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Theoretical Modelling of Thermo-Chemo-Mechanics of Solids: A Review

Bao Qin[1], Zheng Zhong[2]*

(*1. Research Institute of Interdisciplinary Science & School of Materials Science and Engineering, Dongguan University of Technology, Dongguan 523808, China;*
2. School of Science, Harbin Institute of Technology, Shenzhen 518055, China)

Abstract: Multi-field coupling problems involving species transport, heat transfer, substance transformation, and mechanical deformation are prevalent in various scenarios, such as the curing of early-age concretes, the response of soft materials, the oxidation of metals, the lithiation and de-lithiation of lithium-ion batteries, and the self-healing of biological tissues. Thermo-chemo-mechanical coupling dynamics are common characteristics of these problems, making theoretical studies on such processes of significant importance. This work offers a thorough review of advanced theoretical models addressing thermo-chemo-mechanical behavior in solid materials within the theoretical framework of non-equilibrium thermodynamics. First, we outline the thermo-chemo-mechanical coupling phenomena observed in various application scenarios. Then, the theoretical developments of classical continuum mechanics are, phase field method and peridynamics in the contexts of thermo-mechanical coupling, chemo-mechanical coupling, and thermo-chemo-mechanical coupling, respectively. Finally, challenges faced by thermo-chemo-mechanical coupling research are highlighted and prospects and directions for this field are also outlined. This paper helps to understand the history and trends in the development of thermo-chemo-mechanical coupling theory.

Keywords: thermo-chemo-mechanical coupling; continuum mechanics; phase field; peridynamics

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0 Introduction

Multi-field coupling problems in solids are not only widely present in the practical applications of advanced functional materials, intelligent materials, and novel energy transformation and storage systems represented by fuel cells and lithium-ion batteries, but also commonly embedded in the complex behaviors of natural porous media and biological tissues. In these problems, the multi-field coupling characteristics are reflected not only in the response of materials or media to external mechanical, electrical, chemical, and thermal stimuli, but also in their intelligent perception and automatic adjustment to external environments. This is achieved through the superimposed effects of multiple physical fields and the coupling relationships and energy conversion processes among these fields.

Classical multi-field coupling problems in solids primarily involve the processes of heat transfer, electrical (or magnetic) conduction, and deformation in various materials and media, as well as their interactions. Under the combined effects of multiple physical fields, different forms of energy can be converted into one another. For instance, the bi-directional coupling of electricity and heat is manifested in thermo-electric effects, Thomson effect, and Peltier effect. The bi-directional coupling between deformation and heat transfer is evident in thermal expansion (thermal stress) and thermo-elastic effects. Additionally, indirect coupling exists between different processes. For example, Joule heating can induce thermal strain in materials, while thermo-elastic effects can influence electrical (or magnetic)

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* Corresponding author. Zheng Zhong, Ph.D, Professor. Email: zhongzheng@hit.edu.cn.

processes. This type of coupling effect, which involves energy conversion at different levels, requires the constitutive equations of solids to clearly express the interactions between various physical quantities. The spatiotemporal evolution of each physical field must be described by its respective conservation equations and dynamic laws, where the coupling terms accounts for the coupling effect. Moreover, due to the anisotropy, heterogeneity of materials, and specific boundary constraints, the variables can exhibit non-uniformity. The mutual influence among these variables and their impact on the macroscopic properties of solids may occur across different spatial and temporal scales.

Classical multi-field coupling problems typically do not involve chemical processes. This means that during theoretical modeling and numerical analysis, the studied system can be assumed to be a closed thermodynamic system with a fixed and unchanged chemical composition. In this case, there is no species exchange between components, and the system neither receives material inputs from the external environment nor generates or consumes substances internally. However, when chemical processes are considered, coupling problems in solids usually involve the transfer of species, momentum, and energy among various components in an open thermodynamic system. The interaction of solid materials in such complex environments leads to changes in solid structures and energy. Solid structures typically reflect both micro- and macro aspects, for instance, a chemical reaction that leads to chemical bonds and the formation of new bonds represents a change in microstructure of a material, while a chemical reaction that results in the expansion or contraction of a substance's volume indicates a change in its macrostructure. Additionally, chemical reactions can absorb heat from the environment or release heat back into environment again, as well as convert the energy of solids from usable energy to dissipated energy, which indicates changes in energy.

multi-field coupling problems of solids involving chemical processes are accompanied by a series of complex multi-scale phenomena in both time and space, driven by multicomponent materials under various thermodynamic mechanisms. Describing these phenomena requires interdisciplinary integration across mechanics, physics, chemistry, and materials science. Compared to classical multi-physics problems, this significantly increases the difficulty in theoretical analysis, mathematical modeling, equation solving, and experimental validation. For both the design and optimization of novel materials and the assessment and prediction of the short- and long-term performance under coupled fields, it is crucial to have a comprehensive understanding of the interaction mechanisms among various thermodynamic processes involved in thermo-chemical-mechanical coupling phenomena. This understanding includes accurately characterizing the impact of each process on energy and dissipation of systems, ultimately establishing rigorous theoretical descriptions and developing analytical and numerical solution methods. These challenges are not only critical issues of today but also an essential aspect of advancing modern solid mechanics.

Therefore, this work seeks to provide a comprehensive review of thermo-chemo-mechanical coupling theory in solids, with the goal of enhancing readers' insight into the functional and failure mechanisms of equipment and devices. The work is structured as follows: Section 1 introduces the thermo-chemo-mechanical coupling in materials. Section 2 presents a review of theoretical studies on thermo-chemo-mechanically coupled problems. Finally, Section 3 discusses the challenges and prospects in this area.

1 Thermo-Chemo-Mechanical Coupling in Materials

To better understand the interaction mechanisms between thermo-chemo-mechanical coupling phenomena, it is essential to study the coupling process in materials. The interactions between six types of advanced materials under thermal, chemical, and mechanical environments are discussed in this section.

1.1 Response of Soft Smart Materials

Soft smart materials are a unique class of materials that bridge the properties of solids and fluids. They are characterized by their low modulus and remarkable ability to generate significant mechanical responses when exposed to external stimuli, such as heat, light, force, or chemical interactions[1-2]. These materials mainly include polymer colloids[3], hydrogels[4-5], biological soft tissues[6], shape memory polymers [7], dielectric elastomers[8], liquid crystals[9], and foams[10]. Due to their "small excitation, large response" characteristics, they are widely used in soft robotics, drug delivery systems, sensors, and smart actuators. As illustrated in Fig. 1, the synthesis of a lignin-based hydrogel, which holds great promise for biomedical applications and 4D printing, has been achieved[11]. It exhibited exceptional swelling ratios, reaching as high as several thousand percent. The swelling behavior and dimensional changes of the hydrogel were notably influenced by lignin concentration, with significant effects observed from variations in temperature and pH. To effectively foresee the performance of soft materials in service and enhance their functionality during the design and manufacturing stages, it is essential to comprehend the fundamental coupling mechanisms. This requires establishing a comprehensive thermodynamical framework for finite deformation, encompassing species transport, heat transfer, and chemical reactions.

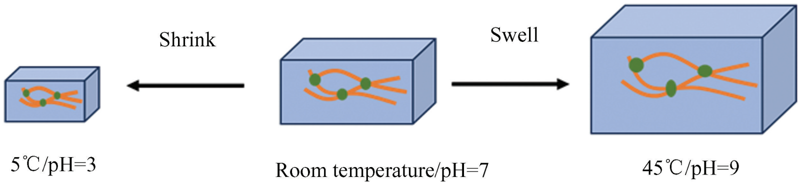


Fig. 1 Examples of pH and temperature responsive hydrogels [11]

1.2 Hydrogen Embrittlement of Metals

Hydrogen Embrittlement (HE) is a phenomenon where the mechanical properties of metallic materials degrade significantly due to hydrogen absorption or diffusion during processes such as smelting, machining, heat treatment, pickling, electroplating, or prolonged use in hydrogen-containing environments[12-13]. HE can lead to sudden accidents, resulting in significant economic losses and posing a serious threat to human safety. It is one of the major hidden risks in the safe production of the hydrogen energy industry[14]. HE typically manifests as delayed fracture under stress, a phenomenon caused by hydrogen atoms diffusing and accumulating at sites of stress concentration [15]. This process reduces the material's ductility and increases its brittleness, making it prone to fracture under static loading after a certain period of time. The factors influencing HE include ambient temperature and pressure, hydrogen purity, concentration, duration of exposure, as well as the material's internal stresses, physical and mechanical properties, microstructure, surface conditions, and the presences of cracks[16]. As illustrated in Fig. 2, the cracking of X70 steel induced by hydrogen is investigated at varying temperatures and hydrogen charging currents[17]. The results indicate that temperature can reduce the susceptibility to HE, while hydrogen concentration significantly affects the fraction of the {110} crystallographic orientation.

