Journal of Engineering Mechanics and Machinery (2022)
Clausius Scientific Press, Canada

DOI: 10.23977/jemm.2022.070407
ISSN 2371-9133 Vol. 7 Num. 4

Microstructure and mechanical properties of $Ni_2FeCo_{0.5}Cr_{0.5}Ta_x$ high-entropy alloys

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Keywords: High-entropy alloy; Microstructure; Mechanical properties

Abstract: High-entropy alloys (HEAs) have attracted much attention for their promising mechanical properties. A new alloy system $Ni_2FeCo_{0.5}Cr_{0.5}Ta_x$ (x = 0, 0.1, 0.3, 0.4, 0.6) with multi-principal elements was designed in this research. These HEAs were prepared by vacuum arc melting method. The crystal structure and microstructure of the HEAs were investigated by X-ray diffraction and scanning electron microscopy. The research results show that the $Ni_2FeCo_{0.5}Cr_{0.5}$ HEA was single-phase face-centered-cubic solid solution, whereas the Ta addition can lead to the formation of Laves phase. Typical cast dendrite and interdendrite structures were observed in the $Ni_2FeCo_{0.5}Cr_{0.5}Ta_x$ HEAs. Vickers hardness and room-temperature compression tests were performed to investigate the effects of Ta adding on the mechanical properties of the new alloy system. The Vickers hardness and the yield strength increase with increasing Ta content.

1. Introduction

The conventional alloys design was often based on one or two principal elements for primary properties, such as Fe-based steels, Mg-based alloys, Al-based alloys and so on. Recently, high-entropy alloys (HEAs), as new series of alloys, are defined as alloys that contain at least five principal elements with each elemental molar ratio between 5 and 35 at.% [1, 2]. With proper composition design, HEAs can possess multiple excellent properties. It has been reported that the face-centered-cubic (FCC) structured HEAs exhibit low strength and high plasticity, and body-centered-cubic (BCC) structured ones show high strength and low plasticity. Thus, the alloying elements are the dominant factor for controlling the microstructure and mechanical properties of HEAs. Many researchers have studied on the effect of alloying elements adding on the microstructure and properties of HEAs [3-7]. For example, Zhou et al.

[8] have investigated the Ti element alloying effect on AlCoCrFeNi HEA and found that the alloy system is composed primarily of the BCC solid solution and possesses excellent room-temperature compressive mechanical properties. He et al. [4, 6] designed a system of CoCrFeNiNbx HEAs, composing of a ductile FCC phase and a hard Laves phase, show excellent integrated mechanical properties of ductility and strength. Therefore, the element adding has huge effects on the microstructures and phases forming of HEAs. It is necessary to investigate different kinds of HEA systems to investigate the relationship between the alloying elements adding and the

microstructure and mechanical properties of HEAs.

In this study, we designed the $Ni_2FeCo_{0.5}Cr_{0.5}$Tax (x = 0, 0.1, 0.3, 0.4, 0.6) HEAs and systematically investigated the effects of Ta adding on the microstructure and properties of the new alloy system. It is aimed to provide a reference study for further physical investigations and basic data for potential application of these alloys.

2. Experimental procedure

The $Ni_2FeCo_{0.5}Cr_{0.5}$Tax HEAs were prepared by a vacuum arc melting furnace under high-purity argon atmosphere with a water-cooled copper hearth. Elements of Co, Cr, Fe, Ni and Ta with purity of 99.95 wt % were used as raw materials. The alloys were reversed and re-melted five times to ensure the chemical homogeneity. The cast ingots were 13 mm in height and 30 mm in diameter. The samples cut from the solidified ingots were used to investigate their microstructure and mechanical properties. The crystal structures of the as-cast alloys were characterized by X-ray diffraction (XRD) with Cu Kα radiation, scanning from 20°to 100°at a scanning r ate of 4°/min. The microstructures of the alloys were analyzed using Scanning Electron Microscope (SEM Hitachi S-4800). The chemical compositions of different phases were calculated from the results of Energy Dispersive Spectrometer (EDS). Vickers hardness was measured using a hardness tester (HVS-1000) under a load of 500 g for 10 s. The Instron 5982 machine was used to test the room temperature compression properties of the as-cast alloys under a strain rate of 5×10^{-4} s^{-1}. We employed at least three cylindrical specimens 6 mm in length and 3 mm in diameter for each sample.

