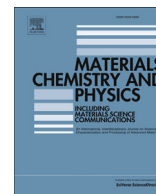




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Effect of alloying on the thermal-elastic properties of 3d high-entropy alloys

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HIGHLIGHTS

- The thermal-elastic properties are studied.
- The influence of alloying elements on the Curie temperature is discussed.
- The Young's moduli along different crystal directions are studied for CoCrFeMnNi.

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ABSTRACT

Using the quasi-harmonic approximation in combination with *ab initio* calculations, we study the temperature dependent elasticity of single-phase face centered cubic (fcc) Co-Cr-Fe-Mn-Ni multi-principle element alloys. Results suggest that the addition of an equimolar alloying element increases the fcc stability due to the increasing valence electron concentration of alloys. The ductility of paramagnetic alloys becomes superior with the increase of temperature. For the CoCrFeMnNi high-entropy alloy, the Young's moduli along different crystal directions are consistent with experiments. The difference between *ab initio* predicted temperature dependent elastic moduli and experiments is discussed.

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1. Introduction

Recently, a new class of materials, high-entropy alloys (HEAs) named by Yeh *et al.*, have attracted extensive attention in scientific literature [1–3]. HEAs are composed of at least four principal alloying elements in equimolar or near-equimolar ratio [4,5], which are also known as multi-principle element alloys. The extensively available experiments suggest that the family of single-phase HEAs include fcc 3d-HEAs mainly composed of 3d transition metals [1,2], the body centered cubic (bcc) refractory-HEAs composed of refractory metals [6], and the hexagonal closed-packed (hcp) rare-earth-HEAs composed of rare-earth elements [7].

Since Cantor *et al.* [8] found the fcc equimolar CoCrFeMnNi HEA, a large number of experimental and theoretical works focused on the Co-Cr-Fe-Mn-Ni based alloys [9–15]. Laplanche [9] and Haglund [10] *et al.* studied the temperature dependent of elastic

moduli and thermal expansion coefficient (TEC) at temperature ($T = 200$ – 1270 K) and the polycrystalline elastic moduli at cryogenic temperature ($T = 50$ – 300 K) of CoCrFeMnNi, respectively. To better understand the CoCrFeMnNi solid solution, Wu and Bei *et al.* [11,12] investigated mechanical properties, recovery, recrystallization, grain growth and phase stability of the Cr-Mn-Fe-Co-Ni based binary, ternary and quaternary alloys. Liu [13] took CoCrFeMnNi as an example to study the microstructure stability and grain growth of HEAs. Lucas *et al.* [14,15] used the vibrating sample magnetometry to determine the high-temperature magnetic applications of the equimolar CoCrFeNi HEA and explored the effects of Cr content on the magnetic properties of CoFeNiCr_x HEAs. Results showed that the Curie temperature of CoFeNiCr_x increases with decrease of Cr content.

Although single-phase HEAs have a simple crystal structure, the atomic random distribution on lattice sites in solid solutions induces the chemical disorder and magnetic disorder. For single-phase 3d HEAs composed of magnetic elements, the Co-Cr-Fe-Mn-Ni alloys show the various magnetic behaviors and different

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Curie temperatures [14–16], due to different magnetic states of alloying elements in their ground state (ferromagnetic (FM) for Fe, Ni, Co, while antiferromagnetic for Cr, multi-magnetic for Mn). As far as we know, the theoretically predicted intrinsic magnetic properties of the Cr-Mn-Fe-Co-Ni multi-principle element alloys are very limited.

Ab initio calculations have been used successfully to predict the fcc stability [17], Young's modulus at low temperature [18] and stacking fault energy [19] for the quinary CoCrFeMnNi HEA. Experiments showed that the binary (CoNi, FeNi), ternary (CoCrNi, CoFeNi, CoMnNi, CrFeNi), quaternary (CoCrFeNi, CoCrMnNi, CoFeMnNi) and quinary (CoCrFeMnNi) alloys all adopt a single-phase fcc solid solutions [12]. From the equimolar binary alloy to equimolar quinary HEA, it is very interesting to study the effect of alloying elements on the elasticity of Co-Cr-Fe-Mn-Ni alloys. In this work we use *ab initio* calculations to investigate the influence of alloying elements on the equilibrium bulk properties of Co-Cr-Fe-Mn-Ni alloys. Meanwhile the thermal-elastic properties as a function of temperature are systematically studied for the single-phase Co-Cr-Fe-Mn-Ni multi-principle element alloys based on quasi-harmonic Debye-Grüneisen approximation.