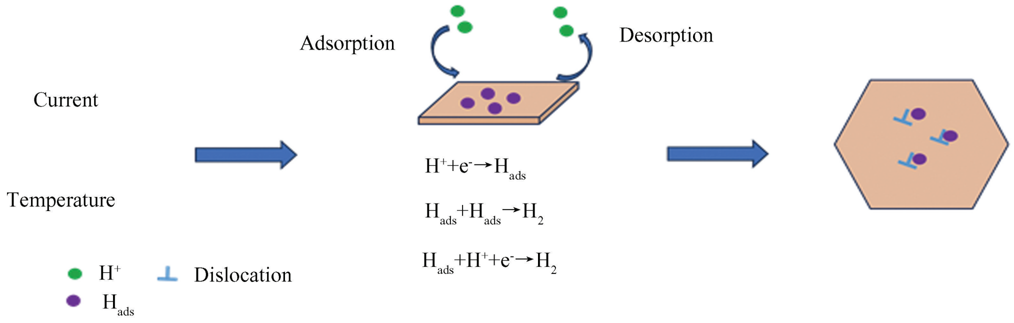


Fig. 2 Examples of hydrogen and temperature sensitive steels [17]

1.3 Lithiation and Delithiation of Silicon

Silicon (Si) electrodes, used as an anode material in lithium-ion batteries (Li-ion batteries), can enable a battery's capacity to reach 4200 mAh/g, far exceeding the capacity of the graphite anode materials commonly used today[18]. Due to their large capacity and abundant availability, silicon electrodes have become the most promising next-generation anode material, capable of meeting the rapidly growing demands of industries such as electric vehicles and portable electronic devices[19-20]. A typical Li-ion battery usually comprises three essential components: the lithium cathode, the electrolyte and the silicon anode[21]. During charging, lithium in the cathode undergoes an electro-chemical reaction at the cathode-electrolyte interface, resulting in the production of lithium ions. These lithium ions then travel through the electrolyte and undergo a subsequent electro-chemical reaction at the electrolyte-anode interface, where lithium atoms are generated. These lithium atoms are then embedded into the silicon electrode, where they chemically react with silicon atoms to form lithium silicide. As a result of the lithium atoms embedding and the creation of lithium silicide, the volume of the silicon electrode can expand up to four times of its original size. When this volumetric change is restricted, substantial stress and plastic deformation are induced within the silicon electrode, often leading to electrode damage and battery failure. Furthermore, experiments reveal that during the initial charging of a Li-ion battery, both crystalline silicon and amorphous silicon develop a two-phase interface within the silicon electrode[22]. On the outer side of the two-phase interface, lithium undergoes an alloying reaction with silicon to form lithium silicide, while on the inner side, lithium has not yet reached the region, and the lithiation reaction has not started. Over time, the two-phase interface gradually expands inward. This two-phase interface often generates large stress gradients and plastic deformation gradients, leading to electrode damage and affecting the safe operation of the battery[23]. As illustrated in Fig. 3, temperature also influences the diffusion of Li atoms and the deformation Si anodes[24]. Therefore, to enhancing the performance and safety of Li-ion batteries, it is crucial to investigate the cyclic behavior of high-energy Si anodes, focusing on mechanical deformation, voltage hysteresis and temperature response.

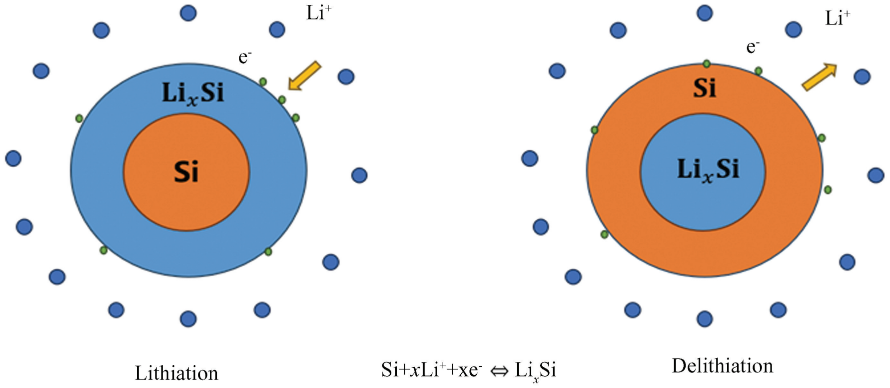


Fig. 3 Examples of lithiation and delithiation in silicon anodes

1.4 Corrosion of Ceramic Materials

Thermal Barrier Coatings (TBCs) are ceramic layers introduced by NASA in the 1950s. These coatings are deposited on the surface of high-temperature alloys on turbine blades to lower the alloys' surface temperature of the alloys, thereby increasing turbine blades' operating temperature and improving engine efficiency[25-26]. Advancements in aerospace are driving higher turbine engine thrust-to-weight ratios, resulting in increased turbine inlet temperatures. Since enhancing the high-temperature resistance of turbine blades by raising the material's maximum operating temperature is challenging, applying TBCs to the turbine base is a more feasible approach. Consequently, the performance and functionality requirements for TBCs are becoming increasingly stringent[27]. A typical TBC consists of a Bond Coating (BC), a ceramic Top Coating (TC), and a thermally grown oxide layer. Yttria-Stabilized Zirconia (YSZ), partially stabilized with Y_2O_3, which is widely used in the ceramic layer. However, it is susceptible to corrosion from Calcium-Magnesium-Alumino-Silicate (CMAS) compounds in high-temperature conditions[28]. As illustrated in Fig. 4, at high temperatures, environmental CMAS becomes molten and adheres to the surface of a ceramic top coating, subsequently penetrating into its microstructure and significantly altering its material properties[29]. The discontinuity in the material caused by CMAS penetration leads to a slight increase in stress around the CMAS deposit-TC interface, the penetrated layer, and the TC-BC interface. The stress concentration shifts from the tip of the microstructure to the areas above and below the tip, which may lead to the formation of a mixed crack type around the microstructures. Additionally, CMAS penetration can lead to an increase in temperature, and the temperature gradient can cause nonuniform CMAS penetration[30]. Therefore, establishing multi-field coupling theories to simulate temperature, stress, and corrosion conditions during the service of thermal barrier coatings can provide guidance and a basis for optimizing and improving the performance of coatings.

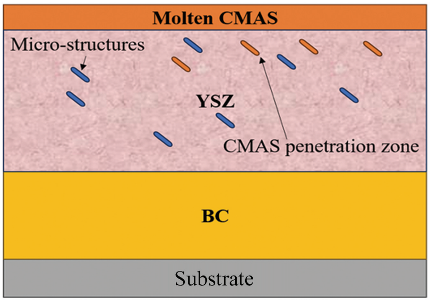


Fig. 4 Examples of CMAS corrosion of ceramic materials

1.5 Curing of Early Age Concretes

Curing of early-age concrete refers to the period from pouring the concrete until it reaches the desired strength and stability as specified in the design. During this period, the concrete undergoes a series of physical-chemical changes, primarily including the hydration of cement, strength development, and volumetric stabilization. In the early-age phase, large volumes of concrete are susceptible to significant internal forces due to temperature-induced deformations and self-shrinkage[31]. These forces can cause the material to transition from the linear creep stage to a nonlinear creep stage. The tricalcium silicate and tricalcium aluminate in the cement react with hydroxide ions (OH^-) in the water, forming hydration products that fill the pores in the concrete, making it harder and increasing its strength. Due to temperature gradients, humidity gradients, irreversible shrinkage, and structural constraints, early-age concrete is prone to curing warping, which can significantly impact its service performance and failure modes[32-34]. As illustrated in Fig. 5, hydration is hindered at lower temperatures and accelerated at higher temperatures[35]. Consequently, under lower temperature conditions, the hydration degree is reduced, resulting in less water consumption and the formation of fewer C-S-H and C-H compounds, which leads to higher porosity. The variations in thermal conductivity can be attributed to factors such as changes in water content, the chemical composition of the solid phase, and porosity (the volume fraction of the solid-phase). Overall, the curing of early-age concrete is a complex multi-physics coupling process, involving chemical, thermodynamic, and mechanical factors, which plays an essential role in determining the concrete's final performance.

