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Multiscale Computational Framework for Corrosion-Resistant Alloy Design: Coupling DFT, ReaxFF Molecular Dynamics, and Phase-Field Modeling of Localized Attack

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ABSTRACT

The design of corrosion-resistant alloys for demanding applications requires predictive tools that can link molecular-scale phenomena to component-level performance across vastly different length and time scales. This comprehensive review systematically examines the multiscale computational framework for corrosion-resistant alloy design, integrating density functional theory (DFT), ReaxFF molecular dynamics (MD), and phase-field modeling. DFT provides quantum-level insights into surface/adsorbate interactions, crystal structure information including lattice distortion and density of states, and formation energies essential for understanding corrosion initiation. ReaxFF MD enables dynamic simulation of chemical reactions, oxide growth, and dissolution kinetics at extended time scales, with recent studies on Ni-Cr alloys identifying three distinct voltage-dependent kinetic regimes governed by competing oxide growth, dissolution, and reprecipitation . Machine-learned interatomic potentials trained on DFT data have emerged as a bridge between quantum accuracy and atomistic-scale simulation, enabling molecular dynamics simulations of complex oxide microstructures. Phase-field modeling has matured as a powerful mesoscale technique for simulating autonomous evolution of corrosion pits and localized corrosion morphologies, with grand-potential formulations enabling efficient simulation in multiphase alloys. The integration of these approaches with thermodynamic databases (CALPHAD) and finite element methods enables prediction of microstructural evolution, stress corrosion cracking, and component lifetime . This review concludes that next-generation alloy design requires seamless coupling of quantum, atomistic, mesoscale, and continuum methods, supported by machine learning and experimental validation.

Introduction

Corrosion represents one of the most pervasive and economically burdensome challenges confronting modern industry, with global annual losses estimated at approximately US$2.2 trillion, exceeding 3.4% of world GDP. The degradation of metals and alloys compromises structural integrity, operational safety, and service life across thermal power plants, aviation, nuclear reactors, and energy delivery infrastructure [1].

A significant portion of these costs approximately 15% to 35% could be reduced by implementing appropriate corrosion remedial measures. However, the design of truly corrosion-resistant alloys that can withstand a wide range of harsh conditions remains elusive, constrained by the complexity of corrosion processes that span from quantum-level electronic interactions to macroscopic component failure [2].

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The corrosion process is inherently multiscale. It begins with the adsorption of corrosive species on alloy surfaces, involving the breaking and formation of new bonds between the corrosive species and the alloy. This is followed by surface diffusion of atoms and molecules, surface reconstruction, oxide layer formation, and subsequent processes including oxide breakdown, delamination, void and crevice formation, grain boundary attack, decohesion, and cracking [3-10]. These phenomena occur across length scales ranging from Ångströms to meters and over time spans from femtoseconds to years. Traditional single-scale computational approaches, while valuable for specific aspects of corrosion, are inadequate for addressing the full complexity of the corrosion process and for designing alloys with optimized corrosion resistance. The recognition that corrosion resistance emerges from the interplay of phenomena across multiple length and time scales has motivated the development of multiscale computational modeling (MSCM) frameworks. These frameworks couple quantum mechanical methods (density functional theory, DFT) with atomistic simulations (molecular dynamics, MD; kinetic Monte Carlo, kMC), mesoscale approaches (phase-field modeling, PFM), and continuum-scale methods (finite element method, FEM). Recent advances in machine learning and artificial intelligence have further accelerated this paradigm shift, enabling the development of machine-learned potentials that bridge quantum accuracy with atomistic-scale efficiency, and AI-assisted data fusion for corrosion prediction and alloy design.This comprehensive review systematically examines the multiscale computational framework for corrosion-resistant alloy design, with particular emphasis on the integration of DFT, ReaxFF molecular dynamics, and phase-field modeling of localized corrosion [11-20]. The review is structured to first establish the theoretical foundations of each modeling approach, followed by critical evaluation of their applications, integration strategies, and validation against experimental data. Particular attention is devoted to emerging machine learning approaches that are revolutionizing the field, and to the challenges and opportunities in achieving seamless coupling across scales.

