

研究タイトル: Studying ‘Physical Chemistry of Materials Degradation’
[材料劣化の物理化学的な研究]



氏名:	田須 ニシス / DAS Nishith	E-mail:	nishith@sendai-nct.ac.jp
職名:	准教授	学位:	博士(工学)
所属学会・協会:	ASME		
研究分野:	Materials Science and Engineering [材料工学]		
キーワード:	Oxidation Mechanism [酸化発生メカニズム]; Corrosion [腐食]; DFT (密度汎関数理論); Multiscale Modeling [マルチスケールモデリング]		
技術相談	<ul style="list-style-type: none"> Understanding of Stress Corrosion Cracking Mechanism [応力腐食割れのメカニズム] 		
提供可能技術:	<ul style="list-style-type: none"> Developing New Materials [新しい材料の開発] 		

研究内容:

The interaction of water with metals at high temperatures leads to the dissolution of metallic atoms and diffusion of dissociated elements, resulting in surface oxidation, a key step in the early stages of corrosion. Understanding these fundamental reactions is essential for improving materials reliability under extreme conditions.

Previous studies show that both oxygen (O) and hydrogen (H) accelerate the oxidation process [1, 2]. Dissociated hydrogen from H₂O diffuses into the metal, becoming negatively charged and initiating localized electron transfer, as shown in Fig. 1. The localized electron transfer process generates strain into the structure. This strain at the surface facilitates oxygen penetration, accelerating the oxidation process [3].

Further research focuses on identifying minor elements that form stable oxide films to improve oxidation resistance. Based on theoretical findings, ultra-high-purity (UHP) iron-based heat-resistant alloys have been developed, showing that adding Zr, Sc, and Nb enhances creep and oxidation resistance under advanced ultra-supercritical (A-USC) conditions [4].

1. N. K. Das, *et al.*, Corros Sci, 50, pp. 1701-1706 (2008).
2. N. K. Das, *et al.*, Corros Sci, 51, pp. 908-913 (2009).
3. N. K. Das, *et al.*, Int J Hydrogen Energ, 38, pp. 1644-1656 (2013).
4. F. Hamdani, *et al.*, Metall and Mat Trans A, 49A, pp.2373-2383 (2018)

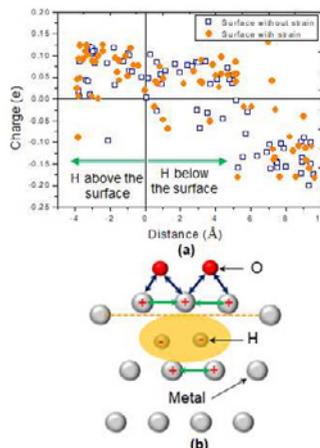


Fig. 1. (a) The calculated H atomic charges in alloys and (b) schematic of H in metals

提供可能な設備・機器:

名称・型番(メーカー)

名称・型番(メーカー)	