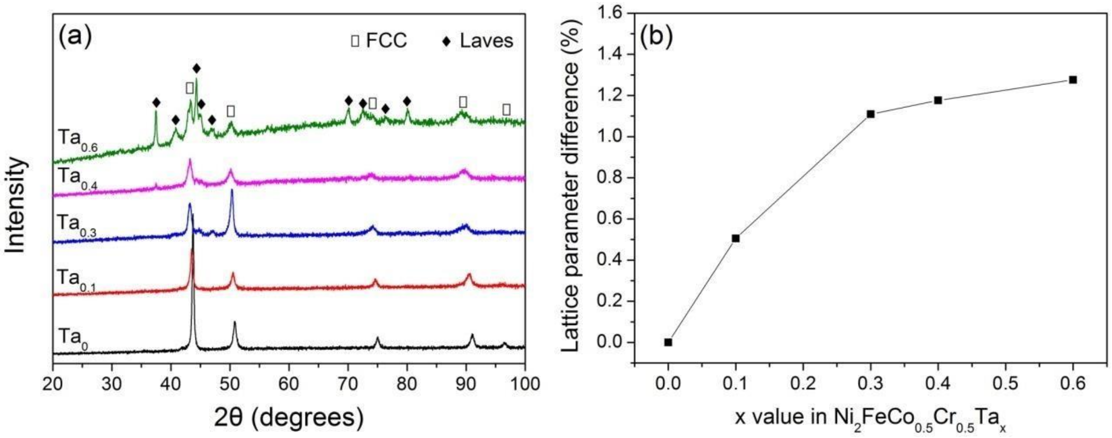

Figure 1: XRD patterns (a) and lattice parameter difference of the FCC matrix as a function of the Ta content (b) in the Ni2FeCo0.5Cr0.5Tax HEAs

3. Results and discussion

The XRD patterns of the as-cast $Ni_2FeCo_{0.5}Cr_{0.5}$Tax HEAs are shown in Figure 1(a). Only diffraction peaks corresponding to FCC crystal structure is observed in the $Ni_2FeCo_{0.5}Cr_{0.5}$ alloy. However, reflections of the Laves phase can be found in $Ni_2FeCo_{0.5}Cr_{0.5}$Tax Ta $_{0.1}$, $Ni_2FeCo_{0.5}Cr_{0.5}$Tax $Ta_{0.3}$, $Ni_2FeCo_{0.5}Cr_{0.5}$TaxT$a_{0.4}$, and $Ni_2FeCo_{0.5}Cr_{0.5}$TaxT$a_{0.6}$ HEAs, and the Laves phase can be identified as Co2Ta-type Laves phases, which is consist with Jiang's results [9]. With increasing the Ta content, the relative intensity of the FCC phase diffraction peaks reduces while the Laves phase diffraction peaks enhance, indicating that the volume fraction of the Laves phase increases with the increment of the Ta concentration. It is noticed that the (111) peak shifts towards a lower 2θ angle with increasing the Ta concentration. The lattice constants of the FCC phase, which were estimated from the (111) peak, were 3.5803, 3.5984, 3.6201, 3.6224, and 3.6261 Å in the $Ni_2FeCo_{0.5}Cr_{0.5}$Tax alloys

Corresponding to x = 0, 0.1, 0.3, 0.4, and 0.6, respectively. The lattice-parameter difference can be expressed as (|a-a0|)/a0, as shown in Figure 1(b), where a0 is the lattice parameter of the FCC matrix in the $Ni_2FeCo_{0.5}Cr_{0.5}$Tax alloy. The lattice-parameter difference increases with the increase of the Ta content indicated that Ta element, with a large atomic radius (Ta 146 pm) than other constituent elements (Fe 126 pm, Ni 124 pm, Co 125 pm, Cr 128 pm), can be partly dissolved into the FCC matrix phase and result in an increase of the lattice parameters.