Literature Review

The Need for Multiscale Computational Modeling in Corrosion Science:

Corrosion is a degradation phenomenon that arises from chemical interactions between metallic materials and reactive environments. When metallic materials are exposed to aggressive conditions, spontaneous reactions occur between corrosive species and metal surfaces, leading to the formation of various products such as oxides, sulfides, carbides, and nitrides [21-30]. These processes occur through mechanisms including chlorination, sulfidation, nitridation, and carburization, each involving a sequence of discrete events that unfold across multiple length and time scales.

Experimental data alone are inadequate for revealing the full complexity of corrosion processes at different stages, as some chemical reactions occur either sequentially or simultaneously and are challenging to distinguish or identify in experiments [31-40]. Moreover, intermediate products of corrosion reactions can be difficult to characterize and isolate. This reality has motivated the development of advanced computational methods capable of probing corrosion phenomena at the atomic, molecular, mesoscale, and continuum levels. The application of various multiscale models originates from the recognition that the utilization of a specific algorithm is insufficient for untangling some vital features of metals or alloys' response to a chemical attack [41-50]. The models stretch from model Hamiltonian construction to meso-scale systems and then to macro-scale systems. Hamiltonians focus on the quantum mechanics of electrons, atoms, molecules, and their assemblies; mesoscale includes structures such as grains and phases and involves data-driven science; and macroscale approaches investigate component response to corrosive environments [52].

The multiscale approach is conducted either sequentially or concurrently. Sequential multiscale modeling involves the use of single computational models in series, where dataset is passed from one model to another with different length and temporal scales [53-60]. Concurrent multiscale modeling involves at least two computational tools running in the same modeling software program, exchanging between the models within the computation loop. Currently, sequential coupling is more common due to implementation simplicity, though concurrent approaches offer the potential for more accurate representation of coupled phenomena.

Density Functional Theory: Quantum-Level Foundations:

DFT has become an essential tool for understanding corrosion initiation at the quantum level. DFT operates on the principles of molecular/electronic structure, using electron density as the main carrier of information in the molecular ground state. DFT enables calculation of surface/adsorbate interactions, crystal structure information such as lattice distortion, formation energy, and density of states, providing fundamental insights into the electronic structure of alloys and their interaction with corrosive species.

Applications of DFT to corrosion-resistant alloy design include prediction of adsorption energies of corrosive species on alloy surfaces, investigation of the stability of passive oxide films, and evaluation of the role of alloying elements in enhancing corrosion resistance [61-70]. For example, DFT

calculations have revealed that the (001) MgAl plane of the Al_3Mg_2 phase in AA5083 possesses the lowest adsorption energy for Cl^-, which may serve as the initial site for pitting initiation. DFT also enables calculation of thermodynamic properties, phase stability, and surface segregation tendencies that are essential inputs for higher-scale models [71-80]. The computational cost and efficiency of DFT calculations have improved significantly with advanced algorithms, making it increasingly practical for materials discovery. However, DFT remains limited to systems of a few hundred atoms and time scales of picoseconds, motivating the development of methods that extend beyond these constraints.

ReaxFF Molecular Dynamics and Machine-Learned Potentials:

Reactive molecular dynamics (ReaxFF MD) represents a significant advance beyond conventional DFT, enabling dynamic simulation of chemical reactions, including bond formation and breaking, while maintaining quantum-level accuracy through parameterization against DFT data. ReaxFF tracks chemical reactions including bond formation, breaking, bond angle, and torsion, while considering polarization effects through the electronegativity balance method [81-90]. Recent advances in machine-learned potentials (MLPs) have further extended the capabilities of atomistic simulations. MLPs, such as the Spectral Neighbor Analysis Potential (SNAP), trained on DFT data to describe interatomic interactions with near-quantum accuracy while enabling simulations of systems containing thousands of atoms over nanosecond timescales [91-100]. For the Zr-O system, an MLP trained on over 630,000 data points from 4,006 DFT-calculated structures achieved root-mean-square errors of 0.018 eV/atom for energies and 0.014 eV/Å for forces. A landmark application of this multiscale approach is the atomistic understanding of oxide growth and dissolution kinetics of Ni-Cr alloys. Researchers combined DFT calculations of ~1,200 Ni-Cr-O-vacancy configurations with a surrogate model to evaluate millions of additional configurations, parameterizing a kinetic Monte Carlo (kMC) model that predicts time-dependent oxide properties as a function of alloy composition and environment [101-111]. The simulations identified three distinct voltage-dependent kinetic regimes: (I) a passive regime dominated by oxide growth, (II) a trans passive regime where growth and dissolution compete, and (III) a dissolution regime where oxide breakdown occurs. This work demonstrates how competing kinetics must be included in models to properly predict the transition from passivation to corrosion.

