

Atomic origin of CO₂-promoted oxidation dynamics of chromia-forming alloys

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Abstract: The development of atomic imperfections within oxide films from high-temperature oxidation of heat-resistant alloys significantly limits the self-protectiveness of the surface oxide, contributing to the failure of energy generating system components such as turbines, engines, and heat exchanges. Directly probing the dynamics of such atomic defects is challenging because of the extreme thermochemical conditions of high-temperature oxidation. Using environmental transmission electron microscopy observations, here we directly capture atomic-scale dynamics of vacancies in growing Cr₂O₃ film during high-temperature oxidation of NiCr alloy in CO₂. Coordinated with theory modeling, we delineate the atomistic mechanisms associated with the effect of interstitial carbon derived from CO₂ on promoting the formation, migration and clustering of atomic vacancies to result in the enhanced alloy oxidation. The identified oxidation mechanism can find broader applicability in utilizing the atmosphere to tune the formation and evolution of atomic-scale defects, thereby affecting the mass transport properties of the growing oxide film.

Keywords: NiCr; High-temperature alloy oxidation; CO₂; In-situ TEM; DFT

Reference

[1] Zhu, Dingding, Jianmin Chen, Jingzhao Chen, Peng Jia, Shadie Zuo, Canying Cai, Jianyu Huang, and Guangwen Zhou. "Atomic Origin of CO₂-Promoted Oxidation Dynamics of Chromia-Forming Alloys." *Acta Materialia* 264 (2024/01/01/2024): 119578.