FCC-to-HCP Phase Transformation in CoCrNi_x Medium-Entropy Alloys

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Abstract

A hybrid first-principles/Monte Carlo simulation is combined with experiments to study the structure and elastic properties of CoCrNi_x ($x = 1-0.5$) alloys. The experimental X-ray diffraction patterns show that the structures have changed from the single-phase face-centered cubic (FCC) structure at $x = 1-0.8$ to the coexistence of FCC and the hexagonal close-packed structures at $x = 0.7-0.5$, which is further confirmed by calculations on mixing energies. The elastic moduli by calculation are basically in agreement with experiments. Room-temperature tension shows that the six alloys have a certain plasticity, the strength and plasticity of the alloys have a linear decrease with the decrease in Ni contents, and the plasticity of the alloys drops from 84 to 23%. Furthermore, first-principles density function theory calculations were employed to reveal the electronic and magnetic structures of alloys. The electron density of states for all alloys is asymmetrical, which illustrates that the alloys are ferromagnetism. It is found that Cr atoms can suppress the ferromagnetism of alloys, since Cr atoms have both positive and negative magnetic moments in all alloys.

Keywords Hexagonal close-packed (HCP) structure · Medium-entropy alloys · Magnetic · Mechanical properties · Phase transformation · High-entropy alloys

1 Introduction

Traditional alloys are based on a single principal element with adding small amount of other elements to enhance particular properties. Recent years, a new class of alloys with multiple principal elements appeared in 2004 [1–5], which are termed as high-entropy alloys (HEAs), were proposed. The definition of HEAs is based on either composition [4] or the magnitude of the mixture entropy [6]. Under the compositional definition, HEAs are defined as those alloys having five or more principal elements with an atomic ratio of each element between 5 and 35% [4]. Under the entropy definition, the distinguishing criterion is the variable of the

system's configuration entropy. When the value of ΔS (the configuration entropy change per mole) is less than R (the gas constant, $R = 8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$), the alloy is at low entropy state, when $R < \Delta S < 1.5R$, it is at medium-entropy state, and thus the system is medium-entropy alloy (MEA), and when $\Delta S > 1.5R$, it is at high-entropy state.

The design of the HEAs can lead to high mixing entropy, which can inhibit the formation of intermetallic compounds and thus promote the formation of the solid solution phases in simple crystal structures, such as face-centered cubic (FCC) [7, 8], body-centered cubic (BCC) [7, 8], or hexagonal close-packed (HCP) [9, 10] lattices. Due to its unique solid solution structure, HEAs often have excellent properties, such as high strength [11], high hardness [12], and high thermal resistance [13]. These excellent properties make HEAs promising as new kinds of metallic alloys.

Several possible mechanisms have been proposed to explain the excellent mechanical properties of HEAs, including lattice distortion and sluggish diffusion. However, due to the multicomponents, there are more experimental difficulties in determining the atomistic details of lattice structures, defect structures, and deformation mechanisms in HEAs. Lu et al. [14] proposed the concept of eutectic high-entropy alloy (EHEA) to solve the problem that large-scale

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production cannot be performed due to the presence of multiple components. Recently, the atomic simulation method has been widely applied to study the features related to the microstructure of HEAs. Among the atomic simulation techniques, the first-principles simulation which is based on density function theory (DFT) is a powerful tool that can be of great help in investigating materials. The calculated results can be served as valuable references for experimental researches. Wang et al. used the first-principles to find that the interlayer adsorption of double-layer MoS_2 is relatively more stable than that of single-layer MoS_2 [15]. It is also found that through first-principle calculations, an increase in the Mo content in CoMo alloys would cause a rapid decrease for Co magnetic moment [16]. By first-principles simulations of HEAs, there are two main different sampling ways: single-phase coherent potential approximation (CPA) [17] and special quasi-hybrid structure (SQS) [18] methods. CPA is capable of handling chemical and magnetic disorder under any component, but its average field properties limit its application. SQS can simulate local pairing and multi-site correlation functions under the constraints of a given unit cell size to select the most stable structure.

The ternary equimolar CoCrNi MEA is based on the CoCrFeMnNi system, widely studied as the most classical system in the field of HEAs and/or MEAs, which has attracted wide attentions. In terms of experiments, there are many studies on its mechanical properties. It has reported that the nanocrystalline CoCrNi alloy obtained by high-pressure torque has an extremely high tensile strength of about 2.2 GPa [19, 20]. And it has been confirmed that the friction stress of the CoCrNi MEA is much larger than that of the conventional alloys, even higher than CoCrFeMnNi HEAs [21]. The CoCrNi MEA has incredible ductility and fracture resistance. It has a low temperature strength of up to 1.3 GPa and an elongation before failure over 70% [22].