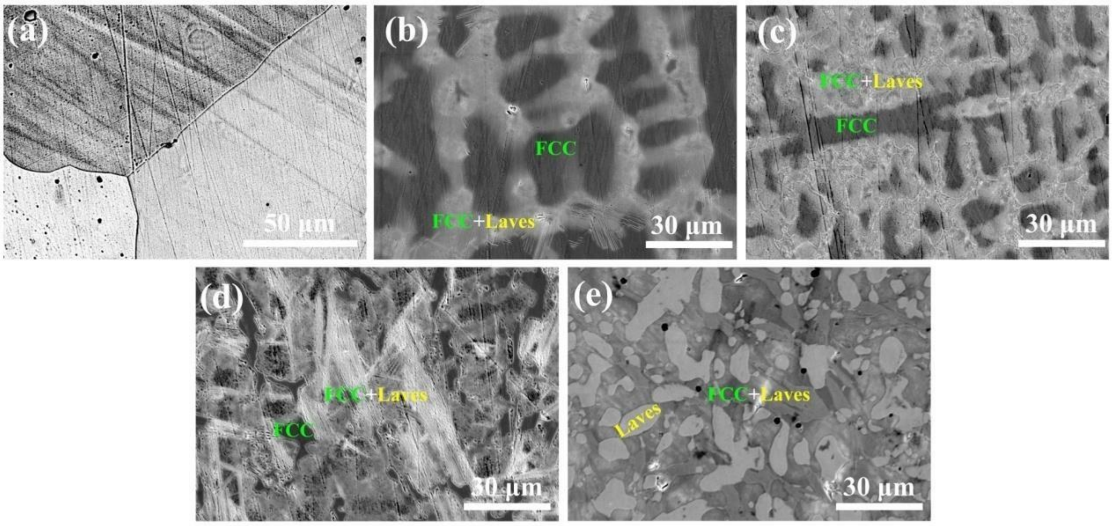

Figure 2: SEM images of the as-cast $Ni_2FeCo_{0.5}Cr_{0.5}Ta_x$ HEAs. (a) x = 0, (b) x = 0.1, (c) x = 0.3, (d) x = 0.4, and (e) x = 0.6.

The microstructure of the present HEAs were displayed in Figure 2. Different morphologies can be observed. The $Ni_2FeCo_{0.5}Cr_{0.5}$ alloy contains large grains and shows single FCC phase. Compared to the $Ni_2FeCo_{0.5}Cr_{0.5}$ alloy, the $Ni_2FeCo_{0.5}Cr_{0.5}Ta_{0.1}$, $Ni_2FeCo_{0.5}Cr_{0.5}Ta_{0.3}$, $Ni_2FeCo_{0.5}Cr_{0.5}Ta_{0.4}$, and $Ni_2FeCo_{0.5}Cr_{0.5}Ta_{0.6}$ HEAs exhibit typical cast dendrite (DR) identified as FCC phase and interdendrite (IR) identified as FCC + Leaves phase structures. These results are consistent with the XRD result. With increasing the Ta content, the IR region reduces and the DR region increases. In order to reveal the chemical component differences between the two phases in the HEAs, EDS was used to analyze chemical composition in the HEAs. For the $Ta_{0.1}$ HEA, the elements contents of the FCC phase (DR region) are 48.53 % (Ni), 22.64 % (Fe), 13.26 (Co),

13.43 % (Cr) and 2.15 % (Ta), respectively. The Laves phase contains 60.79 % Ni,12.94 % Fe, 13.00 % Co, 7.05 % Cr and 6.23 % Ta. The concentration of elements Ni and Ta is obviously enriched in Laves phase. The reason is that the negative mixing enthalpy can make intermetallic compounds form easily. The values of the mixing enthalpy for each atomic pairs [10] of the present HEAs are shown in Table1. It is clear that the enthalpy of mixing between Ta and Ni is the lowest. So they more easily form compounds during solidification.

Vickers hardness and room-temperature compression tests were performed to investigate the effects of Ta additions on the macro-mechanical properties of the as-cast $Ni_2FeCo_{0.5}Cr_{0.5}$ Tax alloy system. Vickers hardness values of the $Ni_2FeCo_{0.5}Cr_{0.5}$Tax HEAs are shown in Figure 3. An increase of the Gd content results in a significant increase in hardness because of the formation of the Laves phase. The compressive engineering stress-strain curves for the $Ni_2FeCo_{0.5}Cr_{0.5}$ Tax HEAs are depicted in Figure 4(a). It was noted that the Ta_0 alloy presented the lowest values of Vickers hardness (191 HV) and yield strength (195 MPa) but demonstrated excellent ductility, which was compressed to 50% height reduction without fracture. When the Ta content increases to

0.1, the Vickers hardness and yield strength (291 HV and 856 MPa, respectively) were obviously higher than those of the Ta0 alloy. And the highest fracture strength reached to 3170 MPa. A further increase of Ta content resulted in the substantial increases of Vickers hardness and yield strength of the present HEAs, while the plastic strain showed significant decreases, as shown in Figure 4(b). The hard and brittle Laves phase could enhance blocking the movement of dislocations. Thus, the formation of the Laves phase significantly enhances the hardness and strength of the HEAs. The similar results can be found in other articles [6, 11, 12]. However, it is obvious that the fracture strength and fracture strain of Ta0.6 alloy decrease rapidly, which was attributed to high volume fraction of the hard/brittle Laves phase. The high Ta content can lead to the brittle fracture.

