Study on the Accelerated Corrosion Mechanism of Tin Bronze under Neutron Irradiation-Groundwater Coupling

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Abstract

Research on the corrosion behavior of packaging container materials in deep geological disposal of high-level radioactive waste is of great significance. Using tin bronze C5191 as a candidate material for packaging containers and BS03 groundwater as a simulated solution, accelerated corrosion experiments on tin bronze materials under neutron irradiation-groundwater coupling were conducted, while first-principles calculations were employed to compute the adsorption energy, Bader charge transfer number, and partial density of states of SO42- in groundwater on CuSn(110) perfect and defect surfaces, thereby explaining the corrosion acceleration mechanism through theoretical calculations. The results indicate that under different experimental conditions, the corrosion rate of tin bronze increased from 0.516 m/a to 17.9 m/a, the adsorption energies of SO42- in groundwater on CuSn(110) perfect and defect surfaces were -5.311 eV and -5.691 eV, respectively, and the Bader charge transfer numbers were -0.3271 and -0.5166, respectively, demonstrating that SO42- more readily interacts with defect surfaces. During co-adsorption, the adsorption energy decreased to -12.391 eV, and the Bader charge transfer numbers increased to -6.0639 and -6.0074, indicating that the radiolysis products of H2O promoted the adsorption of SO42- on metal defect surfaces; the experimental and theoretical calculation results are consistent, proving that the irradiation-groundwater coupling effect significantly accelerates the corrosion rate of tin bronze.

Full Text

Preamble

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Study on the Accelerated Corrosion Mechanisms of Tin Bronze under the Coupled Effects of Neutron Irradiation and Groundwater

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Abstract

[**Background**] The selection of disposal canister materials is crucial in the deep geological disposal of high-level radioactive waste, as metal packaging containers serve as the first engineering barrier to isolate the waste. [**Purpose**] This study aims to investigate the accelerated corrosion mechanisms of tin bronze C5191 under the coupled effects of neutron irradiation and groundwater. [**Methods**] Using tin bronze C5191 as a candidate packaging container material and BS03 groundwater as a simulated solution, corrosion acceleration experiments were conducted under neutron irradiation-groundwater coupling. Additionally, first-principles calculations were performed to determine the adsorption energy, Bader charge transfer numbers, and projected density of states (PDOS) of SO_4^{2-} in groundwater on intact and defective CuSn(110) surfaces, thereby elucidating the corrosion acceleration mechanism through theoretical analysis. [**Results**] The results indicate that under varying experimental conditions, the corrosion rate of tin bronze increased from 0.516 $m \cdot a^{-1}$ to 17.9 $m \cdot a^{-1}$. The adsorption energies of SO_4^{2-} on intact and defective CuSn(110) surfaces were -5.311 eV and -5.691 eV, respectively, with Bader charge transfer numbers of -0.3271 and -0.5166, demonstrating that SO_4^{2-} interacts more readily with defective surfaces. Upon co-adsorption, the adsorption energy decreased to -12.391 eV, and the Bader charge transfer numbers increased to -6.0639 and -6.0074. [**Conclusions**] This study demonstrates that the radiolysis products of H_2O enhance the adsorption of SO_4^{2-} on metal defect surfaces. The experimental and theoretical results are consistent, proving that the irradiation-groundwater coupling effect significantly accelerates the corrosion rate of tin bronze.

Keywords: High-level waste packaging container, Tin bronze, Neutron irradiation, Corrosion acceleration, First-principles

Introduction

Driven by dual-carbon goals, nuclear power technology is flourishing, while the safe disposal of radioactive waste has become an urgent issue to address [1,2].