And CoCrNi alloys are composed of 3d transition metals, and the magnetism has a great influence on many properties. First, the magnetic entropy affects phenomena associated with thermodynamic phase stability, such as ordered disorder [23] and structural phase transitions [24, 25]. In addition, the magnetism may have significant effects on other properties, including mechanical properties [26, 27], electronic properties [28], and heat transfer [29]. Although there are many experimental studies on the CoCrNi MEA, there are only a few reports on the simulation results for the CoCrNi MEA.

In the present study, the integrated experimental and theoretical approaches were used to study the CoCrNi_x ($x = 1-0.5$) MEAs. The systematical heat treatments were conducted to develop the microstructure with the fully homogenous elemental distribution. The prepared sample was then subjected to a tensile test at room temperature using a mechanical testing machine to investigate the

mechanical properties of the alloys. Furthermore, using a hybrid first-principles/Monte Carlo (MC) simulation, the stable MEA structures are constructed, and the elastic parameters, magnetic moment, and density of states (DOS) of CoCrNi_x ($x = 1-0.5$) alloys are calculated. And the effect of the Ni element on the crystal structures and mechanical properties of the alloys is also explored.

2 Methods

2.1 Experimental Procedures

The CoCrNi_x ($x = 1-0.5$) MEAs were prepared by using a pure element having a purity higher than 99.5% by weight (wt%) in an Ar atmosphere in a vacuum arc furnace. To ensure thorough mixing, the ingot was inverted and remelted at least five times. By suction casting, the alloy structure was more uniform. The ingot obtained by the smelting was homogenized at 900 °C for 2 h and then water-quenched, and then the homogenized sheet was rolled in the longitudinal direction of the ingot to a final thickness of 1 mm (reduction rate of 50%) without the cross-rolling and intermediate annealing. In order to remove the deformed substructure after rolling and obtain an equiaxed grains, the rolled sheet was heat-treated at 1200 °C for 2 h to obtain a completely recrystallized microstructure. The recrystallized plate was cut into flat dog-bone samples by a wire electric discharge machine (WEDM). All sides were polished using 100–2000-mesh sandpaper. The tensile test was carried out at room temperature using an Instron mechanical tester.

2.2 Computational Methods

The steps of calculations are as follows: (1) Initial supercell models for the calculation were constructed; (2) a hybrid first-principles/MC simulation was used to generate maximum entropy, with considering the structural energy minimization for a particular crystal structure (e.g., HCP); and (3) based on the stable structures, the elastic modulus, magnetic moment, and electronic DOS were calculated.

The initial structure models of the ternary CoCrNi_x ($x = 1-0.5$) MEAs in different geometric arrangements were considered, including modest-sized bulk samples in the FCC, BCC, and HCP phases. With regards to constructed initial supercells, a MC simulation code was used to generate MEA models guided by the maximum entropy principle [30] that all same-element atoms should disperse homogeneously in the model, and the loops in this code would terminate until all same-element atoms can separate no more far. Hundreds of maximum entropy structures could be generated at the same time. The screening criterion is that the shortest

distances between the same elements should be located in a narrow range, and the narrower, the better [30].

Structural optimizations and total energy calculations were performed using the Vienna Ab Initio Simulation Package (VASP) [31, 32]. The projected augmented-wave (PAW) [33] potentials with the Perdew–Burke–Ernzerhof (PBE) [34] exchange correlation functional were used. A constant kinetic energy cutoff of 350 eV was used for structural optimizations at different crystalline structures. The Brillouin-zone integrations were performed, using the Monkhorst Pack *k*-point meshes. The *k*-point grid used differs depending on the model constructed from the alloys. For the FCC, BCC, and HCP structures, in order to ensure the number of atoms positive, we have built different models for different components, each component has its corresponding *k*-point grid, and these *k*-point grids were found to yield energies that converge to within 2 meV/atom. The configuration that resulted in the lowest energy was used for data analysis.

