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Oxidation of Ni-Cr and Ni-Cr-W Alloys: Transformation from Alloy to Oxide

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The degradation of technical alloys including Ni-based superalloys and steels remains a technological challenge, and depends on the protective oxide layer. Our work focusses on the oxidation of Ni-based superalloys where the a protective oxide layer with chromia provides the corrosion and degradation resistance. [1] The majority of mechanistic studies are centered on transport through the oxide leaving significant gaps in the mechanistic understanding of the initial reaction steps of alloy oxidation. Our presentation will give comprehensive view of the oxidation processes on Ni-Cr-(W,Mo) surfaces. [2]
We use operando and in-situ experiments to capture the initial oxidation steps at the pristine alloy surface combining NAP-XPS, XPEEM, XPS, and STM experiments and DFT calculation. This work straddles the complexity gap by using single crystal thin films [3] as well as polycrystalline cast alloys with a wide composition range Ni-5Cr to Ni-30Cr, and the ternaries Ni-15Cr-6W, and Ni-15Cr-6Mo (all (at%)). The use of thin films is achieves a variation in alloy composition with relative ease, and offers NiCr(100) and NiCr(111) surfaces. [4] Our work identified using NAP-XPS the surface chemical reactions central to understand the role of minor alloying elements (MAE) such as W, and M where a relatively small addition of a specific element has an outsized impact on oxidation. [5] With NAP-XPS experiments [2] in combination with DFT it was shown that MAE is tied to the formation of preferential adsorption sites at the W-Cr bridge site thus favoring the nucleation of the coveted chromia over NiO. Variation in oxidation parameters p(O2) (10-9 to 10-2 mbar) and T (200 ℃ to 600 ℃) isolate kinetic limiters, which include an enhanced bulk diffusion through alloying with W, and an unexpectedly short diffusion length for O-atoms for T<300℃. [6] Polycrystalline, large grain (up to 1 mm) cast alloys gives access to a wide range of surface orientation, [7] far beyond the low index surfaces of model systems. The relevance of crystallographic orientation on oxide nucleation and chemistry will be discussed based on XPEEM, and STM experiments.

REFERENCES
[1] V. Maurice, P. Marcus. Prog. Mater. Sci., 95, 132-171 (2018)
[2] C. Volders, V.A. Angelici, I. Waluyo, A. Hunt, L. Árnadóttir, P. Reinke. npj Materials Degradation, 6, 52 (2022)
[3] G. Ramalingam, P. Reinke. Journal of Applied Physics, 120, 225302 (2016)
[4] W.H. Blades, M.R. Barone, P. Reinke. npj Materials Degradation, 5, 1-10 (2021)
[5] K. Lutton Cwalina, C.R. Demarest, A.Y. Gerard, J.R. Scully. Curr. Opin. Solid State Mater. Sci., 23, 129-141 (2019)
[6] R. Ramanathan, G. Ramalingam, J.H. Perepezko, P. Reinke, P.W. Voorhees. ACS Applied Materials & Interfaces, 10, 9136-9146 (2018)
[7] K. Gusieva, K.L. Cwalina, W.H. Blades, G. Ramalingam, J.H. Perepezko, P. Reinke, J.R. Scully. J. Phys. Chem. C, 122, 19499-19513 (2018)

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Surface Science

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