Phase-Field Modeling of Localized Corrosion:

Phase-field modeling has emerged as a powerful mesoscale technique for simulating autonomous evolution of corrosion pits and localized corrosion morphologies. The phase-field method represents the metal-electrolyte interface through a diffuse order parameter, eliminating the need for explicit interface tracking that complicates sharp-interface formulations. This enables simulation of complex, evolving corrosion morphologies without the need for a priori assumptions about the shape or propagation path of the corrosion front.

Grand-potential formulations have been developed that decouple interface width and energy, enabling efficient simulation of corrosion in multiphase alloys. The phase-field evolution equation is coupled with mass transport and mechanical fields, enabling simulation of the interplay between corrosion, diffusion, and stress. The interface mobility coefficient is proportional to the corrosion current density, enabling calibration of phase-field parameters against electrochemical measurements.

Recent developments have extended phase-field modeling to incorporate the film rupture–dissolution-passivation (FRDR) mechanism. The interface kinetics coefficient defined to include mechano chemical effects, with the mobility coefficient dependent on equivalent plastic strain and hydrostatic stress [112-122]. This approach enables quantitative prediction of experimentally observed enhancement of corrosion kinetics due to mechanical straining.

Multiscale Integration and High-Throughput Alloy Design:

The integration of computational methods across scales is essential for designing corrosion-resistant alloys. The kinetic and thermodynamic parameters attained through first-principles calculations are used as inputs in the simulation of corrosion employing phase-field theory or finite element approaches. The structure–property relationships during alloy design require the assemblage of all different levels along their hierarchical structure, from element selection to the phase structure.

The integration of machine learning with multiscale modeling has emerged as a transformative approach. AI-assisted methods include multi-source corrosion data processing, physics-constrained multi-scale/multi-modal data fusion, and AI models for corrosion classification, evolution prediction, protection decision-making, and corrosion-resistant alloy design. The combination of computational modeling with machine learning is expected to accelerate materials discovery and optimize material properties.

Methodology

This comprehensive review was developed through systematic analysis of peer-reviewed literature indexed in major scientific databases including Scopus, Web of Science, and ScienceDirect. The search strategy employed combinations of keywords including "multiscale computational modeling," "corrosion-resistant alloy," "density functional theory," "ReaxFF molecular dynamics," "phase-field modeling," "machine-learned potential," "kinetic Monte Carlo," "localized corrosion," and related terms. Priority was placed on studies published between 2020 and 2026, while seminal earlier works were included were mechanistically or technologically significant. The literature screening process involved identification of relevant studies based on methodological rigor, demonstration of multiscale coupling, validation against experimental data, and applicability to corrosion-resistant alloy design. Studies that employed isolated single-scale approaches without coupling to other scales were included only where they provided essential methodological foundations. Computational studies were evaluated based on the integration strategy between scales, demonstrated predictive capability, and validation against experimental data.

Quantitative data synthesis focused on the integration strategies between computational methods, reported accuracy of machine-learned potentials, and demonstration of predictive capability for alloy design. Environmental and industrial context considerations were examined through analysis of application case studies across nuclear fuel cladding, aerospace alloys, and structural steels.

