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High Entropy MAX phase and MXene for Radioactive Waste Management

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1. Introduction

MAX phase refers to metal-like ceramics consisting of early transition metals (M), 13-15 group elements (A), and Carbon or Nitrogen (X). It is used as a high-temperature structure material due to high elastic stiffness, thermal conductivity, thermal shock resistance, oxidation resistance, etc. In nuclear engineering, Zr-based MAX phases such as Zr_2AlC or Zr_3AlC_2 are considered as one of the candidate materials for accident tolerant fuels[1].

By selectively etching A element layers in a MAX phase, new two-dimensional transition metal carbides or nitrides nanomaterials can be obtained, which called MXene. MXene has a high surface area, electrical conductivity, and good optical properties, so it is applied to the catalyst, energy storage, EMI shielding, or heavy metal ion decontamination[2]. Especially in the nuclear field, MXene has been studied for decontamination or disposal of nuclear waste such as Cs-137, Sr-90, and U [3].

High-entropy materials composed of 4-5 elements with similar atomic ratios are also promising materials in the nuclear field due to their high-temperature properties and high irradiation resistance. The concepts of high entropy were only limited in alloy systems, but it has been gradually extended to ceramic materials such as oxides, carbides, and nitrides[4]. Recently, high entropy MAX phase and MXene were also developed and showed high tailored properties[5]. In this study, we synthesized new compositions of high entropy MAX and MXene for radioactive waste management applications.

2. Experiment

2.1. Synthesis of High Entropy MAX phase

Based on DFT calculation results, 2 high entropy MAX phase, $(T,V,Nb,Ta)_2AlC$ and $(Ti,V,Zr,Ta,)_2AlC$, were chosen and synthesized. Element powders, Ti, V, Nb, Ta, Al, C or Ti, V, Zr, Ta, Al, C, were mixed in the atomic ratio of 1:1:1:1:2:2 and ball milled in a polypropylene jar for 18 h. The milled powders were annealed in an Ar atmosphere at 1500 °C for 4 hr. As shown in Figure 1,

2.2 Synthesis of High Entropy MXene

The synthesized MAX powder were ground in a mortal and pestle and sieved through a 200 mesh test sieve. The sieved MAX powder were poured into LiF/HCl mixture solution and stirred for 24 h at 60 °C. Then the Al layer in the MAX phase were selectively etched and monolayered $(T,V,Nb,Ta)_2C$ and $(T,V,Nb,Ta)_2C$.

In future work, various properties suitable for radioactive waste management applications such as radionuclide adsorption will be studied with the high entropy MAX phase and MXene.

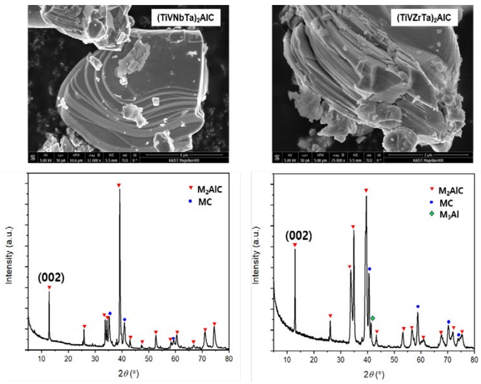

Figure 1. SEM image and XRD patterns of the high entropy MAX phase

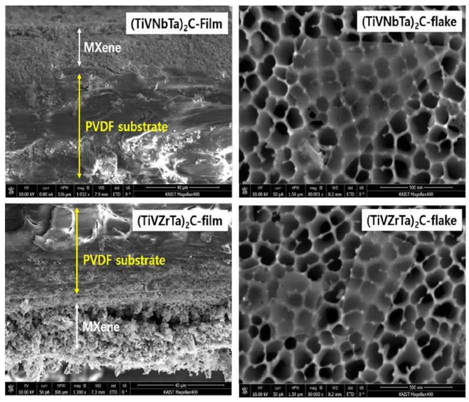

Figure 2. SEM image of the high entropy MXene

3. Summary

Two advanced materials, MAX phase and MXene, were prepared in the form of high entropy phase more suitable for radioactive waste management applications. Two compostions of high entropy MAX phase, $(Ti,V,Zr,Ta,)_2AlC$ and $(Ti,V,Zr,Ta,)_2AlC$, determined from the first principle calculations were successfully synthesized. Also, High entropy MXene were prepared by selective etching of their high entropy MAX phase.

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