3 Results and Discussion

3.1 Crystal Structures

The X-ray diffraction (XRD) patterns of CoCrNi_x ($x=1-0.5$) MEAs are displayed in Fig. 1. For multicomponent alloys, many of the complex phases or intermetallic compounds would normally form during solidification. But it can be clearly seen from the experimental results in Fig. 1 that the CoCrNi alloy is a single-phase FCC structure, which is consistent with the previous experimental reports [35], and it can be clearly indicated from the XRD results that the CoCrNi_{0.9} and CoCrNi_{0.8} alloys also have single-phase FCC structures. However, as the Ni content continues to decrease, a HCP structure begins to exhibit. The alloys all have HCP besides FCC when $x=0.7-0.5$. And as the Ni content is getting lower and lower, the peak intensity of the HCP is getting higher and higher, and the volume fraction

of the HCP is gradually increased. This is mainly because Ni content decreases in the system, and the content of Co is relatively increased. The Co element has the HCP structure and the element Ni has the FCC structure; as a consequence, the increase in Co and the decrease in Ni lead to the formation of the HCP structure.

To understand the structures of CoCrNi_x ($x=1-0.5$) MEAs from a computational perspective, we calculated the mixing energies of alloys. The mixing energies of alloys are one of the key parameters controlling the solid solution phase formation. The mixing energy is defined with respect to the total energies of the alloy components in all three structures (BCC, FCC, and HCP). The mixing energy calculated as

$$E_{\text{mixing}} = E_{\text{alloy}} - \sum_i c_i E_i^{\text{FCC/BCC/HCP}} \quad (1)$$

where E_{alloy} is the total energy per atom of the alloy with FCC, BCC, or HCP structure, and $E_i^{\text{FCC/BCC/HCP}}$ is the equilibrium energy of the *i*th alloy component calculated for the corresponding structure. c_i stands for the concentration.

The calculated mixing energies for CoCrNi_x ($x=1-0.5$) MEAs are summarized in Table 1. And the mixing energies against the composition of the alloys in FCC and HCP structures are presented in Fig. 2. It can be found from Table 1 that the mixing energies of the BCC structures are positive and obviously higher than the other two structures, that is,

Table 1 Mixing energies of CoCrNi_x ($x=1-0.5$) MEAs (eV/atom)

	BCC	HCP	FCC
CoCrNi	1.112	−0.418	−0.435
CoCrNi _{0.9}	1.180	−0.367	−0.379
CoCrNi _{0.8}	1.227	−0.308	−0.315
CoCrNi _{0.7}	1.314	−0.264	−0.269
CoCrNi _{0.6}	1.357	−0.217	−0.221
CoCrNi _{0.5}	1.390	−0.168	−0.171

Fig. 1 XRD patterns of CoCrNi_x ($x=1-0.5$) MEAs

Fig. 2 Mixing energies of CoCrNi_x ($x=1-0.5$) MEAs

the BCC structures are unstable state, while the FCC structures are the most stable among the three structures for the six components. That is consistent with the experimental results, the alloys are mainly FCC structures. Furthermore, it is found from the XRD patterns that the HCP structures appear on the FCC matrix when $x=0.7-0.5$. Although FCC structures are the most stable structures for all six components, the mixing energies of FCC and HCP structures are very close (within 4%). Consequently, there is a possibility that the HCP will appear in the alloys. Specifically, the discrepancy between FCC and HCP mixing energies in the CoCrNi_x ($x=1, 0.9, 0.8, 0.7, 0.6, 0.5$) alloys is 3.91%, 3.17%, 2.22%, 1.86%, 1.81, and 1.75%, respectively. With the decrease in the Ni content, the energy gap between both FCC and HCP structures narrows gradually. This means that the possibility of HCP structures appear in the alloys increases; once exceeding a certain critical value, HCP would appear on the matrix of the FCC. The trend of calculated mixing energies offers a simulation sight to understand the results in the experiment XRD pattern, that is, the HCP structures begin to appear in the CoCrNi_x ($x=0.7-0.5$) alloys.

By comparing the mixing energies, the FCC structure is the most stable phase, and XRD also shows that when $x=1-0.8$, the alloys are single FCC, although at $x=0.7-0.5$, the HCP structures appear in the alloys, but the structures of the alloys are mainly FCC. So we selected the FCC structures to model and calculate their properties.