Currently, deep geological disposal is the most widely recognized method for high-level radioactive waste internationally [3,4]. As the first engineering barrier in contact with high-level radioactive waste [5,6], the long-term safety and effectiveness of disposal canisters are paramount. Irradiation and groundwater corrosion are critical factors affecting canister lifespan and safety. Researchers worldwide have investigated the irradiation behavior of candidate materials such as industrial pure titanium [7], titanium alloys [8,9], carbon steel [10], stainless steel [11], and nickel-based alloys [12]. Tin bronze has also been considered as a candidate material due to its excellent mechanical properties, thermal stability, and resistance to hydrogen embrittlement [13,14]. Given that geological repositories for high-level radioactive waste require timescales exceeding ten thousand years, safety assessment is essential. Under extreme conditions, packaging container materials may remain in environments with coupled neutron irradiation and groundwater for extended periods, warranting attention to the irradiation effects and corrosion acceleration mechanisms of tin bronze. Current neutron source designs are diverse and increasingly mature [15,16], facilitating irradiation experiments on canister materials. Johansson et al. [17] conducted corrosion experiments on copper-cast iron canisters and found that bentonite type is a crucial factor affecting sulfide production, with sulfides and sulfate-reducing bacteria on material surfaces significantly influencing corrosion. Björkbacka et al. [18] demonstrated that copper corrosion accelerates under γ irradiation at 0.37 and 0.77 $kGy \cdot h^{-1}$, as hydroxyl radicals produced by γ irradiation oxidize copper, with localized corrosion features arising from anodic reactions at corrosion centers and cathodic reactions in surrounding areas. Gao et al. [14] showed that tin content, microstructure, and environmental factors such as anion species in corrosive media (Cl^-, SO_4^{2-}, HCO_3^-, NO_3^-) and pH affect the initial corrosion behavior of tin bronze. Shen et al. [19] simulated corrosion behavior of reactor alloy materials using quantum mechanics-based density functional theory, calculating system energy changes, chemical bond reconstruction, and charge transfer to analyze adsorbate behavior on crystal surfaces. Chen et al. [20] applied first-principles calculations based on density functional theory and semi-classical Boltzmann transport theory to investigate interface stability, electronic structure, bonding properties, and thermoelectric transport performance of CuSn/Cu interfaces with different crystallographic orientations, calculating ideal adhesion forces for various interfaces.

While numerous studies have addressed groundwater corrosion experiments for high-level waste disposal canisters, research on irradiation-groundwater coupling effects and microscale simulations remains limited. This paper employs first-principles calculations to further investigate the corrosion mechanisms of tin bronze at the atomic scale. By combining experiments with theoretical calculations, neutron irradiation-corrosion experiments were conducted on tin bronze C5191 in simulated solutions with varying Cl^- and SO_4^{2-} concentrations. Simultaneously, first-principles calculations using MedeA-VASP software based on density functional theory were performed to analyze the adsorption behavior of SO_4^{2-} and water radiolysis products on material surfaces, providing refer-

ence for studying corrosion behavior of high-level waste canister materials under irradiation-corrosion coupling.

1. Materials and Methods

1.1 Materials and Instruments

Tin bronze C5191 was selected as the experimental material, with chemical composition shown in Table 1 . The material was cut into cylindrical specimens of $ $10 mm × 10 mm with a thickness of 5 mm, then progressively polished with sandpaper (2000#, 3000#, 5000#, 7000#) and polishing paste (10000#). After cleaning with deionized water, degreasing with anhydrous ethanol, and drying, the samples were weighed, numbered, and stored sealed.

A solution containing Cl^- and SO_4^{2-} sodium salts was prepared to simulate groundwater from the 500 m deep BS03 borehole in the Beishan area of Gansu Province [21]. Using the average concentrations (Cl^-: 1261.3 mg/L, SO_4^{2-}: 1259.7 mg/L) as the standard solution, concentrations were increased to 4×, 8×, and 16× (hereinafter denoted as 1×, 4×, 8×, and 16×).

The main instruments used in the experiments included: a 600 kV ns pulsed neutron generator (China Institute of Atomic Energy), CP124C electronic analytical balance (Ohaus Shanghai Instruments), PHS-3C precision pH meter (Shanghai Zhiguang Instruments), sandpaper (Shanghai Hongce Instrument Technology), polishing paste (Hangzhou Kraftwell Industrial), and Nova NanoSEM 450 field emission scanning electron microscope (SEM, FEI Czech).

