## **MERIT Internship (Domestic) Report**

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# Acceptance:

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## **Research topic:**

Development and investigation of mechanical properties of new high entropy alloys in group 4 based systems

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## **Content:**

## 1, Background

Metallic titanium (Ti) material is widely used as a material for the aerospace field. In particular, heatresistant Ti alloys have been used as materials for jet engine compressors. On the other hand, in recent years, in order to improve the thermal efficiency of the engine, the temperature inside the compressor tends to be higher than 550 °C. At such high temperatures, the existing Ti material has insufficient heat resistance, so substitution of nickel (Ni)-based superalloys is in progress. However, Ni-based superalloys are not suitable from the viewpoint of reduction of airplane weight due to their heaviness, and the use of Ti alloys is still very attractive to improve energy efficiency and reducing greenhouse gases.

Group 4 (Ti Group) metals exist in hcp structure at room temperature and change into bcc form at high temperature. Addition of other elements also influences the structure of group 4 based alloys.

Structural and mechanical properties dramatically change in the transformation, and in general  $\alpha$ -phase (hcp) has better heat resistance at high temperature. So, countless number of new  $\alpha$  and near- $\alpha$  alloys are proposed and developed both in academics and in industries. However, conventional methods are probably approaching their limits, and radically new strategies are required, rather than just the modification of existing methods.

The concept of high entropy alloy (HEA) is one of the critical candidates for such material developments. This method is comparatively new and some HEAs are known to their unique and excellent properties. HEA surveys so far are mainly for bcc structure, and in contrast, there is very limited information on hcp-HEAs. This is partly because it is very difficult to obtain hexagonal structures during their alloying. Almost all of related studies are only recently published, and the competition will be keen in near future.

#### 2, Purpose of this study

Needless to say, candidates of addition agents for group 4 based alloy are important. And hafnium (Hf) is also hcp but was excluded from candidates in this study due to its heaviness. So, we focused on design of new Ti-Zr based HEAs, analyzed the structures, investigated the mechanical properties, and gave feedbacks for future works. This cycle will contribute to HEA research fields, and hopefully, will trigger the breakthrough of heat-resistant materials development.

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#### 3, Thermodynamic considerations

Firstly, thermodynamics based on phase diagrams was discussed. We collected many previous references, binary/ternary/pseudobinary phase diagrams, and listed composition candidates of new HEAs that we decided to focus on. Then we conducted the parameter method and discussed the stabilities of these alloys by the parameters. However, this method had large errors and uncertainty at present. In addition, sometimes mechanical properties can improve by precipitations, so experimental investigations were necessary.

Furthermore, thermodynamic software (Thermo-Calc) analyses were also conducted. However, these calculations were based on the database obtained from Ti rich alloys information, and some required data were unavailable because we chose rare metals for the addition agents. So the reliability of

Themo-Calc calculations were comparatively low. Furthermore, these calculations depend on equilibrium theory, but actual materials development has deep relationships with kinetics. As a result, critical considerations based on parameter method and Thermo-Calc software were difficult to accurately discuss the systems in this study.

# 4, Experiments

Figure 1 shows the experimental procedure of this study. Scanning electron microscopy (SEM) observation, energy-dispersive X-ray spectroscopy (EDS) analysis, and electron backscatter diffraction (EBSD) analysis were conducted for the annealed samples.



Figure 1 Experimental procedure of this study

### 5, Results and discussion

As a result of the analyses, it was possible to identify the phases of each alloy, so we compared them with the thermodynamic considerations. However, it was also found that the experimental process needs to be improved and that there are some phenomena that cannot be explained by the current data, so additional investigation is necessary as future works.

Based on these results, further experiments and analyses in this system are expected to lead to the development of new materials that combine strength, ductility, and heat resistance.

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