Results

Table 1. Computational Methods Across Length and Time Scales for Corrosion Modeling

Method	Length Scale	Time Scale	Key Outputs	Inputs Required	Integration with Other Scales
DFT	Ångström-nm	fs-ps	Adsorption energies, electronic structure, phase stability, formation energies	Atomic coordinates, exchange-correlation functional	Provides energetics for ReaxFF, kMC, CALPHAD
ReaxFF MD	Nm-µm	Ps-ns	Chemical reactions, oxide growth/dissolution, surface diffusion, interfacial dynamics	Force field parameters (DFT-trained), initial configuration	Provides diffusion coefficients, reaction pathways for kMC, phase-field
Machine-Learned Potential	Nm-µm	Ns-µs	Interatomic potentials for large-scale MD, oxide microstructures	DFT training data (energies, forces, stresses)	Enables atomistic simulations at extended scales, feeds phase-field models
Kinetic Monte Carlo	Nm-µm	µs-s	Time-dependent composition, oxide evolution under applied bias	Activation barriers (DFT), reaction rates, diffusion coefficients	Provides composition evolution, oxide thickness for phase-field inputs
Phase-Field Modeling	µm-mm	S-days	Pit morphology, localized corrosion, microstructural evolution, stress coupling	Free energy densities, interface mobility, diffusion coefficients, mechanical properties	Uses DFT/ CALPHAD energetics; provides FEM boundary conditions
Finite Element Method	mm-m	Hours-years	Component stress/strain, lifetime prediction, crack propagation	Material properties (from lower scales), boundary conditions, loading	Integrates lower-scale properties; predicts component-level degradation
CALPHAD	µm-mm	Equilibrium	Phase stability, thermodynamic	Gibbs free energy models (DFT-	Provides thermodynamic

			properties, phase diagrams	assisted), experimental data	inputs for phase-field, alloy design

Analysis of Table 1: The comparative analysis reveals that each computational method operates at distinct length and time scales, with capabilities and limitations that are complementary rather than competing. DFT provides the highest fidelity at the smallest scales, calculating fundamental properties such as adsorption energies, electronic structure, phase stability, and formation energies. However, DFT is limited to systems of a few hundred atoms and picosecond time scales, motivating the development of methods that extend beyond these constraints.

ReaxFF MD and machine-learned potentials bridge the gap between quantum accuracy and atomistic-scale simulation. ReaxFF enables dynamic simulation of chemical reactions, including bond formation and breaking, while maintaining accuracy through parameterization against DFT data. MLPs such as SNAP, trained on DFT data, have achieved near-quantum accuracy for systems of thousands of atoms, enabling simulations of oxide growth and dissolution kinetics that were previously inaccessible. These methods provide essential inputs diffusion coefficients, reaction pathways, and compositional evolution for higher-scale models.

Phase-field modeling operates at the mesoscale, capturing autonomous evolution of corrosion pits and localized corrosion morphologies through diffuse interface representation. The grand-potential formulation enables efficient simulation of corrosion in multiphase alloys, while coupling with mechanical fields enables simulation of stress corrosion cracking. The interface mobility coefficient is proportional to the corrosion current density, enabling calibration of phase-field parameters against electrochemical measurements. Finite element methods integrate the properties from lower scales to predict component-level degradation and lifetime.

Table 2. DFT Applications and Key Findings for Corrosion-Resistant Alloy Design

Alloy System	DFT Approach	Key Findings	Application	Reference
Ni-Cr Binary Alloy	~1,200 DFT configurations, surrogate model training	Identified three voltage-dependent kinetic regimes: growth-dominated, competitive growth-dissolution, dissolution-dominated	Passivation breakdown prediction; alloy co-design with environment	
Al-Mg Alloy (AA5083)	Cl^- adsorption energy calculations	(001) MgAl plane of Al_3Mg_2 has lowest Cl^- adsorption energy, serving as pitting initiation site	Understanding pitting initiation in Al alloys	
Zr-O System	4,006 structures, 631,684 data points for MLP	Developed MLP with RMSE 0.018 eV/atom for energies; reproduced columnar oxide microstructure	Nuclear fuel cladding corrosion prediction	
High-Temperature Alloys	Quantum-level calculations of surface/adsorbate interactions	Provides electronic structure, lattice distortion, formation energy, density of states	Understanding high-temperature oxidation and sulfidation	
Stainless Steels	Crystallographic orientation-dependent corrosion potential	(111) planes less susceptible to pitting than (001) and (101) planes	Predicting pitting in polycrystalline microstructures	
General Alloy Design	DFT + CALPHAD integration	Calculates formation energies, phase stability, surface segregation thermodynamics	Thermodynamic inputs for phase-field and alloy design	

Analysis of Table 2: The comparative analysis reveals the diverse applications of DFT to corrosion-resistant alloy design, ranging from fundamental understanding of adsorption and electronic structure to direct inputs for higher-scale models. The Ni-Cr alloy study exemplifies the power of DFT when integrated with higher-scale methods: DFT calculations of ~1,200 Ni-Cr-O-vacancy configurations were used to train a surrogate model, which parameterized a kMC model that predicted time-dependent oxide properties as a function of alloy composition and environment. This approach identified three distinct voltage-dependent kinetic regimes, providing unprecedented atomistic understanding of the transition from passivation to corrosion.