1.2 Irradiation-Corrosion Conditions

Corrosion experiments were divided into non-irradiated and neutron-irradiated groups. The non-irradiated group involved immersing non-irradiated metal samples in simulated solution. The neutron-irradiated group included three conditions: (1) both metal and solution irradiated, (2) metal irradiation only, and (3) solution irradiation only. The neutron irradiation environment was provided by the 600 kV ns pulsed neutron generator at the China Institute of Atomic Energy. During irradiation, the simulated solution and metal samples were positioned in the outer and inner periphery of the target position, respectively, with neutron flux rates of 3.50$×10^{7}$ $n \cdot cm^{-2} \cdot s^{-1}$ for metal samples and 1.73$×10^{6}$ $n \cdot cm^{-2} \cdot s^{-1}$ for the solution. The irradiated surface served as the working surface. Pretreated tin bronze samples were immersed in simulated solutions of varying concentrations to replicate the corrosion environment of disposal canisters in groundwater, with the working surface facing upward. Each sample group contained 20 mL of simulated solution with an initial pH of 7.80$±$0.02. After 30 days of immersion at ambient temperature, samples were removed, acid-cleaned, dried, and weighed. The corrosion status of non-irradiated and neutron-irradiated samples before and after immersion in different concentration solutions is shown in Figure 1 [Figure 1: see original paper].

The corrosion rate of tin bronze was determined using the chemical immersion method [22]. The corrosion rate v ($\mathrm{m \cdot a^{-1}}$) is expressed as:

$$v = \frac{8.76 \times 10^4 \times \Delta m}{\rho \times s \times t}$$

where Δm is the mass loss after corrosion (g), is the sample density ($\mathrm{g \cdot cm^{-3}}$), s is the sample surface area ($\mathrm{cm^2}$), and t is the corrosion time (h).

1.3 Calculation Methods and Model Establishment

The calculations in this study were based on first-principles methods using density functional theory (DFT) [23], with Medea-VASP software employed for simulating intact and defective CuSn(110) surfaces. The exchange-correlation interaction between electrons was treated using the generalized gradient approximation (GGA) with the PBE functional. Optimized CuSn crystal cells were cleaved to create surfaces and establish adsorption models, as shown in Figure 2 [Figure 2: see original paper]. For structural optimization, the plane wave cutoff energy was 450 eV, the Brillouin zone k-point mesh was set to $1\$\times3\times3, the integration method for CuSn(110) surfaces was Methfessel-Paxton with a smearing width of 0.2 eV, the force convergence criterion was 0.02 eV \cdot nm^{\{-1\}}, and the self-consistent field (SCF) convergence precision was 1.0\times10^{\{-5\}}\$$ eV. After optimization, the CuSn unit cell lattice parameters were a=b=4.19, c=5.09, which are close to reference values [24] of a=b=4.12, c=5.13, confirming the reliability of the structure.

2. Results and Discussion

2.1 Corrosion Behavior Analysis

2.1.1 Corrosion Rate The relationship between mass loss, corrosion rate, and solution concentration for tin bronze under different irradiation conditions is shown in Figure 3 [Figure 3: see original paper]. Under identical solution concentrations, condition 1 (both metal and solution irradiated) exhibited the greatest mass loss, reaching a maximum of 0.001 g at 16× solution concentration. Under the same irradiation conditions, the corrosion rate of tin bronze increased nonlinearly with solution concentration. At 16× concentration, the corrosion rate of non-irradiated tin bronze increased by 19.9%. As evident from Figure 3, when both metal and solution were irradiated, the corrosion rate of tin bronze was highest at all concentrations and increased most rapidly, reaching a maximum value of 17.9 $\mathrm{m \cdot a^{-1}}$. The corrosion rate under metal irradiation conditions was higher than under solution irradiation alone. When the irradiation effects on metal coupled with radiolysis products from water, the metal corrosion acceleration was most severe [25]; moreover, irradiation-induced defects on the metal surface had a greater impact on corrosion than water radiolysis products.