1.6 Self-Healing of Biological Tissues

Self-healing capability enables organisms to repair damaged cells and tissues, maintain organ function, defend against external threats, adapt to environmental changes, promote growth and development, and influence evolution and population adaptability [36]. Bones are filled with micro-cracks that form and grow due to the daily stresses placed on them. As the primary structural material in our bodies, bone is relatively weaker than many engineering materials, but it has one key advantage — its ability to repair itself. Small cracks, which develop and grow under cyclic stresses through the mechanism of fatigue, can be detected and repaired before they grow large enough to pose a significant risk[37-38]. As illustrated in Fig. 6, Osteoblasts, a type of stem cell, play a crucial role in the healing of fractured human bones by forming mineralized calluses (primarily $Ca_{10}(PO_4)_6(OH)_2$) that bridge the fracture interfaces at body temperature[39]. Inspired by bones, researchers are dedicated to integrating self-regeneration or self-healing abilities to materials such as polymers[40], alloys[41], ceramics[42] and cements[43] in order to extend their durability, reliability, and lifespan. Additionally, temperature can play a crucial role in the self-healing process of materials. For example, microbial self-healing cementitious materials require an optimal incubation environment to activate bacteria, which then produce calcium carbonate to seal cracks[44]. The self-healing process is governed by complex interactions across multiple physical fields, including mechanical deformation, species transport, heat transfer and chemical reactions. To further the development of self-healing materials and enhance our understanding of the underlying mechanisms, it is essential to create an effective multi-field coupling model that captures the damage and chemical reaction-driven self-healing processes.

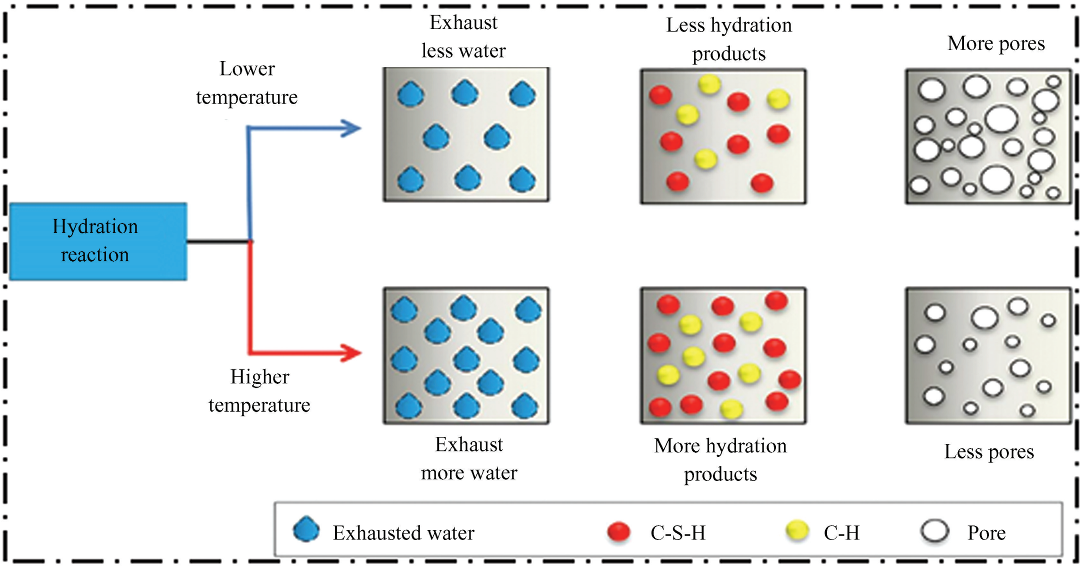


Fig. 5 **Examples of temperature effect on hydration reaction of concrete**[35]

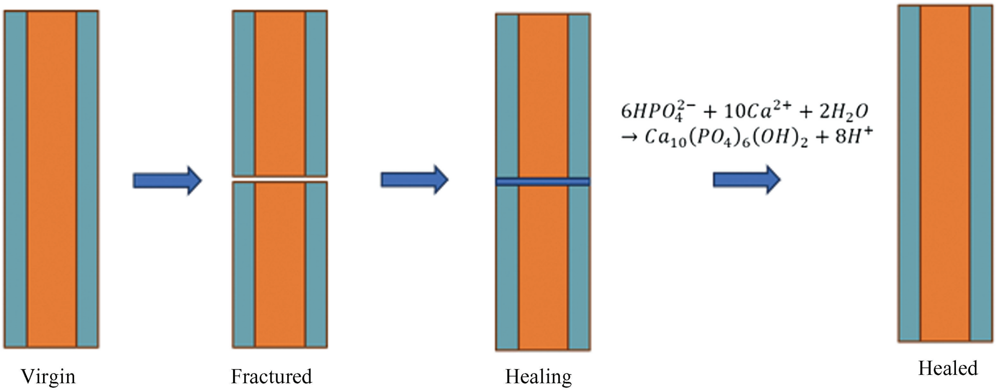


Fig. 6 **Inspiration from self-healing of bones**

From the above introduction, it is evident that with the rapid advancement of science, technology, and society, existing industrial equipment is facing increasingly complex operating environments, accompanied by higher demands for service life and reliability. Advanced materials often operate in environments that involve thermal, chemical, and mechanical interactions, which can significantly impact their performance and functionality. By conducting in-depth research on multi-physical field coupling problems, readers can gain insights into the mechanisms underlying changes in solid structures and energy. This, in turn, provides a deep insight into the functional and failure mechanisms of equipment and devices. The following section will introduce recent advances in theoretical models within the thermo-chemo-mechanical coupling field.

2 Recent Advances in Theoretical Modelling

The development of non-equilibrium thermodynamics (or thermodynamics of irreversible processes) laid the foundation for the establishment of a rigorous theoretical framework for coupled multi-field problems. In this context, the local equilibrium hypothesis of linear non-equilibrium thermodynamics allows for the extension of static thermodynamics to continuum thermodynamics. The temperature and entropy in various irreversible processes retain the definitions from equilibrium thermodynamics, thus enabling the thermodynamic laws to be expressed in integral forms involving these additive quantities. At the same time, the state variables can be locally represented at any given time, and the relationships between them remain unchanged from those in equilibrium thermodynamics, even when the system deviates from equilibrium. Non-equilibrium thermodynamics also indicates that entropy is generated non-negatively at any moment and position within the system, and the rate of entropy production can be expressed as a function of the irreversible process variables. This, in turn, determines the derivation of the constitutive equations, reflecting the system's dynamic response to internal or external changes, which is the Classical Continuum Mechanics (CCM) employing non-equilibrium thermodynamics. The theoretical framework of CCM is presented in Table 1 based on the work of Anand and Govindjee[45]

Table 1 Theoretical framework of classical continuum mechanics (CCM)

Laws	Formulas
The mass balance	$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0$
The balance of linear momentum	$\boldsymbol{\sigma} \cdot \nabla + \rho b = \rho \dot{\boldsymbol{v}}$
The balance of angular momentum	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{T}}$
The first thermodynamic law	$\rho_R \dot{e} = \boldsymbol{S} : \dot{\boldsymbol{E}} + q_R - \nabla_R \cdot \boldsymbol{j}_R^q$
The dissipation inequality	$\rho_R (\vartheta - \frac{\partial e}{\partial s}) \dot{s} + (\boldsymbol{S} - \rho_R \frac{\partial e}{\partial \boldsymbol{E}^{\mathrm{r}}}) : \dot{\boldsymbol{E}}^{\mathrm{r}} + \boldsymbol{S} : \dot{\boldsymbol{E}}^{i} - \frac{\boldsymbol{j}_R^q}{\vartheta} \cdot \nabla_R \geqslant 0$
The state equations	$\vartheta = \frac{\partial e}{\partial s}, \boldsymbol{S} = \rho_R \frac{\partial e}{\partial \boldsymbol{E}^{\mathrm{r}}}$
The evolving equations	$\dot{\boldsymbol{E}}^{i} = \boldsymbol{L}^{i} : \boldsymbol{S} + \boldsymbol{L}^{i\vartheta}(-\nabla_R \vartheta), \dot{\boldsymbol{j}}_R^q / \vartheta = \boldsymbol{L}^{\vartheta i} : \boldsymbol{S} + \boldsymbol{L}^{\vartheta}(-\nabla_R \vartheta)$

