

研究タイトル: Designing 'Corrosion Resistant' Materials using Computational Chemistry Methods [計算科学による「耐食材料」の開発]

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研究分野: Computational Materials Science [計算材料科学]

キーワード: DFT (密度汎関数理論); Materials Genome (マテリアルゲノム)

技術相談

提供可能技術:



研究内容:

研究課題

Understanding fundamental mechanism of oxidation

Hydrogen- accelerated oxidation

Designing new materials

研究シーズ

The interaction of water with metal in high temperature environments leads to the dissolution of metallic atoms and the diffusion of dissociated elements. Subsequently, oxidation takes place at the surface. The metal surface oxidation is an important step for the early stage of corrosion. Thus, it is desirable to get better description and deeper insight into the basic features of chemical reaction of water with metal surface. Atomic scale studies indicate that both O and H can accelerate the surface oxidation process [1,2]. For example, the dissociated H from H<sub>2</sub>O can quickly diffuse into the structure and become negatively charged species, as shown in Fig. 1. The negatively charged H initiates a localized electron transfer process by taking electron; which generates localized strain in the metal surface. This process can help dissociated O to penetrate deeper into the structure. As a result, the subsurface hydrogen accelerates the early stage of oxidation [3]. A further study is carried out to find some minor elements that can form a stable oxide film on the metal surface. Based upon theoretical finding, ultra high purity (UHP) iron-based heat-resistant alloys are developed [4]. The alloy demonstrates that the addition of Zr, Sc and Nb significantly improve the creep and oxidation resistance under the advanced ultra-supercritical (A-USC) condition.

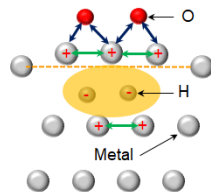


Fig. 1 a schematic representation of H in metals

1. N. K. Das, *et al.*, Corr. Sci., 50, pp. 1701-1706 (2008).
2. N. K. Das, *et al.*, Corr. 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).

提供可能な設備・機器:

名称・型番(メーカー)