2.1.2 Corrosion Morphology The original sample morphology is shown in Figure 4 Figure 4: see original paper, with all SEM images magnified 1500×. The pretreated material surface was smooth and flat with minor scratches. The micro-morphology of non-irradiated tin bronze after 30 days of immersion in standard and 16× concentration groundwater simulated solutions is shown in Figures 4(b) and 4(c). At standard concentration, surface corrosion was not obvious, while in 16× concentration solution, the metal surface exhibited dense corrosion pits, consistent with the result shown in Figure 3 that the corrosion rate was highest at 16× concentration.

The micro-morphology of materials after 30 days of immersion under three irradiation conditions in standard, 4×, 8×, and 16× concentration solutions is shown in Figure 5 [Figure 5: see original paper]. After neutron irradiation, sample surface roughness increased and holes appeared. Irradiation produces primary knock-on atoms that undergo cascade collisions, generating numerous vacancies and self-interstitial defects that gradually evolve into visible defects such as voids and dislocation loops over time [26]. The results show that tin bronze underwent primarily localized corrosion, with varying degrees of corrosion observed at all concentrations. Under condition 1 (both metal and solution irradiated), large corrosion pits aggregated at 16× concentration, while under conditions 2 and 3, corrosion pits were smaller and more dispersed. Although corrosion pits were also present on tin bronze surfaces under conditions 2 and 3, the corrosion was slightly less severe than under condition 1. As observed in Figures 5(a4, b3), fewer corrosion pits aggregated on the tin bronze surface, with slight corrosion traces near scratches. Under identical simulated solution concentrations, irradiation significantly accelerated tin bronze corrosion.

2.2 Adsorption Mechanism Analysis

2.2.1 SO_4^{2-} Adsorption on Intact and Defective CuSn(110) Surfaces Residual neutrons and γ radiation from high-level radioactive waste cause irradiation damage such as atomic displacement in metal canister materials [27]. In first-principles calculations, a defective CuSn(110) surface (missing 2 Sn atoms from the surface layer) was constructed to simulate irradiation damage. The optimized adsorption models are shown in Figures 2(a) and 2(b). Adsorption energy E ds was calculated to investigate adsorption characteristics on material surfaces:

$$E_{\text{ads}} = E_{\text{post-ads}} - E_{\text{pre-ads}} - E_x$$

where E ds is the adsorption energy, E ds is the total optimized energy after adsorption, E ds is the total optimized energy before adsorption, and E is the optimized energy of the adsorbate.

The Hole site was selected on both intact and defective CuSn(110) surfaces for SO_4^{2-} adsorption. The adsorption energy of SO_4^{2-} on the intact CuSn(110)

surface was -5.311 eV, while on the defective surface it was -5.691 eV. Both values are less than 0, satisfying the thermodynamic condition for spontaneous adsorption. In all cases, the adsorption energy on defective surfaces was lower, indicating that defective surfaces are more susceptible to adsorption and form more stable adsorption configurations. Since irradiation creates defective metal surfaces that more readily interact with anions in solution, this corresponds with the experimental conclusion that irradiation accelerates metal surface corrosion.

Bader charge transfer calculations for SO_4^{2-} on intact and defective CuSn(110) surfaces were performed to analyze atomic charge changes in the adsorption system, with results shown in Table 2 . Cu13, Cu16, Sn15, and S exhibited electron gain, while O showed electron loss. The total charge transfer numbers were -0.3271 and -0.5166 for intact and defective surfaces, respectively. The defective surface lost more electrons than the intact surface, indicating stronger interaction between SO_4^{2-} and metal atoms on defective surfaces. This charge transfer promotes the formation of Cu-O bonds between O in SO_4^{2-} and Cu on the surface during adsorption, stabilizing the adsorbed system.

To further analyze the interaction of SO_4^{2-} with metal surfaces at the electronic level, Figure 6 [Figure 6: see original paper] shows the projected density of states (PDOS) before and after adsorption, with the dashed line indicating the Fermi level (E=0 eV). The PDOS peaks of SO_4^{2-}-p orbitals are primarily distributed between -9 and -2 eV, overlapping and hybridizing with the PDOS peaks of Cu13-d and Cu16-d orbitals, promoting Cu-O bond formation. The SO_4^{2-}-s orbital showed no overlap with Cu atomic orbitals, indicating that interaction with surface Cu atoms is mainly mediated by SO_4^{2-}-p orbitals. After adsorption, the PDOS of Cu13-d and Cu16-d orbitals shifted to lower energy levels, particularly at peak positions hybridized with SO_4^{2-}-p orbitals, where the peaks were lower than before adsorption. This corresponds to the reduced system energy after adsorption, forming a more stable adsorption system. Moreover, the PDOS energy of the defective CuSn(110) surface was slightly lower than that of the intact surface, confirming the adsorption energy calculations.