The Phase Field Method (PFM) is a robust computational technique used to simulate the evolution of micro-structures in materials, particularly when dealing with complex phenomena like phase transitions[46], crack propagation[47-48], and other interfacial phenomena[49-50]. It is widely applied in material science, mechanics, and other fields involving dynamic changes in structure or composition. The core idea of PFM is to represent the interfaces or boundaries between different phases (e. g., solid-liquid, solid-solid, or different material phases) by a smooth, continuous field that varies spatially and temporally. Instead of directly modeling the sharp boundaries, the method uses a "phase field" variable, typically denoted as ϕ, which is a scalar field that smoothly transitions between different phases. Fig. 7 presents a schematic of a diffuse crack in a one-dimensional domain[51]. This field variable distinguishes between multiple phases via a smooth transition, where ϕ $[0, 1]$ denotes the undamaged state ($\phi = 0$) and the fully damaged state ($\phi = 1$) of the material. PFM can also be derived from the framework of non-equilibrium thermodynamics. As illustrated in Table 2, we extend the derivation of the fracture phase field constitutive relations based on the previous Fig. 8.

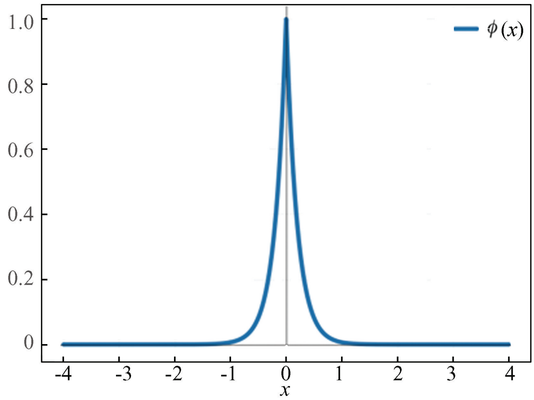


Fig. 7 Schematic representation of a diffuse crack in one dimensional domain

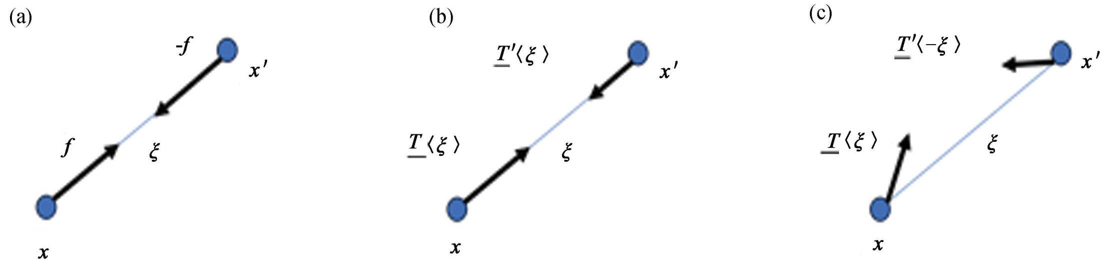
Peridynamics (PD) is a non-local theory proposed by Silling[52] at the Sandia National Laboratories in the United States. Based on the concept of non-local internal force integration, it converts the differential equations of continuum mechanics into integral form. This approach uses a unified mathematical framework to describe both continuous and discontinuous spaces, avoiding issues such as the non-existence of local spatial derivatives in discontinuous regions.

PD can be classified into three types based on the development of force densities (as shown in Fig. 8): Bond-Based Peridynamics (BB-PD), Ordinary State-

Based Peridynamics (OSB-PD), and Nonordinary State-Based Peridynamics (NOSB-PD)[53]. BB-PD involves equal and opposite forces between pairs of points, making it suitable for simple bond-based models. OSB-PD, on the other hand, allows for unequal pairwise force densities and can model more complex material behaviors by considering the entire horizon of each point. NOSB-PD extends this concept further by introducing force densities in arbitrary directions, modifying the forces based on additional material properties or internal states, which enables the modeling of highly complex, nonlinear material behaviors. The formulations in PD can also be derived from non-equilibrium thermodynamics and proven to be thermodynamically consistent, similar to CCM[54-56]. For instance, Schaller et al.[56] proposed a thermodynamically consistent formulation for open systems within the framework of continuum-kinematics-inspired PD, which has been compared with the formulation in CCM, as shown in Table 3.

Table 2 Theoretical framework of phase field method (PFM)

Laws	Formulas
The first thermodynamic law	$\rho_R \dot{e} = \boldsymbol{S}:\dot{\boldsymbol{E}} + q_R - \nabla_R \cdot \boldsymbol{j}_R^q + \nabla_R \cdot (\boldsymbol{G} \cdot \dot{\phi})$
The dissipation inequality	$\rho_R\left(\vartheta - \frac{\partial e}{\partial s}\right)\dot{s} + \left(\boldsymbol{S} - \rho_R \frac{\partial e}{\partial \boldsymbol{E}^{\mathrm{r}}}\right):\dot{\boldsymbol{E}}^{\mathrm{r}} + \boldsymbol{S}:\dot{\boldsymbol{E}}^{i} + \left(\rho_R \frac{\partial e}{\partial \phi} - \nabla_R \cdot \boldsymbol{G}\right)\dot{\phi} + \left(\boldsymbol{G} - \boldsymbol{\rho_R} \frac{\partial \boldsymbol{e}}{\partial \nabla_{\boldsymbol{R}} \boldsymbol{\phi}}\right):\nabla_{\boldsymbol{R}} \dot{\boldsymbol{\phi}} - \frac{\boldsymbol{j}_R^q}{\vartheta} \cdot \nabla_R \vartheta \geqslant 0$
The state equations	$\vartheta = \frac{\partial e}{\partial s}, \boldsymbol{S} = \rho_R \frac{\partial e}{\partial \boldsymbol{E}^{\mathrm{r}}}, \boldsymbol{G} = \rho_R \frac{\partial e}{\partial \nabla_R \phi}$
The evolving equations	$\dot{\boldsymbol{E}}^{i} = \boldsymbol{L}^{i}:\boldsymbol{S} + \boldsymbol{L}^{i\vartheta}(-\nabla_R \vartheta), \dot{\boldsymbol{j}}_R^q/\vartheta = \boldsymbol{L}^{\vartheta i}:\boldsymbol{S} + \boldsymbol{L}^{\vartheta}(-\nabla_R \vartheta)$ $\dot{\phi} = \boldsymbol{L}^{p}\left(\rho_R \frac{\partial e}{\partial \phi} - \nabla_R \cdot \boldsymbol{G}\right)$



Bond-Based Peridynamics (BB-PD)

Ordinary State-Based Peridynamics(OSB-PD)

Nonordinary State-Based Peridynamics(NOSB-PD)

Fig.8 Three kinds of PD[53]

CCM, PFM, and PD can all be unified within the framework of non-equilibrium thermodynamics. Their characteristics, advantages, and disadvantages are summarized in Table 4. Although the theory of nonequilibrium thermodynamics provides the basic methods for theoretical modeling of coupled problems, simulating these complex coupled behaviors requires a thorough understanding of the interaction mechanisms between various thermodynamic processes, as well as a reasonable characterization of each process's contribution to the system's free energy and dissipation. Existing theoretical models have extensively discussed species transport-deformation problems for various materials, with some also addressing the coupling of chemical reactions, such as oxidation and degradation, with heat transfer and deformation. These chemo-mechanical coupling methods either follow traditional theories for reactive systems of fluid mixtures, where the mass fractions of all components are treated as independent state variables to describe the chemical processes, or they reasonably distinguish the effects of species transport and chemical reactions on the solid's free energy and dissipation processes. The following is a review of some thermo-chemo-mechanical coupling theoretical models within the framework of non-equilibrium thermodynamics.