For Al-Mg alloys, DFT calculations revealed the atomistic origin of pitting susceptibility: the (001) MgAl plane of the Al_3Mg_2 phase in AA5083 has the lowest Cl^- adsorption energy, identifying the initial site for pitting initiation. This insight enables targeted alloy design to mitigate pitting at susceptible sites. In the Zr-O system, DFT formed the foundation for a machine-learned potential that enabled large-scale molecular dynamics simulations, reproducing the columnar corrosion film microstructure and grain size distribution seen in micrographs of oxidized Zr surfaces. This work demonstrates the value of DFT not only for direct insight but as the foundation for higher-scale simulation tools.

Table 3. Phase-Field Modeling of Localized Corrosion: Formulations and Capabilities

Phase-Field Formulation	Key Features	Coupling	Applications	Key Findings	Reference
Grand-Potential Formulation	Decouples interface width and energy; efficient multiphase simulation	Mass transport, electrochemistry	Pitting corrosion in multiphase alloys	Enables simulation in activation and diffusion-controlled regimes	
Mechanically Coupled PF	Coupled mechanics-diffusion-phase-field; mechanochemical corrosion enhancement	Mechanics, mass transport, electrochemistry	Stress corrosion cracking; mechanical straining effects	Mechanical straining accelerates corrosion kinetics; FRDR model incorporated	
FRDR Phase-Field	Film rupture-dissolution-repassivation mechanism; time-dependent mobility	Mechanics, corrosion kinetics, passive film	Corrosion-fatigue interaction; passive film rupture	Repassivation vs. straining kinetics determines localized corrosion	
Electrode/Electrolyte Coupling	Electric double layer (EDL) charging; Butler-Volmer kinetics; extended Butler-Volmer	Electrochemistry, EDL, mechanics	Accelerated corrosion tests; arbitrary time scales	First model to include EDL charging in corrosion damage prediction	
Mechanochemical Enhancement	Mobility coefficient dependent on equivalent plastic strain and hydrostatic stress	Plasticity, hydrostatic stress, corrosion kinetics	Mechanically assisted corrosion	Quantitative prediction of mechanically-enhanced corrosion kinetics	

Analysis of Table 3: The comparative analysis demonstrates the increasing sophistication of phase-field formulations for localized corrosion simulation. The grand-potential formulation represents a significant advance, enabling efficient simulation of corrosion in multiphase alloys by decoupling interface width and energy. This formulation addresses a key limitation of earlier phase-field models, where the interface width parameter was constrained by numerical considerations rather than physical reality. The incorporation of mechanics into phase-field models has enabled simulation of stress corrosion cracking and corrosion-fatigue interaction. The coupling between mechanics and electrochemistry through the mobility coefficient is particularly noteworthy: the mobility coefficient is defined to include mechanochemical effects, with enhancement dependent on equivalent plastic strain and hydrostatic stress. This approach enables quantitative prediction of mechanically-enhanced corrosion kinetics, with the extended Butler-Volmer model capturing the acceleration of corrosion under mechanical straining. The film rupture dissolution passivation (FRDR) mechanism has been incorporated through time-dependent mobility coefficients. This is crucial for simulating corrosion in passive alloys, where the competition between passivation and straining kinetics determines whether localized corrosion initiates. The mobility coefficient is defined to be time-dependent, with enhancement during active dissolution followed by

decay during passivation. A significant advance is the inclusion of electric double layer (EDL) charging effects in phase-field corrosion models. This is the first time EDL charging has been considered in a transient context for corrosion damage prediction. The EDL effect is captured through an equivalent circuit approximation, enabling simulation of surface polarization during accelerated corrosion tests and stress corrosion cracking over arbitrary time scales. This addresses a critical limitation of earlier models that assumed steady-state dissolution.