3.2 Mechanical Properties

According to the Hooke's law, there are three independent elastic constants c_{11} , c_{12} , and c_{44} for the cubic lattice. These constants are related to the bulk elastic modulus $B=(c_{11}+2c_{12})/3$ and the tetragonal shear modulus $c'=(c_{11}-c_{12})/2$. An isotropic system is described by the bulk modulus B and the shear modulus G . For the shear modulus G ,

we adopted the arithmetic Hill average $G=(G_R+G_V)/2$ of the Voigt and Reuss bounds defined by [36]

$$G_R = \frac{5(c_{11}-c_{12})c_{44}}{4c_{44}+3(c_{11}-c_{12})} \quad (2)$$

$$G_V = \frac{c_{11}-c_{12}+3c_{44}}{5} \quad (3)$$

The Young's modulus E and Poisson's ratio ν can be obtained from the values of B and G by the relations

$$E = \frac{9BG}{3B+G} \quad (4)$$

$$\nu = \frac{3B-2G}{2(3B+G)} \quad (5)$$

The simulation results of three cubic constants c_{11} , c_{12} , and c_{44} (GPa), the tetragonal shear modulus c' (GPa), the bulk elastic modulus B (GPa), the shear modulus G (GPa), the Young's modulus E (GPa), Poisson's ratio ν , and the B/G ratio are listed in Table 2. The experimental test results are also given. The simulation results of bulk elastic modulus B , the shear modulus G , the Young's modulus E , Poisson's ratio ν , and the B/G ratio are also plotted in Fig. 3. The present theoretical tool has been employed to study the elastic constants of elemental metals and has been found that it has the accuracy of the most common DFT tools. Unfortunately, we could not find any published experimental data on the single-crystal elastic parameters of these MEAs.

The theoretical single-crystal elastic constants satisfy dynamical stability conditions, namely $c_{44}>0$, $c_{11}>|c_{12}|$, and $c_{11}+2c_{12}>0$ [37] for all alloys. Accordingly, all MEAs considered here are predicted to be mechanically stable.

From Table 2, it can be found that the calculated E of the CoCrNi alloy is 265.78 GPa and the experiment result

Table 2 Simulation results of three cubic constants c_{11} , c_{12} , and c_{44} (GPa), the tetragonal shear modulus c' (GPa), the bulk elastic modulus B (GPa), the shear modulus G (GPa), the Young's modulus E (GPa), Poisson's ratio ν , and the B/G ratio

	c_{11}	c_{12}	c_{44}	c'	B	G	E	ν	B/G
CoCrNi	291.144	168.035	145.812	61.555	209.071	103.166	265.780	0.288	2.027
CoCrNi ^{exp}					203.127	98.605	239.374	0.307	2.060
CoCrNi _{0.9}	289.615	168.564	149.345	60.526	208.914	103.962	267.511	0.287	2.010
CoCrNi _{0.9} ^{exp}					201.364	101.167	246.811	0.303	1.990
CoCrNi _{0.8}	275.136	175.459	148.155	49.839	208.685	105.820	271.559	0.283	1.972
CoCrNi _{0.8} ^{exp}					200.278	102.972	261.493	0.282	1.945
CoCrNi _{0.7}	292.022	168.380	146.139	61.821	209.594	108.829	278.316	0.279	1.926
CoCrNi _{0.7} ^{exp}					208.742	109.634	278.645	0.274	1.904
CoCrNi _{0.6}	304.563	165.484	151.275	69.540	211.844	110.74	282.922	0.277	1.913
CoCrNi _{0.6} ^{exp}					214.751	114.837	282.379	0.268	1.870
CoCrNi _{0.5}	315.125	137.512	154.855	73.807	216.716	115.015	293.179	0.275	1.884
CoCrNi _{0.5} ^{exp}					219.331	123.444	305.014	0.263	1.777

Fig. 3 Schematic diagram of physical parameters (B, G, E, ν , and B/E) as a function of the Ni content

is 239.374 GPa, which has a certain degree of discrepancy from the previously reported 222 GPa [38]. But the discrepancy between the experimental and simulation results is approximately within 10%. It shows that the simulation results are credible. It is also found that with the decrease in x , the experimental and simulation results show the same trend; G and E are increased. We can also discover that as the Ni content decreases, B/G and ν show a downward trend. As it is well known when $B/G \geq 1.75$ or $\nu \geq 0.26$, the materials have a certain plasticity. Here, the B/G of all alloys is larger than 1.75, and the ν is larger than 0.26, so all alloys should have plasticity. And with the decrease in x , the plasticity is getting worse and worse. It is predicted by simulation that the alloys have a certain plasticity and decrease with the decrease in x . Next, we carried out the room-temperature tensile tests and confirmed the predicted results.