Table 3 Comparison of governing equations in PD and CCM

Laws	Formulas
The balance of linear momentum	
PD	$\rho_R D_t v = \int_{H_0} \boldsymbol{p}_0^l d V^l + \boldsymbol{b}_{\boldsymbol{R}}^{\mathbf{ext}}\textbf{subject to}\int_{\boldsymbol{B}_0}\int_{\boldsymbol{H}_0} \boldsymbol{p}_0^l d V^l dV = \int_{\partial B_0} t_0^{\text{ext}} dA$
CCM	$\rho_R D_t \boldsymbol{v} = \nabla\cdot \boldsymbol{P} + \boldsymbol{b}_R^{\text{ext}}\text{subject to}\boldsymbol{P}\cdot\boldsymbol{N} = t_0^{\text{ext}}$
The balance of angular momentum	
PD	$\int_{H_0} \boldsymbol{\xi}\times\boldsymbol{p}_0 d V^l = 0$
CCM	$\varepsilon : [\boldsymbol{F}\cdot\boldsymbol{P}^{\mathrm{T}}] = 0$
The first thermodynamic law	
PD	$\int_{H_0} \rho_R D_t u^l d V^l = -\int_{H_0} q_0^l d V^l + F_0^{\text{ext}} + \int_{H_0} \boldsymbol{p}_0^l \cdot D_t \boldsymbol{\xi}^l d V^l \text{subject to}\int_{B_0}\int_{H_0} q_0^l d V^l dV = \int_{\partial B_0} Q_0^{\text{ext}} dA$
CCM	$\rho_R D_t u = -\nabla\cdot\boldsymbol{Q} + F_0^{\text{ext}} + \boldsymbol{P}:\nabla\cdot\boldsymbol{F} \text{ subject to } \boldsymbol{Q}\cdot\boldsymbol{N} = Q_0^{\text{ext}}$
The balance of entropy	
PD	$\vartheta\int_{H_0} \rho_R^l D_t s^l d V^l = -\int_{H_0} q_0^l d V^l + F_0^{\text{ext}} + \vartheta S_0 + D_0 \text{ subject to}\int_{B_0}\int_{H_0} q_0^l d V^l dV = \int_{\partial B_0} Q_0^{\text{ext}} dA$
CCM	$\vartheta\rho_R D_t s = -\nabla\cdot\boldsymbol{Q} + F_0^{\text{ext}} + \vartheta S_0 + D_0\text{subject to } \boldsymbol{Q}\cdot\boldsymbol{N} = Q_0^{\text{ext}}$
The dissipation inequality	
PD	$D_0 = \int_{H_0} \rho_R^l D_t \boldsymbol{\xi}^l d V^l - \int_{H_0} \rho_R^l D_t \psi^l d V^l - \vartheta S_0 \geqslant 0$
CCM	$D_0 = \boldsymbol{P}:\nabla\cdot D_t\boldsymbol{F} - \rho_R D_t\psi - \vartheta S_0 \geqslant 0$

Table 4 Comparison of different methods

Model	Features	Advantages	Disadvantages
CCM	Based on the assumption of material continuity, describing the mechanical behavior of objects. Assumes the material is homogeneous and continuous, ignoring the microstructural effects. Suitable for most macroscopic material and structural analysis.	Simple and efficient, suitable for common engineering problems. Clear mathematical formulation, mature computational models. Handles most macroscopic problems effectively.	Ignores microstructural and local effects. Cannot accurately describe complex phenomena like fracture and phase transitions.
PFM	Introduces a phase field variable to describe the distribution and evolution of different phases in materials. Suitable for describing complex phenomena such as phase transitions and crack propagation. Based on partial differential equations.	Can accurately describe complex processes like phase transitions, crack propagation, and interface evolution. Suitable for multiscale problems and captures microstructural effects.	High computational cost, especially in high-dimensional and complex scenarios. Requires precise modeling of phase field variables for reasonable results.
PD	Uses molecular dynamics or atomic-scale methods to describe the behavior of solid materials at the microscopic level. Considers the microstructure and local effects of materials. Often requires significant computational resources.	Can accurately capture physical phenomena at the microscopic scale, such as material fracture, friction, and microstructural evolution. Simulates realistic material behavior.	Computationally complex and time-consuming, typically limited to small-scale and short-time simulations. Requires extensive atomic-level data input, making model setup complex.

2.1 Thermo-Mechanically Coupling Models

Duhamel and Neumann made significant contributions to the early development of thermoelasticity theory in the 19th century[57-58]. They established fundamental equations to describe the interactions between thermal and mechanical effects, primarily focusing on thermal expansion under small deformation conditions. These foundational works provided a basis for integrating thermodynamics with solid mechanics. Although Duhamel proposed the thermoelastic equations coupling deformation fields and temperature fields as early as 1837, it was until 120 years later, with the publication of papers by Biot[59] and Lessen[60] in 1956, that new impetus was brought to this area of research. In the years following the publication of Biot's paper, numerous significant studies on coupled thermoelasticity emerged. For example, Weiner[61] published a proof of the uniqueness of solutions for coupled thermoelastic equations. Chadwick and Sneddon[62], and Lockett[63], analyzed wave propagation (including Rayleigh waves) in thermoelastic media. In classical thermoelastic mechanics, the temperature problem is first solved, and then the stress is derived from the Duhamel-Neumann equation. However, both theoretical analyses and experiment results demonstrate that displacement body displacement changes with temperature variations, and vice versa. Therefore, it is necessary to consider the time derivative of the first stress invariant in the equations of motion and heat conduct. The coupled thermoelastic theory, along with the generalized thermoelastic theory proposed later by Lord and Shulman[64] in 1967, became a central focus of research in this area.

In the 1950s and 1960s, the introduction of irreversible thermodynamics significantly advanced thermo-mechanical coupling theories. The work of Prigogine et al.[65] established an intrinsic connection between heat flux and stress. The internal variable method emerged to describe material behavior under thermo-mechanical interactions, including creep and stress relaxation[66-67]. From the late 20th century to the present, research expanded to high-temperature environments and large deformation scenarios. Thermo-viscoelastic and thermo-viscoplastic models rapidly evolved to capture time-dependent behaviors. Researchers developed precise thermo-mechanical coupling theories for metals and polymers under high-temperature and large-strain conditions. For instance, Dippel et al.[68] developed a three-dimensional thermo-mechanically coupled material model for elastomers at finite deformations. This model effectively captures the temperature dependence of mechanical properties and accounts for self-heating of the elastomers caused by dynamic deformation. Anand et al.[69] developed a thermo-mechanically coupled elasto-viscoplasticity model to describe the large deformation behavior of amorphous polymers, accounting for both strain rate and temperature dependencies. When further refined[70], this model holds significant potential for simulating the thermo-mechanical behaviors of components and structures made from such materials, as well as for aiding in the analysis of various polymer processing operations. Shao et al.[71] established a theoretical model to predict the variation of the Taylor-Quinney coefficient in glassy polymers within the thermodynamic framework of internal state variables. The established approach simultaneously accounts for both strain-softening and strain-hardening processes. Krairi et al.[72] introduced a novel constitutive model to characterize the response of thermoplastic polymers under non-isothermal conditions. This model integrates linear viscoelasticity, viscoplasticity, and thermal effects, all formulated within the framework of non-equilibrium thermodynamics. The thermo-viscoelastic response is captured by general hereditary integrals, while the viscoplastic component accounts for both isotropic and kinematic hardening effects. Wang et al.[73] proposed a coupled thermo-mechanical constitutive model for concrete, designed to characterize its mechanical behaviors at varying temperatures, all within a thermodynamic framework. The model creatively incorporates the coupling of thermal effects, thermo-plastic hardening and damage evolution within the energy potential function.