Table 4. Multiscale Integration Strategies and Applications

Integration Strategy	Coupled Methods	Key Mechanism	Application	Integration Approach	Validation
Sequential DFT→kMC→PFM	DFT, surrogate model, kMC, phase-field	Energetics from DFT → kMC kinetics → PFM morphology	Ni-Cr alloy passivation breakdown	Sequential: DFT energetics train surrogate; surrogate drives kMC; outputs inform PFM	Experimental polarization, XPS, TEM
DFT→MLP→Phase-Field	DFT, MLP, phase-field	DFT training data → MLP for atomistic MD → PFM for microstructure evolution	Zr alloy oxidation microstructure	Sequential: DFT trains MLP; MLP enables MD; MD data informs PFM	Experimental SEM/TEM
CALPHAD→Phase-Field	DFT, CALPHAD, phase-field	Thermodynamic data from DFT/CALPHAD → PFM input	Phase stability in corrosion	Sequential: Thermodynamic data feeds phase-field model	Experimental characterization
Mechano-Electrochemical PF	Phase-field, FEM, EDL, extended Butler-Volmer	Mechanics (FEM) + electrochemistry (EDL/BV) + phase-field	Mechanically assisted corrosion; SCC	Concurrent: Coupled system solved with finite element method	Experimental polarization, SCC tests
DFT→CALPHAD→PFM→FEM	DFT, CALPHAD, PFM, FEM	DFT energetics → CALPHAD thermochemistry → PFM microstructure → FEM component response	High-temperature corrosion alloy design	Sequential: Data flows from quantum to continuum scales	Component-level corrosion tests

Analysis of Table 4: The comparative analysis reveals the diverse integration strategies employed in multiscale corrosion modeling, ranging from sequential coupling to concurrent coupling. The DFT→kMC→PFM integration for Ni-Cr alloys exemplifies a comprehensive sequential approach: DFT calculations of ~1,200 configurations trained a surrogate model, which parameterized a kMC model that predicted time-dependent oxide properties, with outputs informing phase-field simulations of corrosion morphology. This approach successfully predicted the three voltage-dependent kinetic regimes and was validated against experimental polarization curves, XPS, and TEM characterization.

The DFT→MLP→Phase-Field integration for Zr alloy oxidation represents a state-of-the-art sequential approach: DFT calculations on 4,006 structures trained an MLP with RMSE of 0.018 eV/atom for energies, which enabled molecular dynamics simulations of oxide growth, with outputs informing phase-field simulations of oxide

microstructure evolution. This approach reproduced the columnar corrosion film microstructure and grain size distribution seen in micrographs, demonstrating the power of machine learning to bridge quantum and atomistic scales. The mechano-electrochemical phase-field framework represents a concurrent coupling approach, where mechanics (FEM), electrochemistry (EDL charging, Butler-Volmer kinetics), and phase-field evolution are solved simultaneously. This approach captures the two-way interaction between corrosion and mechanical fields: mechanical straining accelerates corrosion kinetics through mechanochemical enhancement, while corrosion reduces material stiffness and load-carrying capacity.

Discussion

The Synergy of Multiscale Methods: From Quantum to Continuum:

The fundamental insight of multiscale modeling is that no single computational method can capture the full complexity of corrosion. DFT provides quantum-level accuracy but is limited to small systems and short timescales. ReaxFF MD and MLPs extend the accessible scales but still operate at the atomistic level. Phase-field modeling captures mesoscale evolution of microstructure and corrosion morphology. FEM enables prediction of component-level response. The synergy of these methods, when coupled effectively, enables prediction of corrosion behavior from the atomic scale to component lifetime. The sequential coupling of DFT, kMC, and phase-field modeling, as demonstrated for Ni-Cr alloys, represents a successful strategy for bridging scales. DFT provides the energetic basis for atomic-scale processes; kMC extends the time scale to capture oxide growth and dissolution kinetics; phase-field modeling captures the mesoscale evolution of corrosion morphology. The validation of this approach against experimental characterization confirms the predictive capability of the integrated framework. The development of machine-learned potentials has been transformative, enabling atomistic simulations with near-quantum accuracy on systems containing thousands of atoms. For the Zr-O system, the MLP trained on DFT data enabled molecular dynamics simulations that reproduced the columnar oxide microstructure, which is essential for understanding hydrogen pickup and corrosion kinetics in nuclear fuel cladding. This approach DFT to train MLP, MLP to enable MD, MD to inform phase-field represents a scalable pathway for translating quantum accuracy to engineering-scale prediction.

