Engineering Materials against Molten Chloride Corrosion

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Molten salts enable numerous industrial applications, yet trace impurities such as moisture severely accelerate corrosion. Because traditional phase stability diagrams disregard these impurities, we present a holistic computational framework for impurity-inclusive, three-dimensional phase stability (Pourbaix) diagrams in molten chlorides. Applied to transition metal systems, these diagrams quantitatively predict that boride phases offer exceptional thermodynamic stability and corrosion resistance against oxygenated species. Guided by these computational predictions, we demonstrate two kinds of engineered materials – siliconized stainless steel 316 and Inconel 625 metal-matrix composites reinforced with 2wt% TiB_2 or ZrB_2 via laser powder-bed fusion. Upon exposure to NaCl–KCl–$MgCl_2$ at 800°C for 300 h, both materials exhibit solid corrosion resistance against molten chlorides, while the unmodified alloy exhibited a maximum chromium-depletion depth of 71.3 μm. Specifically, the siliconized SS316 formed a robust surface silicide layer that effectively suppressed the outward diffusion and dissolution of vulnerable base metals. Parallelly, the grain boundary strengthening with Mo-rich boride precipitates reduced this depth to 12.5 μm in the TiB_2-reinforced alloy. CALPHAD and Pourbaix-diagram calculations confirm that these borides remain thermodynamically stable, effectively shielding grain boundaries from intergranular attack. Ultimately, this combined computational and experimental approach provides explicit purification targets and a practical design strategy for developing advanced, corrosion-resistant alloys for molten salt environments.

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