2.2.2 Co-adsorption of SO_4^{2-} and Water Radiolysis Products on CuSn(110) Surfaces While high-level radioactive waste causes defects in canister materials, groundwater in the near-field can permeate bentonite and directly contact the canister, becoming decomposed by irradiation according to equations (3)-(5). Radiolysis produces radical and molecular products ($\cdot$OH, $\cdot$O, etc.) with oxidizing properties that alter the redox conditions in the repository near-field [28].

This study selected $\cdot$OH and $\cdot$O as research objects due to their significant impact on corrosion acceleration. Figures 2(c) and 2(d) show co-adsorption models of water radiolysis products with anions on metal surfaces, investigating co-adsorption on defective surfaces. Adsorption energy calculations yielded -9.572 eV for SO_4^{2-} co-adsorbed with $\cdot$OH on defective CuSn(110) surfaces and -12.390 eV for co-adsorption with $\cdot$O. The lower adsorption energy for SO_4^{2-}

with ·O indicates a more stable adsorption system.

Bader charge transfer calculations for co-adsorption systems are shown in Table 3 . Negative values indicate electron gain; ·O and ·OH gained electrons while Cu atoms lost electrons. The total charge transfer for SO_4^{2-} co-adsorbed with ·O on defective CuSn(110) surfaces was -6.0074, lower than the net charge transfer of -5.4098 for co-adsorption with ·OH, indicating that the SO_4^{2-}-·O co-adsorption model is more stable.

PDOS analysis of co-adsorption systems is shown in Figure 7 [Figure 7: see original paper]. Energy distribution shifted to lower energy regions after adsorption, with reduced peak intensities, indicating lower overall system energy. When SO_4^{2-} co-adsorbed with water radiolysis products on defective CuSn(110) surfaces, the p orbitals of SO_4^{2-}-·OH were distributed primarily near -4 to -1 eV, overlapping with Cu d-orbitals in this region. The presence of adsorbates reduced the original peak intensities of substrate atoms, exhibiting hybridization coupling. The PDOS peaks of SO_4^{2-}-·O p-orbitals showed greater amplitude and peak-to-valley distance, with more pronounced changes, indicating that ·O had a greater influence on the adsorption system and interacted more strongly with Cu atoms. This is consistent with the experimental observation that irradiation accelerates metal surface corrosion.

Conclusion

This study investigated the corrosion acceleration mechanism of tin bronze under neutron irradiation-groundwater coupling. Experiments revealed that irradiation significantly accelerates tin bronze corrosion, with the corrosion rate reaching 17.9 $m \cdot a^{-1}$ when both samples and simulated solution were irradiated—34.7 times higher than the non-irradiated rate of 0.516 $m \cdot a^{-1}$. First-principles calculations demonstrated that irradiation-induced metal surface defects increased Bader charge transfer by 57.9% and reduced system adsorption energy by 5.7%. Water radiolysis product ·O further reduced the adsorption energy of SO_4^{2-} on defective CuSn(110) surfaces to -12.390 eV, enabling SO_4^{2-} to adsorb more readily on metal surfaces and accelerate material corrosion. Both experimental and theoretical simulations confirm the corrosion acceleration phenomenon of tin bronze under irradiation-groundwater coupling, providing reference for material selection of high-level waste disposal canisters.

Author Contributions

Yang Bo: Conceptualization, experimental guidance, research design, analysis of experimental results, writing—original draft, review & editing, final approval. Zhang Meng: Literature investigation, research design, data analysis, figure preparation. Chen Moru: Experimental characterization, model establishment. Zhao Shi: Data curation, model validation. Wei Qianglin and Liu Yibao: Theoretical calculation guidance, project supervision, review & editing, final approval.