Over the past decade, PFM has gained significant attention due to its numerous advantages. As a continuous approach, PFM deals fracture as a phase transformation, avoiding the crack-tip singularities commonly found in discontinuous approaches. This framework directly determines crack profiles by solving governing equations, eliminating the need for special fracture criteria. PFM has been extensively applied to failure analyses, especially for 3D modeling and multi-crack scenarios. The first exploration of multi-field problems including thermal effects in PFM was carried out by Sicsic et al.[74] and Bourdin et al.[75]. Subsequent studies focused on advancing computational methods and applying them to a variety of materials including ceramics[76], concrete[77] and rock[78], showcasing its versatility in addressing complex fracture phenomena. For example, Kumar[79] developed a thermodynamically consistent framework for a thermo-mechanically coupled PFM tailored to thin-walled structures, enabling the incorporation of three-dimensional constitutive thermo-mechanical equations for material behavior. To address common numerical challenges, such as Poisson and volumetric locking pathologies, the proposed models are enhanced with an Enhanced Assumed Strain (EAS) formulation, ensuring more accurate and stable simulations. Yue et al.[80] introduced a thermo-mechanical model for mixed-pattern fractures using PFM. This model effectively addresses challenges in simulating thermally induced cracking, particularly for complex fracture modes. To account for various failure patterns under thermo-mechanical conditions, the constitutive formulation incorporates a unified failure criterion that considers both tensile and shear strengths, enhancing this model's versatility in predicting diverse fracture behaviors.

PD offers unique advantages for solving solid material and structural failure problems in engineering mechanics, enabling the effective simulation of thermo-mechanical crack initiation, propagation, and branching in materials like rock and concrete. For example, Guan et al.[81] developed a thermo-mechanical coupled BB-PD model that incorporates complete thermomechanical anisotropy by incorporating an anisotropic mechanical BB-PD framework. Employing a staggered coupling strategy, the key parameters in both physical fields are dynamically updated, which allows for accurate computation of mechanical behavior under thermo-mechanical coupled conditions. Zhang et al.[82] proposed a comprehensive thermo-mechanically coupled model that incorporated the frost heave influence through OSB-PD theory, allowing for the analysis of cracking behaviors in frozen rocks. To enhance the OSB-PD model's constitutive equations, they incorporated a coupling term to capture the interactions between thermal and structural effects, as well as an equivalent pressure density term to account for the frost heave phenomenon. Yang et al.[83] proposed a thermo-mechanically coupled PD model to simulate the thermo−mechanically coupling material behaviors and thermally induced fracture in solid materials. They implemented a novel multi-horizon scheme, where the thermal field was solved using a horizon different from that of the mechanical field. This approach enables applications of distinct degrees of non-locality to different physical fields, enhancing this model's flexibility and accuracy.

2.2 Chemo-Mechanically Coupling Models

According to the different coupling scales of diffusion and reaction in space and time, the processes can be classified into three categories: diffusion-dominated, reaction-dominated, and diffusion-reaction jointly dominated. In the diffusion-dominated case, the reaction kinetics is limited by the rate at which reactants diffuse to the reaction interface. This means that the transport speed of the reactants through space is slower than the actual chemical reaction rate, making it the rate-limiting step of the overall reaction. In the reaction-dominated case, the reaction kinetics is limited by itself, i.e., the rate at which reactants are converted to products. In this scenario, the reactants can rapidly reach the reaction interface, but the activation energy barrier of the chemical reaction is high, resulting in a slower reaction rate. In the diffusion-reaction jointly dominated case, both the reaction rate and the diffusion rate are not fast enough, and together, they determine the overall reaction rate.

The species transport in the solid phase and the chemical reactions undergoing between these species and the solid are closely coupled with the material's heat transfer and deformation processes. While both of these processes can result in changes in the material's composition and cause volumetric expansion or contraction, thus affecting the material's macroscopic mechanical behavior, their effects on the solid's microstructure and material properties are not the same, and their interactions with stress (or strain) also differ. Considering the varying coupling scales of diffusion and reaction across space and time in different scenarios, models for species diffusion-deformation coupling, chemical reaction-deformation coupling, and diffusion-reaction-deformation coupling are introduced accordingly.

2.2.1 *Species diffusion-deformation coupling models*

The initial exploration of species transport-deformation coupling problems in solids can be traced back to the late 19th century in the work of Gibbs[84], who established a thermodynamic theory for the finite deformation of elastic solids capable of absorbing liquids, assuming that both solids and liquids were in equilibrium. Biot[85] linked a similar thermodynamic theory to Darcy's law to describe fluid movement within porous elastic solids, resulting in the theory of poroelasticity, which remains commonly employed in the analysis of various species diffusion-deformation phenomena, including clay consolidation and biological tissue deformation. Bowne and Truesdell[86] also developed a theory of mixtures, providing balance equations for mass, momentum, and energy for each component, and derived the global entropy inequality for the mixture system from the second law of thermodynamics. Rice and Cleary[87] applied poroelastic theory to solve fundamental stress-diffusion coupling problems. Larché and Cahn[88], building on Gibbs' theory, proposed linear and nonlinear theories for describing solvent-absorbing polymer materials and solute atom vacancy diffusion in crystals. Subsequently, Weitsman's theory[89] bridges concepts of Gibbs, Larché-Cahn, and Truesdell, as it uses irreversible thermodynamics to give the global equilibrium equations for a solid solvent-solute mixture, but it does not provide corresponding evolution equations for each component. This theory explains how stress in elastic and viscoelastic polymer materials aids the diffusion of moisture. Valançon et al.[90] also used irreversible thermodynamics to establish a coupled theory for describing water and gas transport in polymers.

As the applications of these hyperelastic polymers continue to expand, theoretical research on them has also deepened. From the early studies on species transport-deformation coupling in gels by Tanaka et al.[91], to more recent works by Duda et al.[92], Hong et al.[93-94], and Chester [95-96], various diffusion-deformation coupling models have emerged that can more comprehensively describe problems such as swelling, dehydration, and stress-induced osmotic flow in these materials. For example, Hong et al.[97], Wallmersperger et al.[98], and Boissonade[99] considered the influence of charges and extended the field theory models to polyelectrolyte gels. Among them, Hong et al.[97] incorporated the effects of polymer network stretching, solvent, ion, and polymer mixing, as well as colloidal polarization in their electrochemical-finite deformation coupling theory, and analyzed the coupled deformation of gels under electrochemical environments through numerical examples. Anand[100] formulated a PFM that couples Cahn-Hilliard-type species diffusion under large elastic-plastic strains of a material. This framework considers swelling and phase segregation effects induced by the diffusive species, providing a comprehensive approach to describe these interactions. Pan and Zhong[101] applied polymer swelling theory to natural fiber-reinforced composites and used the internal variable thermodynamics approach to describe the deterioration of mechanical properties in materials induced by moisture absorption. All of these theoretical models employed stress-coupled species diffusion control equations and constitutive relations for solids with chemical constraints to express the coupling between mechanical deformation and species diffusion.

Meanwhile, with the rapid development of new energy conversion and storage devices such as Li-ion batteries and fuel cells, there has been a growing understanding of the solid-state diffusion-stress coupling problem in solid electrode and electrolyte materials. For example, in Li-ion batteries, during the charging and discharging process, lithium ions embed into or de-intercalate from the electrode material, causing changes in the electrode volume. This volumetric change can induce significant internal stresses within the battery structure, which, in turn, alters the movement of lithium ions. This mutual coupling process ultimately impacts the electrochemical performance of the battery. Such species transport-stress bidirectional coupling issues are commonly presented in various solid electrode materials. Christensen and Newman[102] were among the first to investigate volumetric changes of spherical particles due to lithium intercalation, as well as the solute concentration and stress distribution. Swaminathan et al.[103] developed a theory of electro-chemo-elastic coupling for point defect ionic solids, explaining the bidirectional couplings between mechanical and electrochemical forces. Haftbaradaran et al.[104] established a continuum model to describe the nonlinear behavior of high-concentration lithium-ion diffusion-deformation coupling in electrode materials under high stress. Zuo and Zhao[105] established a PFM that couples finite deformation, lithium diffusion, crack propagation and stress evolution. This model can be used to investigate the stress evolution of spherical silicon particle in consideration of elastic softening and plastic flow at finite deformation. Di Leo et al.[106] developed a PFM coupling Cahn-Hilliard-type species diffusion in the case of large deformation and applied it to describe phase-separating in Li−ion electrodes. Zhang et al.[107] proposed a variational framework that integrates multi-field dissipative phenomena to model large plastic deformation and fracture induced by diffusion and mechanical constraints during the two-phase lithiation of silicon electrodes. Wang and Tong[108] developed a multi-physics PD model that integrates mechanical deformation, Li-ion diffusion and crack growth to analyze postponed fracture in electrodes of Li-ion battery. Their model effectively simulates lithium-ion accumulation near crack tips due to stress field concentrations and captures material embrittlement caused by lithium reactions.