The room-temperature tensile results are shown in Fig. 4. When the $x=0.5$, the plasticity of the alloy is only 23%, but the CoCrNi alloy has a room-temperature plasticity of up to 84%. The element Ni itself has a certain degree of plasticity, and as the Ni content in the system decreases, the effect that the element Ni can provide is gradually weakened, resulting in a gradual decrease in the plasticity. And as the Ni content decreases gradually, the strength of the alloys also shows a steady downward trend, and the tensile strength gradually decreases from 800 to 570 MPa.

3.3 Electronic Properties

Based on the equilibrium FCC structures, the electronic structures of these alloys are studied. Spin-polarized electron DOS for the CoCrNi_x ($x=1-0.5$) MEAs is shown in

Fig. 4 Room-temperature tensile stress-strain curves of CoCrNi_x ($x=1-0.5$) MEAs

Fig. 5. Overall speaking, the electron DOS of the alloys is relatively symmetrical, and the number of spin-ups and spin-downs can cancel each other, thereby lowering the magnetic properties of the alloys. The overall DOS of the alloys also changes as the Ni content changes. As illustrated in the figure, when x is 1 and the energy is -2 eV, the spin-up portion of the alloy has a downward recess, and the spin-down portion almost appears to be in a smooth state. When x is 0.5, the electron DOS of the alloy is relatively symmetrical. In general, with the decrease in x , the spin-up and spin-down distribution of electron DOS become more and more symmetrical, which means as the Ni content decreases, the ferromagnetism of these alloys is getting increasingly suppressed.

Fig. 5 Spin-polarized electronic DOS for the CoCrNi_x ($x=1-0.5$) MEAs

Fig. 6 Average magnetic moments of total elements and each element for CoCrNi_x ($x=1-0.5$) MEAs

3.4 Magnetic Properties

The average magnetic moments of total elements and each element for CoCrNi_x ($x=1-0.5$) MEAs are shown in Fig. 6. It can be seen from the figure that the average total magnetic moment gradually decreases with x , which is consistent with the results of the electron DOS; the smaller the x is, the more relatively symmetrical the DOS of the alloys is, as illustrated in Sect. 3.3. And the average magnetic moments of Co and Ni decrease with the decrease in Ni contents, while the magnetic moment of Cr shows non-monotonicity. In order to reveal this magnetic moment trend, the magnetic moments of individual atoms are further investigated.

The local magnetic moment of individual atoms in CoCrNi_x ($x=1-0.5$) alloys at zero temperature is shown in Fig. 7. For all alloys, Co and Ni atoms only exhibit positive (ferromagnetic) moments, while some Cr atoms carry small negative (antiferromagnetic) moments. And the magnetic moments of Co and Ni decrease with decreasing Ni concentration, which is owing to the decrease of Ni content leads to the relative increase of Cr content. In general, Cr can suppress the ferromagnetism of Co and Ni. A reduction in average magnetic moments for Co and Ni from 1.66 and 0.67 μB in elementary element drops to 1.6 and 0.6 μB in equimolar CoCrNi MEA, as shown in Fig. 6. Similar phenomenon was also found in previous studies [39]; Zuo et al. [39] found that when Cr was added to CoMnFeNi HEAs, the magnetic moment of the alloy have become smaller. In Fig. 7, it is found that as x decreases, the magnetic moments of Co and Ni in the alloys become lower and lower, indicating that the inhibitory effect of Cr is gradually increasing.

4 Conclusion

The hybrid first-principles/Monte Carlo simulation method combined with experiment was employed to study the CoCrNi_x ($x=1-0.5$) MEAs. Through the calculation of the mixing energy, it is found that the FCC is the most stable structure, but the discrepancy of mixing energies between HCP and FCC structures is very small (within 4%). And with the decrease in Ni content, the discrepancy is gradually reduced. So maybe when the discrepancy between the two is small enough, the HCP structure would appear in the FCC

Fig. 7 Predicted local magnetic moments of individual atoms in CoCrNi_x ($x = 1-0.5$) MEAs at zero temperature

matrix. It can also be found from XRD patterns that the alloy is FCC when $x = 1-0.8$, and HCP appears as $x = 0.7-0.5$. The plasticity of the alloys decreases with the decrease in x , and compared with the experimental results, the conclusions are consistent. The electronic structures and magnetic moments of the alloys are investigated, and it is predicted that the antiferromagnetism of Cr can suppress the magnetic moments of the alloys.

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