References

1. ZHANG Yuqing. Thinking of constructing new-type energy system for fulfillment of carbon peak and carbon neutrality goals[J]. Petroleum Science and Technology Forum, 2024, 43(2): 8-14. DOI: 10.3969/j.issn.1002-302X.2024.02.002.

2. Wang L, Gao R, Nam O H, et al. Sustainability-oriented prioritization of nuclear fuel cycle transitions in China: a holistic MCDM framework under uncertainties[J]. Nuclear Science and Techniques, 2024, 35(09): 152-168. DOI: 10.1007/s41365-024-01504-3.

3. Wang J, Chen L, Su R, et al. The Beishan underground research laboratory for geological disposal of high-level radioactive waste in China: planning, site selection, site characterization and in situ tests[J]. Journal of Rock Mechanics and Geotechnical Engineering, 2018, 10(3): 411-435. DOI: 10.1016/j.jrmge.2018.03.002.

4. Rodriguez-Dono A, Olivella S, Mokni N. Assessment of a high-level spent nuclear fuel disposal model[J]. Environmental Geotechnics, 2018, 7(1): 42-58. DOI: 10.1680/jenge.18.00017.

5. Tan Y, Xu X, Ming H. Analysis of double-layered buffer in high-level waste repository[J]. Annals of Nuclear Energy, 2022, 165: 108660. DOI: 10.1016/j.anucene.2021.108660.

6. Zhu J, Wang T, Zhang H, et al. Alkaline buffer characteristics and mechanism of Gaomiaozi bentonite in high-level radioactive waste repository[J]. Environmental Earth Sciences, 2023, 82(13): 346. DOI: 10.1007/s12665-023-10928-w.

7. Panin A V, Kazachenok M S, Kretova O M, et al. The effect of electron beam treatment on hydrogen sorption ability of commercially pure titanium[J]. Applied Surface Science, 2013, 284: 750-756. DOI: 10.1016/j.apsusc.2013.07.166.

8. Wei Q, Li Y, Huang Y, et al. Corrosion behavior of high-level waste container materials Ti and Ti–Pd alloy under long-term gamma irradiation in Beishan groundwater[J]. Chinese Physics B, 2021, 30(5): 056109. DOI: 10.1088/1674-1056/abf03b.

9. T. Ishida et al. Radiation damage studies on titanium alloys as high intensity proton accelerator beam window materials[M]. Japan: Koichi Sato and Eiichi Wakai, 2020. DOI: 10.7566/JPSCP.28.041001.

10. K. Daub, X. Zhang, J. J. Noël, et al. Gamma radiation-induced carbon steel corrosion[J]. ECS Transactions, 2019, 33(25): 15-24. DOI: 10.7566/JPSCP.28.041001.

11. Z. Jiao, J. Hesterberg, G. S. Was. Effect of post-irradiation annealing on the irradiated microstructure of neutron-irradiated 304L stain-

less steel[J]. Journal of Nuclear Materials, 2018, 500: 220-234. DOI: 10.1016/j.jnucmat.2017.12.030.