2.2.2 *Chemical reaction-deformation coupling models*

Metals and alloys are widely used as structural materials in various industrial fields. When exposed to oxidizing atmospheres at high temperatures, their surfaces gradually oxidize to form a brittle oxide layer, which leads to changes in the material's composition and properties. This process is also accompanied by a continuously increasing oxidation strain, further affecting the material's mechanical behavior. A large number of researchers have developed theoretical models to describe the stress evolution in metal substrates and oxide layers at high temperatures. For example, Zhao and Huntz[109] analyzed the deformation problem during single-sided oxidation of certain metal materials, while Evans[110] investigated the nonlinear creep behavior of oxidized metals and theoretically predicted the stress evolution process of the metal and oxide layers. The earliest research on the mechanisms of oxidation strain generation can be traced back to Pilling and Bedworth[111], who argued that the difference in molar volumes between metals and their oxides was the cause of isotropic oxidation deformation. Clarke[112-113] introduced the fundamental assumption, known as the Clarke assumption, which posits that the oxidation is driven by the inward diffusing oxygen and the outward diffusing metal, explaining the variation of oxidation strain and suggesting that the growth rate of the oxide layer thickness is directly proportional to the lateral strain rate of the oxide layer. This assumption was subsequently widely accepted and applied in later research. For example, Panicaud et al.[114] used Clarke's model to predict the temporal variation of oxidation stress at constant temperatures, while Favergeon et al.[115] established a mesoscopic model to address the diffusion-stress coupling issue during the high-temperature oxidation of zirconium alloys.

With the rapid development and application of polymers, mechanochemistry methods have gradually been applied to polymer preparation and processing, such as ultrasonic irradiation, pan milling, and high-speed stirring. Due to the characteristics of polymer chains, including their long molecular length, multiple structural hierarchies formed by covalent bonds, and sensitivity to stress and temperature, they are prone to activation, degradation, cross-linking, and copolymerization under stress. This provides new pathways for the preparation, modification, and processing of polymer materials. Despite extensive research discussing the design, synthesis, and performance characterization of mechanochemically responsive polymers, only a few studies have established theoretical models capable of describing the interaction between the macroscopic stress state of specific mechanochemically responsive polymers and mechanochemical reactions. For instance, Silberstein et al.[116], Wang et al. [117] and Silberstein et al. [118] developed respective elastic and viscoelastic mechanical models for glassy mechanochemically responsive polymers and stress-responsive elastomers. These models employed reaction kinetics with the concentration of chemically responsive groups as the basic variable to quantify the mechanochemical reaction process and linearly relate the force on polymer chains to the reaction activation energy[119]. However, these results only align with some experimental findings. Recently, Takaffoli et al.[120] established a viscoelastic theory that more thoroughly characterizes the strain rate-dependent behavior and the coupling interactions of mechanochemical reactions in mechanochemically responsive polymers. They employed the generalized Maxwell model to represent the viscoelastic response of polymer chains in elastomers. As experimental methods provide an increasingly deep and enriched understanding of various behaviors in mechanochemically responsive polymers, developing a general theoretical model that can reasonably and rigorously describe the mechanical-chemical coupling phenomena observed in experiments has become a trend in the field of mechanochemistry research.

2.2.3 *Diffusion-reaction-deformation coupling models*

In addition to the diffusion-stress coupling, the reaction-diffusion-deformation coupling in the thermal oxidation process is a more critical aspect of the aging issue in polymers and other materials. Consequently, many related theoretical models have been developed[121]. In particular, Colin et al.[122-123] proposed a mechanical description of the reaction-diffusion phenomenon at the molecular scale for thermal oxidation. Olivier et al.[124-125] established a reaction-diffusion-mechanical coupling model based on irreversible thermodynamics to describe the stress localization behavior that ultimately leads to fiber-matrix separation during the thermal oxidation of composites. Gigliotti et al.[126], building on Olivier's work, compared the experimental and theoretical predictions of thermal oxidation shrinkage strain in carbon fiber-epoxy composites. However, these studies provide a limited description of the reaction-diffusion and mechanical coupling effects, as they only present the effect of the chemical process on the mechanical state of solids, with minimal discussion on how the material's stress-strain state influences the reaction-diffusion process. A more comprehensive theoretical framework for polymer oxidation was developed by Gigliotti and Grandidier[127], and later expanded by Gigliotti et al.[128]. They derived a CCD (Classical Continuum Damage) model and developed a thermo-chemo-mechanically coupling model for the thermal oxidation of polymer-based composites. This model specifically examines the impact of strain and strain gradient distribution on the oxygen diffusion-reaction process within polymers. Wang et al.[129] coupled stress with oxidation reaction-diffusion through a stress-coupled reaction kinetics equation and diffusion equation, establishing an elastoplastic model for zirconium oxidation-diffusion-stress coupling. Rajagopal et al.[130] introduced independent internal variables and their dynamic equations in his CCM model to quantify polymer damage caused by reactions, thereby describing changes in the material's mechanical properties. This approach disregards material transfer and specific chemical reaction processes, instead focusing on the alterations in the material's macroscopic mechanical properties.

PFM and PD have become popular for addressing diffusion-reaction-mechanically coupled problems due to their advantage in capturing microstructural evolution, such as crack initiation. Wang et al.[131] proposed a reaction-diffusion PFM that incorporates two forms of Li (one for diffusion and the other for alloying reaction) to explore remaining unclear fundamental mechanism. This model combines both Li diffusion and alloying reaction, and also couples with elasto-plastic deformation. It allows for the exploration of the role of the inactive phase in the morphology and stress variations of Se-doped Ge electrodes during lithiation. Mathew et al.[132] established a PFM that uses the Allen-Cahn equation to characterize the evolution of the non-conserved phase field variable, and the Cahn-Hilliard equation to describe the dynamics of concentration field, for modelling the diffusion-controlled stress corrosion cracking process. Luo et al.[133] established a diffusion-mechanically coupling PFM, in which the PFM is applied to predict the fracture of sulfate-damaged concrete. The PFM transforms the discrete sharp crack surface into a regularized crack, facilitating its coupling with the species transport model. Liu et al.[134] proposed a fully coupled PD model to analyze the reaction-diffusion-mechanical behavior of sulfate attack in concrete. Since ion diffusion and chemical reactions occur simultaneously, sulfate ions in the concrete are described by reaction-diffusion equations. This model indicates that the swelling force generated by reaction products is the dominate driving force behind macrocrack propagation during the transport process.

2.3 Thermo-Chemo-Mechanically Coupling Models

The research on thermo-chemo-mechanical coupling issues related to solid species transport, heat transfer, mechanical deformation, and chemical reactions, as reviewed above, encompasses numerous fields of modern science, technology, and industrial applications. However, to simplify analysis, the aforementioned studies and related theoretical models focus on specific types of problems and consider only certain coupling phenomena or some indirect coupling effects. For example, studies on species transport−deformation coupling in smart materials and biomaterials typically consider only the coupling between species diffusion and stress, while neglecting or greatly simplifying the effects of temperature and chemical reactions. Similarly, models addressing high-temperature oxidation of materials often only examine the chemical reaction expansion effect under isothermal conditions, ignoring expansion strains induced by the diffusion medium or neglecting the influence of stress on the reaction kinetics. Over the course of the last two decades, the study on thermo-chemo-mechanical coupling modeling is rapidly increasing.

