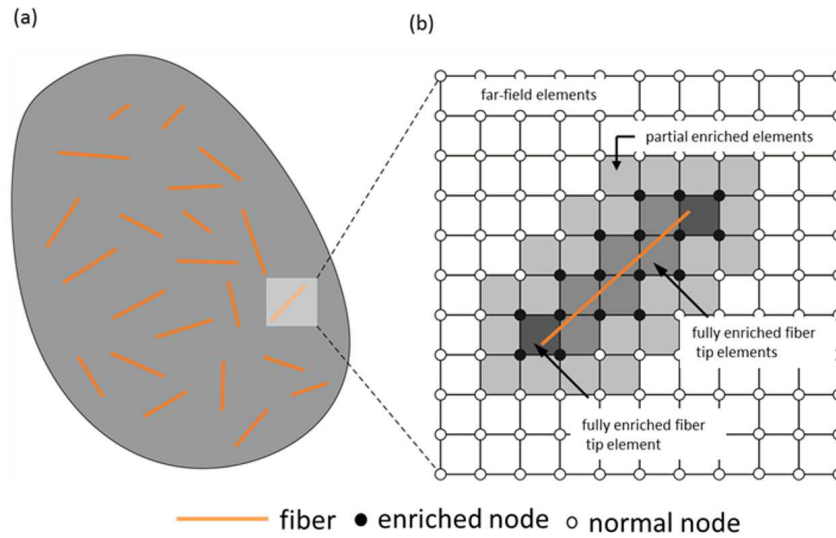
FIG. 11: (a) The scheme of a 2D fiber-reinforced problem and (b) the XFEM mesh for a single-fiber redraw from Pike and Oskay (2014)

fracture (Akisanya and Fleck, 1992; Hutchinson and Suo, 1992; Ryoji and Jin-Quan, 1992). However, the interfacial fracture behavior for multiphase materials (like concrete) under moisture environments is not yet well explained. Previously, the interface fracture was tested on trilayer specimens: carbon FRP, epoxy adhesive, and concrete [shown in Fig. 12(a)] (Au and Büyüköztürk, 2006a,b; Lau and Büyüköztürk, 2010) under different moisture environments. It was found that the fracture toughness of the trilayer material system dropped dramatically because of the presence of moisture, which was studied by MD [Fig. 12(b)]. Results of simulation showed that the adhesive strength between epoxy and silica was reduced with the decrease of the energy barrier E_b. However, a coupling between MD and FEM is required to characterize the interface mechanism at different scales.
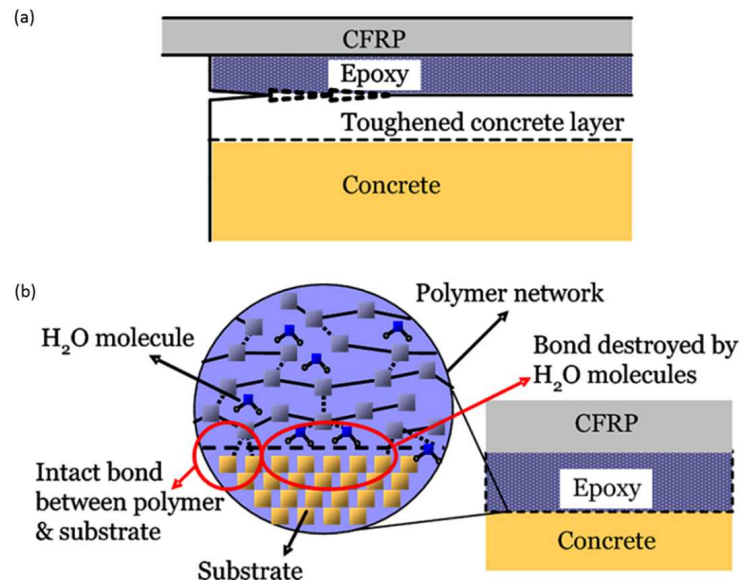
FIG. 12: (a) Plasticization of an epoxy-penetrated concrete layer and (b) weakening of the bond between epoxy and concrete, copyright from Büyüköztürk et al. (2011)

5. SUMMARY AND PROSPECTIVE

5.1 Summary

Numerical modeling, especially the multiscale modeling method, always performs an important role in describing the mechanical properties of HPC and HPFRC. The concurrent multiscale models are more efficient approaches to characterize different mechanisms with different models compared to the sequential multiscale models. The common multiscale methods often use homogenous methods and consider concrete as homogenous or simple two-phase composite materials in representative volume element (RVE) to simulate the problems by quantitates. In contrast, HPC performance consists of more than two phases and the mechanical properties are determined by multiscale and multifield, not only by physical models. So, the multiscale modeling integrates the material and structural mechanics and describes the performance of HPC more accurately. On the other hand, the image reconstruction technology (such as x-ray, μCT) provides an opportunity to establish real models instead of hypothetical ones. The real multiscale modeling can be built to analyze the multiphysics behavior of HPC and HPFRC.

5.2 Prospective

As the HPC is a complex multiphase material, the structure can change because of hydration heat and the different components used. Therefore, the multiscale homogenous approach should take the time-scale, scholastic, and the chemical admixtures into account. The multiscale XFEM can describe the multiple phase materials and track the dynamic boundary of inclusion (such as aggregate, C-S-H gel, fiber) with the level-set method and can be applied instead of FEM.

For HPFRC, a multiscale structure model based on XFEM has been built, but the failure of fiber and debonding is not considered. The nanoscopic chemomechanical interactions at the fiber-matrix interface in carbon nano- and microfiber is reinforced with cement composites. A multiscale computational framework for modeling the mechanical response of nano- and micro- reinforced concrete is cementitious composites.

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