Table 1: Mixing enthalpy of different atom pairs, H^{mix} (kJ/mol), in the $Ni_2FeCo_{0.5}Cr_{0.5}Ta_x$ HEAs calculated by Miedema's approach [10]

Element	Ta	Co	Cr	Fe	Ni
Ta	-	-24	11	-15	-29
Co	-	-	-4	-1	0
Cr	-	-	-	-1	-7
Fe	-	-	-	-	-2
Ni	-	-	-	-	-

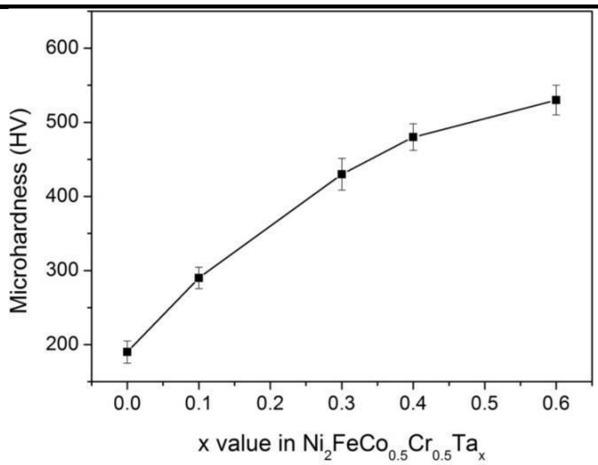

Figure 3: Vickers hardness of the as-cast Ni2FeCo0.5Cr0.5Tax HEAs.

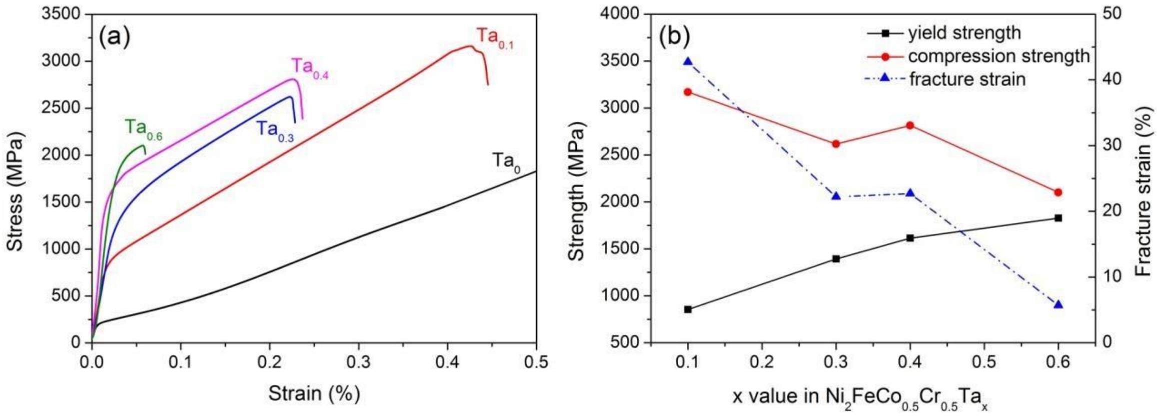

Figure 4: (a) Compressive engineering stress–strain curves of the Ni2FeCo0.5Cr0.5Tax HEAs. (b) Compressive strength, yield strength and fracture strain of the $Ni_2FeCo_{0.5}Cr_{0.5}Ta_x$ HEAs.

4. Conclusions

In this work, a typical single FCC crystal structure is indentified in the $Ni_2FeCo_{0.5}Cr_{0.5}$ HEA. With the addition of Ta element, besides the FCC phase, Laves phase also formed in the HEAs. Furthermore, the microstructure of the $Ni_2FeCo_{0.5}Cr_{0.5}Ta_x$ alloys is typical cast dendrite and interdendrite structures. The Vickers hardness and yield strength of the present HEAs increases as the increase of the Ta element content, which due to the formation of the hard Laves phase.

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