Materials Design for Tellurium Capture in Molten Salt Reactors via Atomic-Scale Thermodynamic Modeling

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1. Introduction

Tellurium (Te), a fission product in molten salt reactors (MSRs), segregates at grain boundaries (GBs) and induces intergranular cracking in structural alloys [1]. Conventional mitigation approaches such as alloy development and protective coatings reduce Te-induced damage but cannot prevent Te accumulation in circulating salts [2,3]. To address this challenge, absorber materials that selectively capture Te are required.

This study aims to establish a computational framework to evaluate candidate materials for Te capture at the atomic scale. By focusing on the thermodynamic driving forces of Te adsorption and segregation, we provide quantitative criteria to identify metals with strong affinity for Te and assess their potential as the absorbers in MSR environments.

2. Methods and Results

Atomic-scale thermodynamic modeling was performed to evaluate the behavior of Te in candidate absorber materials for MSR environments. All calculations used the Preferred Potential (PFP, v5.0.0), a neural network interatomic potential trained on density functional theory (DFT) datasets, enabling large-scale simulations with high accuracy and efficiency [4]. We employed the chemical potential (μ_{Te}) as the descriptor of Te stability at different atomic sites. The relative difference in μ_{Te} between two sites represents the thermodynamic driving force for Te adsorption and migration. As illustrated in Fig. 1, Te interaction with the absorbers follows two representative diffusion paths: (1) adsorption onto the surface from the salt, and (2) segregation from the surface into grain boundaries (GBs).

Structural models were constructed to calculate site-specific μ_{Te} values using atomic-scale simulations (Fig. 2). Surface models were prepared using low-index planes of FCC, BCC, and HCP structures, with Te placed at representative adsorption sites. GB models were generated as symmetric tilt grain boundaries (STGB) for representative FCC, BCC, and HCP systems, with each GB slab containing ≥25 Å atomic thickness. These structural configurations provide a systematic framework to quantify the site-specific driving forces for Te capture.

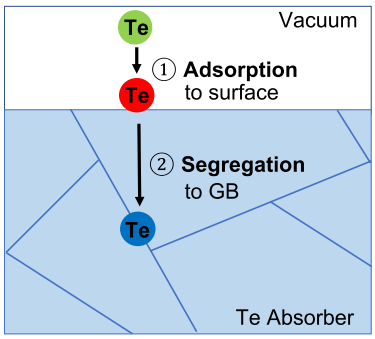

Fig. 1. Diffusion paths of Te in absorbers: (1) adsorption to the surface, (2) segregation to the grain boundary (GB).

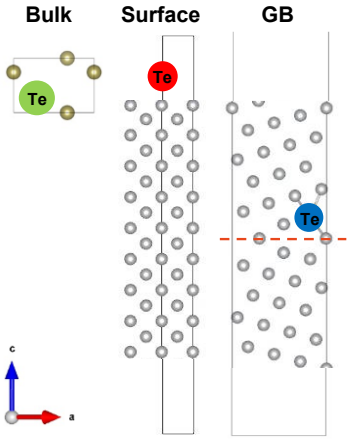

Fig. 2. Structure modeling for calculating site-specific chemical potential of Te at surface and GB sites.

The thermodynamic driving forces were defined as:

(1) $\Delta\mu_{adsorption} = \mu_{Te\ (surface)} - \mu_{Te\ (bulk)}$

(2) $\Delta\mu_{segregation} = \mu_{Te\ (GB)} - \mu_{Te\ (surface)}$

Figure 3 summarizes the ranking of candidate metals according to these two factors. Elements such as Ta, W, Mo, Nb, V, and Mn exhibit stronger Te adsorption than Fe and Ni, which are commonly used structural materials in MSRs. In addition, Nb shows the most favorable segregation tendency from surface to GB, indicating its strong ability to capture Te into

subsurface regions. These results provide a systematic screening of candidate metals for Te absorbers and highlight the importance of considering both surface adsorption and GB segregation to select Te absorber materials.

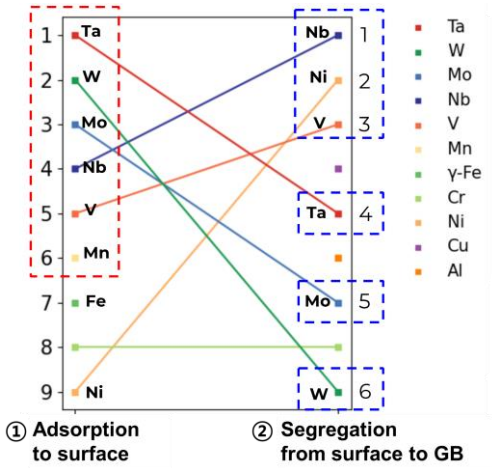

Fig. 3. Ranking of candidate materials based on Te adsorption and segregation: red box highlights metals with stronger surface adsorption than Fe and Ni; blue box shows relative ranking for GB segregation tendency.

3. Conclusions

This study employed atomic-scale thermodynamic modeling to evaluate candidate materials for Te capture in MSRs. By comparing site-specific chemical potentials at surfaces and GBs regions, we identified the driving forces that govern Te adsorption and segregation. The results reveal clear differences among metals, indicating that certain candidates exhibit stronger surface affinity and more favorable GB segregation than conventional structural alloys such as Fe and Ni. These findings demonstrate that thermodynamic modeling can provide an efficient framework for screening absorber materials and guiding future experimental validation.

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