In early years, some theoretical work in CCM (Classical Continuum Mechanics) has continuously advanced on fully thermo-chemo-mechanically coupled problems in solids. For instance, Rambert et al.[135-136] first established a CCM model for the multi-field coupling problem of polymer materials. Their studies differentiated the effects of stress/strain magnitude and stress/strain gradient on the mass transfer process, indicating that the stress gradient promotes the diffusion process of gases and moisture within the polymer. André and Wriggers[137] developed a CCM model incorporating viscous and inelastic effects. This model focuses on describing the reaction kinetics and thermo-mechanical behavior during the vulcanization process of rubber materials. Hu and Shen[138], starting from the Gibbs equation of an open thermodynamic system and the second thermodynamic laws, established a CCM model for thermo-chemo-mechanical coupling in solids and its variational principle, using linear phenomenological laws to express the coupling relationships among irreversible strain rates, heat flux vector, diffusion flux vector, and chemical reaction rate. Anand and his colleagues[139-140] developed a CCM model for finite deformation, fully three-dimensional problems. This model couples high-temperature elastic-viscoplastic deformation of materials with oxygen and hydrogen diffusion, ultimately leading to chemical reactions. Zhang and Zhong[141-142] proposed a thermodynamic theoretical framework for thermo-chemo-mechanical interactions in chemically active solids. They introduced the reaction extent and diffusion concentration as two kinds of independent variables to reflect the impact of chemical reactions and material diffusion on system energy, allowing explicit expression of changes in the solid's microstructure caused by chemical reactions. Later, Zhang et al.[143] used the displacement potential method to solve the thermo-chemo-elastic coupling model, obtaining analytical solutions under steady-state and quasi-static conditions. They analyzed the impact of solid-state chemical reactions and material diffusion on the deformation of core-shell structures, verifying the applicability of their analytical method. Qin et al.[144-145] extended Zhang's theory to large deformation plasticity problems and developed an exponential reaction kinetics model that considers the effects of strain, enabling the description of chemical processes far from equilibrium in multi-field coupling problems. Salvadori et al.[146] established a thermo-chemo-mechanical coupling framework for small deformations based on non-equilibrium thermodynamics, focusing on trapping reactions. The concentration of diffusing substances was divided into two parts: one part is trapped and cannot participate in the diffusion process, while the other part remains free and can diffuse. Zhao et al.[147] developed a thermodynamically consistent continuum-level oxidation model that integrates diffusion, oxidation reactions and large viscoelastic deformation. This model effectively simulates oxidation processes in complex geometries, eliminating the need for artificial interface marking and tracking. The multi-field coupling behavior in early-age concrete is crucial, gaining significant attention[148-152]. For example, Wang et al.[153] developed an chemo-thermo-mechanical damage model for early-age concrete, integrating concepts from CCM and continuum damage mechanics. The evolution laws governing mechanical damage are derived from work-conjugate elastoplastic damage energy release rates, effectively capturing the effects of microcrack closure and reopening, anisotropy, and concrete aging in relation to the degree of hydration.

PFM significantly advanced studies on simulating early-age cracking behavior in concrete and thermo-chemo-mechanical behaviors of other materials. For example, Nguyen et al.[154] considered the coupled effects among cement hydration, heat transfer, and the crack phase field, developing a chemo-thermo-mechanical multi-field coupled PFM. This model effectively captures the influence of the competition between autogenous shrinkage and thermal expansion/contraction on the evolution of early-age concrete cracks. Afshar et al.[155] developed a PFM at finite strain theory for solid mechanics problems involving the coupling of species transport within a host material, sharp interface reactions between the species and the host, as well as mechanical deformation and stress. The theory distinguishes between diffusion-limited and reaction-limited kinetics, providing insight into how sharp reaction fronts develop in each case. Additionally, the phase-field formulation allows for the application of wetting boundary conditions, which are crucial for accurately simulating experimentally observed reaction front morphologies. Min et al.[156] proposed a chemo-thermo-mechanical coupled PFM, enabling the complete fracture process of thermal barrier coatings to be captured. This contribution represents a significant advancement over existing PFM. The model considers the couplings among material oxidation, thermal conduction and damage, with the fundamental differential equations derived in strict accordance with the laws of thermodynamics.

At the present, PD model for chemo-thermo-mechanically coupling problems has also become a research hotspot. Sun et al.[157] proposed a chemo-thermo-mechanically coupled PD – FEM model for predicting fracture in early-age concrete, accounting for interactions in thermal transfer, hydration heat, creep, strength evolution, fracture, and the impact of cracks on temperature and hydration fields. This chemo-thermo-mechanically coupled problem is solved in a staggered manner within the classical finite element and NOSB-PD framework. This approach enables the seamless accommodation of fracture in early-age concrete, with NOSB-PD providing an elegant treatment of discontinuities. Li et al.[158] proposed a thermo-chemo-mechanically coupled BB-PD model, integrating the ceramics oxidation kinetics with thermo-mechanical BB-PD. Unlike classical thermo-mechanically coupled models, the proposed model accounts for the effects of the reaction extent on the erosion resistance of ceramic materials, providing a more comprehensive understanding of their behavior under high-temperature conditions. Xiang et al.[159] derived the constitutive equations governing mass, linear momentum, and energy to describe the interactions among various fields. Additionally, they formulated evolution equations to govern the fluxes of species and heat. These equations are systematically constructed based on the principles of chemical kinetics and the inequality of energy dissipation, ensuring a thermodynamically consistent framework. Zhou et al.[160] proposed a thermo-hydro-chemo-mechanically coupled PD model for fractured rock masses to simulate fluid-driven cracking as well as the effects of water pressure and temperature under thermo-hydro-chemo-mechanically coupled conditions. This model is capable of simulating issues such as fluid−driven cracks and chemical corrosion.

3 Challenges and Prospects

This paper has provided a corresponding review of the thermo-chemo-mechanical theoretical models within the framework of non − equilibrium thermodynamics, including CCM, PFM, and PD. The thermo-chemo-mechanically coupled model based on CCM was one of the earliest established frameworks. It effectively describes the coupling interactions among temperature conduction, species transportation, and mechanical deformation. However, its main limitation lies in its inability to handle discontinuities, such as cracks. The thermo-chemo-mechanical PFM employs the Cahn-Hilliard equation to describe the evolution of conserved field concentrations and the Allen-Cahn equation to depict the dynamic changes in non-conserved field damage. This makes it particularly effective for addressing thermo-chemo-mechanical coupling problems involving phase transitions and cracks. The thermo-chemo-mechanical PD model, which replaces differential operators with integral formulations, naturally captures fracture behaviors such as crack initiation, propagation, and branching under coupled thermo-chemo-mechanical effects. As a result, PD has become a research hotspot in recent years. However, it has the drawback of high computational cost, especially considering multi-physics coupling. In the future, thermo-chemo-mechanical coupling theoretical models still face several challenges and opportunities in the following three areas.

First, studies indicate that temperature can induce thermal expansion and create inhomogeneous stress fields, resulting in thermal fatigue or cracking. Chemical reactions, such as oxidation, corrosion, or phase transformation, can degrade material strength and toughness. Additionally, mechanical loading exacerbates microcrack propagation and fracture, particularly under cyclic or impact conditions. Recently, Yin et al.[161] proposed a model to study the interfacial evolution and the stress state of the crack tip in chemically active environments, using the transition-state theory. Noii et al.[162] developed a PFM to address fatigue failure in Li-ion battery electrode particles, focusing on fractures caused by lithium diffusion. These studies primarily focus on chemo-mechanical coupling failure, neglecting the critical role of temperature. However, thermo-chemo-mechanical coupling significantly impacts material performance and stability, especially under extreme conditions such as high temperatures, high pressures, or rapid chemical reactions, which can accelerate material failure. Developing a comprehensive thermo-chemo-mechanically coupled model to describe material failure in multi-field environments remains both a challenging and promising area of research.

Second, machine learning and data-driven approaches have been increasingly applied to thermo-mechanically or chemo-mechanically coupling modeling, significantly enhancing predictive capabilities in complex scenarios. Nguyen et al.[163] employed machine learning approaches to estimate the compressive strength of ultra-high-performance concrete and the effect of temperature on its compressive strength is also investigated. Zeng et al.[164] employed a deep learning method to predict chemo-mechanical damage from PFM simulation video sequences. thermo-chemo-mechanical models are expected to integrate with efficient algorithms for real-time simulation and multi-objective optimization.

Finally, a meso-macroscopic multi-scale approach is commonly employed by researchers[165] to investigate thermo-chemo-mechanical coupling behaviors in materials. Future advancements aim to develop self-consistent theories that seamlessly integrate quantum, atomic, microscopic, and macroscopic scales, further enriching the understanding and modeling of thermo-chemo-mechanical interactions.

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