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学位論文紹介
Doctoral Thesis Introduction

Exploring New High-Entropy Materials for Functional Applications

機能性材料への応用を目指した新しい高エントロピー材料の探索

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1. Introduction

High-entropy materials include high-entropy alloys (HEAs) and high-entropy ceramics are materials with five or more than five principal elements. They have an entropy of mixing more than 1.5R (R: gas constant) which leads to their low Gibbs free energy and corresponding high stability. High-entropy materials have shown considerable potential for various applications due to their superior properties such as high lattice strain, lattice defect, and cocktail effect. In this research work, arc melting and high-pressure torsion (HPT) were used to fabricate and processing of some high-entropy alloys and ceramics which then were examined for Vicker hardness and applications for nickel-metal hydride batteries, and photocatalytic activity for water splitting to produce the O_2 and H_2.

2. Introducing an ultra-hard high-entropy alloy

A carbon-doped AlTiFeCoNi HEA was produced by arc melting and then processed by HPT to improve the Vickers hardness. The material had three phases FCC, BCC and $L2_1$ in agreement with CHALPHAD calculation. It was treated by HPT to improve the structure and Vicker hardness. XRD results showed the $L2_1$ phase transformed to BCC phase after HPT processing. An effective grain refinement occurred after the HPT treatment was confirmed by transmission electron microscopy (TEM) and electron backscatter diffraction (EBSD) analysis. This HEA showed a Vicker hardness of 630 Hv which increased significantly to 950 Hv after HPT as high as some ceramics.

3. High-entropy hydrides as nickel-metal hydride batteries

$Ti_xZr_{2-x}CrMnFeNi$ HEAs with different Ti to Zr ratios were fabricated using arc melting and investigated as anode materials for nickel-metal hydride batteries for the first time. All HEAs had C14 Laves phase with a minor fraction of the B2 phase which the C14 phase includes the Ti and Ni-poor coarse grains and the B2 phase contains the Ti and Ni-rich small grains. Lattice parameters of HEAs decreased by increasing the Ti to (Ti + Zr) atomic ratio. The result of the nickel-metal hydride battery test showed the sample with Ti to (Ti + Zr) atomic ratio of 0.4 has the highest discharge capacity of around 80 $mAhg^{-1}$ with considerable cyclic stability.

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4. Heterostructured high-entropy oxide photocatalyst

HPT was used to produce a high-entropy oxide (HEO) with $TiZrNbTaWO_{12}$ composition then examined for photocatalytic water splitting. The material contains five different phases including one orthorhombic phase, two monoclinic phases, and two tetragonal phases which can generate ten types of heterojunctions. The synthesized HEO showed higher light absorbance compared with corresponding binary oxides and could successfully generate O_2 under visible light. However, the relevant binary oxides either can not produce O_2 under visible light or has lower efficiency compared with this HEO.

5. Low bandgap high-entropy oxynitride photocatalyst

By considering the high potential of oxynitride photocatalysts for water splitting and superior properties and high stability of high-entropy materials a high-entropy oxynitride (HEON) with a narrow bandgap of 1.6 eV was fabricated by HPT. This HEON was evaluated for photocatalytic water splitting. The result showed extremely higher light absorbance compared with related HEO and binary oxides. Finally, it could successfully evolute the H_2 under UV irradiation even better than Ga_6ZnON_6 as a typical oxynitride for water splitting.

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List of Publications

[1] P. Edalati, A. Mohammadi, Y. Tang, R. Floriano, M. Fuji, K. Edalati, Phase transformation and microstructure evolution in ultrahard carbon-doped AlTiFeCoNi high-entropy alloy by high-pressure torsion, Mater. Lett. 302 (2021) 130368.
[2] P. Edalati, A. Mohammadi, Y. Li, H. W. Li, R. Floriano, M. Fuji, K. Edalati, High-entropy alloys as anode materials of nickel-metal hydride batteries, Scr. Mater. 209 (2022) 114387.
[3] P. Edalati, Y. Itagoe, H. Ishihara, T. Ishihara, H. Emami, M. Arita, M. Fuji, K. Edalati, Visible-light photocatalytic oxygen production on a high-entropy oxide by multiple-heterojunction introduction, J.

Photochem. Photobiol. A 443 (2022) 114167.
[4] P. Edalati, X. F. Shen, M. Watanabe, T. Ishihara, M. Arita, M. Fuji, K. Edalati, High-entropy oxynitride as a low-bandgap and stable photocatalyst for hydrogen production, J. Mater. Chem. A9 (2021) 15076–15086.

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Curriculum Vitae

Parisa Edalati obtained Bachelor's and Master's degrees in Chemical Engineering at Ferdowsi University of Mashhad, Iran in 2014 and 2018, respectively. She received her Doctoral degree in Applied Chemistry and Life Sciences at Nagoya Institute of Technology, Japan in 2023.