12. M. A. Stopher. The effects of neutron radiation on nickel-based alloys[J]. Materials Science and Technology (United Kingdom), 2017, 33(05): 518-536. DOI: 0000-0003-1816-7805.
13. Mao Z, Zhang D Z, Jiang J, et al. Processing optimisation, mechanical properties and microstructural evolution during selective laser melting of Cu-15Sn high-tin bronze[J]. Materials Science and Engineering: A, 2018, 721: 125-134. DOI: 10.1016/j.msea.2018.02.051.
14. Gao T, Wu Y, Wang J. Mechanism of incipient annular corrosion of high-tin bronze in simulated soil solution[J]. Corrosion Engineering, Science and Technology, 2023, 58(5): 464-474. DOI: 10.1080/1478422X.2023.2202062.
15. WANG Jia, ZHANG Zixiong, LI Kaixuan, et al. Scheme design for neutron beam shaping assembly based on D-Be compact fast neutron source[J]. Nuclear Techniques, 2024, 47(12): 7-15. DOI: 10.11889/j.0253-3219.2024.hjs.47.120201.
16. ZHANG Zixiong, LI Kaixuan, WEI Qianglin, et al. Simulation study of medical isotope production using electron accelerator-driven photoneutron source[J]. Nuclear Techniques, 2024, 47(09): 37-44. DOI: 10.11889/j.0253-3219.2024.hjs.47.090203.
17. Johansson A J, Lilja C, Sjögren L, et al. Insights from post-test examination of three packages from the MiniCan test series of copper-cast iron canisters for geological disposal of spent nuclear fuel: impact of the presence and density of bentonite clay[J]. Corrosion Engineering, Science and Technology, 2017, 52(sup1): 54-60. DOI: 10.1080/1478422x.2017.1296224.
18. Björkbacka Å, Hosseinpour S, Leygraf C, et al. Radiation induced corrosion of copper in anoxic aqueous solution[J]. Electrochemical and Solid-State Letters, 2012, 15(5): C5. DOI: 10.1149/2.022205esl.
19. SHEN Chuankai, ZHANG Baoliang, LIU Wenguan, et al. Research status of density functional theory in corrosion of reactor alloy materials[J]. Nuclear Techniques, 2024, 47(10): 4-17. DOI: 10.11889/j.0253-3219.2024.hjs.47.100001.
20. Chen J, He X, Hou Z, et al. The differences in bonding properties and electrical, thermal conductivity between the preferred crystallographic orientation interface of Cu_3Sn/Cu[J]. Surfaces and Interfaces, 2024, 104152. DOI: 10.1016/j.surfin.2024.104152.
21. ZHENG Min, ZHANG Qichao, HUANG Yanliang, et al. Determination of representative ground-water for corrosion assessment of candidate materials used in Beishan area preselected for high-level radioactive waste disposal repository[J]. Journal of Chinese Society For Corrosion and Protection, 2016, 36(02): 185-190. DOI: 10.11902/1005.4537.2015.055.

22. XU Qiufa, GAO Kewei, PANG Xiaolu, et al. Effects of Cl^-, SO_4^{2-} and CO_3^{2-} ions on corrosion resistance of carbon steel in groundwater solution[J]. Transactions of Materials and Heat Treatment, 2015, 36(7): 166-173. DOI: 1009-6264(2015)07-0166-08.

23. Clark S J, Segall M D, Pickard C J, et al. First principles methods using CASTEP[J]. Zeitschrift für Kristallographie-Crystalline Materials, 2005, 220(5-6): 567-570. DOI: 10.1524/zkri.220.5.567.65075.

24. Muller J, Laïk B, Guillot I. α-CuSn bronzes in sulphate medium: Influence of the tin content on corrosion processes[J]. Corrosion Science, 2013, 77: 46-51. DOI:10.1016/j.corsci.2013.07.025.

25. ZHANG Jieru, YANG Bo, PAN Haiying, et al. Corrosion mechanism of iron-based materials adsorption Cl^- in high level radioactive waste packaging containers[J]. Nuclear Techniques, 2021, 44(10): 12-18. DOI: 10.11889/j.0253-3219.2021.hjs.44.100301.

26. TIAN Zhen, LI Congcong, WU Yuan, et al. Research progress in multi-principal element alloys for nuclear structure materials on irradiation damage[J]. Journal of Materials Engineering, 2024, 52(1): 1-15. DOI: 10.11868/j.issn.1001-4381.2023.000600.

27. Sun C. A short review of defect superlattice formation in metals and alloys under irradiation[J]. Journal of Nuclear Materials, 2022, 559: 153479. DOI: 10.1016/j.jnucmat.2021.153479.

28. WEI Qianglin, LIU Yibao, YANG Bo, et al. Corrosion behavior of Q235 carbon steel in simulated groundwater in Gansu Beishan area with high-strength γ irradiation[J]. Atomic Energy Science and Technology, 2019, 53(01): 59-66. DOI: 10.7538/yzk.2018.youxian.0643.

Note: Figure translations are in progress. See original paper for figures.