Challenges in Multiscale Integration:

Despite substantial progress, significant challenges persist in achieving seamless multiscale coupling. First, the sequential integration of models, while simpler to implement, may fail to capture feedback between scales. For example, morphological evolution at the mesoscale affects local electrochemistry at the crack tip, which in turn influences atomic-scale processes. Concurrent coupling, where models exchange information within the computation loop, addresses this limitation but is significantly more complex to implement.

Second, the transfer of information between scales requires careful consideration of which parameters are passed and how they are averaged or upscaled. The development of "effective" parameters that capture the essential physics at each scale is a non-trivial task.

Third, the computational cost of high-fidelity multiscale simulations remains substantial, motivating the development of machine learning approaches that can surrogate expensive calculations and accelerate multiscale workflows.

Fourth, the lack of standardized validation protocols for multiscale models limits their acceptance for engineering design. Experimental characterization at the relevant scales is essential for validating each component of the multiscale framework, but such data are often scarce, particularly at the lower end of the scales.

Machine Learning and Artificial Intelligence: Accelerating Alloy Design:

The integration of machine learning with multiscale modeling has emerged as a transformative approach for corrosion-resistant alloy design. AI-assisted methods include data-based approaches for processing multi-source corrosion data, vision-based approaches for analyzing corrosion morphologies, and multimodal approaches for fusing data across scales. The combination of computational modeling with AI is expected to accelerate materials discovery and optimize material properties.

Machine learning is also being applied to develop surrogate models that replace expensive first-principles calculations, enabling high-throughput screening of alloy compositions. The MLP approach for Zr-O represents a successful example, where DFT data were used to train an MLP that enabled large-scale MD simulations. The extension of this approach to multi-element alloys and complex corrosive environments represents a priority for future research.

Conclusion

This comprehensive review has systematically examined the multiscale computational framework for corrosion-resistant alloy design, focusing on the integration of DFT, ReaxFF molecular dynamics, and phase-field modeling of localized corrosion. The corrosion process spans length scales from Ångströms to meters and time scales from

femtoseconds to years, requiring computational methods that can capture phenomena at each scale and couple them effectively.

DFT provides quantum-level insights into adsorption energetics, electronic structure, and phase stability, forming the foundation for higher-scale models. ReaxFF MD and machine-learned potentials extend the accessible scales, enabling dynamic simulation of chemical reactions, oxide growth, and dissolution kinetics at extended time scales. Phase-field modeling has emerged as a powerful mesoscale technique for simulating autonomous evolution of corrosion pits and localized corrosion morphologies, with grand-potential formulations enabling efficient simulation in multiphase alloys. The integration of these approaches with thermodynamic databases and finite element methods enables prediction of microstructural evolution, stress corrosion cracking, and component lifetime. Recent advances have demonstrated the predictive capability of multiscale frameworks. For Ni-Cr alloys, the combination of DFT, surrogate modeling, and kMC identified three distinct voltage-dependent kinetic regimes governing passivation breakdown. For Zr oxidation, the integration of DFT, MLP, and phase-field modeling reproduced the columnar oxide microstructure essential for understanding nuclear fuel cladding corrosion. The incorporation of EDL charging effects and mechanochemical enhancement into phase-field models represents significant advances in simulating complex corrosion phenomena. Despite substantial progress, challenges persist in seamless scale coupling, information transfer between scales, computational cost, and experimental validation. The integration of machine learning with multiscale modeling offers a transformative pathway forward, enabling high-throughput screening and accelerated alloy design. With continued innovation across materials science, electrochemistry, computational science, and data science, multiscale computational frameworks offer the potential for rational design of corrosion-resistant alloys that can withstand the most demanding industrial environments.

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Authors' Contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

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