The rest of the paper is organized as follows. In Section 2, we present the methodology and give the most important details of the numerical calculations. In Section 3, we show the results of the equilibrium bulk properties and elastic properties of different magnetic states and discuss the effect of alloying element on the Curie temperature and the thermal-elastic properties of Co-Cr-Fe-Mn-Ni alloys. Finally, some conclusions are drawn in Section 4.

2. Theoretical methodology

The exact muffin-tin orbitals (EMTO) method is an efficient *ab initio* approach to solving the Kohn–Sham equation [20] which employs large overlapping potential spheres for the exact single-electron potential and the full charge density method further improves the accuracy of full potential total energy [21]. The substitutional disorder in both chemical and magnetic degrees of freedom [22,23], is treated by the coherent potential approximation (CPA) which use an effective medium in single site approximation. For the self-consistent calculations, we employed the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional form of generalized gradient approximation (GGA) to compute the charge density and total energy [24]. The Green's function was calculated for 24 complex energy points from the bottom of the valence bands to the Fermi level. In the irreducible wedge of the fcc Brillouin zone, we used 240 inequivalent k points, allowing to maintain a 10^{-2} mRy/atom accuracy in the total energy. We employed the disorder local magnetic moment (DLM) [25] picture to describe the paramagnetic (PM) state of the present HEAs. The DLM resembles a random spin configuration with zero averaged magnetization, while allowing the presence of finite local magnetic moments on each lattice site above the magnetic transition temperature [26–28].

There are only three independent elastic constants c_{11} , c_{12} , and c_{44} in the cubic lattice. Based on the equilibrium volume and bulk modulus derived from the forth-order Birch-Murnaghan equation of state (i.e. energy as a function of volume), the elastic constants c_{11} , c_{12} and c_{44} were obtained through by calculating the total energy as a function of volume-conserving lattice strains [29,30]. Combining the three elastic constants c_{11} , c_{12} , c_{44} with the Voigt–Reuss–Hill averaging method [31,32], we can calculate the polycrystalline elastic moduli (shear modulus G , Young's modulus E), Poisson's ratio ν and Zener ratio A_Z [21].

We used the quasi-harmonic Debye-Grüneisen approximation to compute the TEC based on the equation of state and the *ab initio*

calculated Poisson ratio, then we calculated the equilibrium volume and bulk modulus at given temperature, and further the temperature dependent elastic constants and polycrystalline elastic moduli were estimated with the method of elastic calculations [21]. The quasi-harmonic approximation is a simple and effective method to account for the lattice vibrational information, without the phonon density of state for solid solutions. In the quasi-harmonic Debye-Grüneisen model, the harmonic approximation at any given crystal structure is assumed, even if it does not correspond to the equilibrium structure. Note that we also considered the contributions of electronic entropy and magnetic entropy to Gibbs energy implemented in quasi-harmonic approximation.

3. Results and discussion

3.1. Equilibrium bulk properties

Fig. 1 shows the equation of states of the paramagnetic (PM) Cr-Mn-Fe-Co-Ni alloys. Although the Fe, Co and Ni alloying elements have similar Goldschmidt atomic radii [33], their binary solid solutions have different equilibrium Wigner-Seitz (WS) radii (see Fig. 1 and Table 1), for example the PM CoNi alloy has smaller WS radius than FeNi. Interestingly their WS radii of binary solid solutions are very close to the average WS radii derived from the experimental lattice parameters of alloying elements via Vegard's law [34]. For CoCrNi, CoFeNi and CoMnNi ternary alloys, *ab initio* calculations predict the similar WS radius to each other, which are slightly smaller than the average WS radii. The EMTO predicted WS radius of CrFeNi is much smaller than the experimental average one. The difference between *ab initio* calculations and experimental average may be due to *ab initio* performed at $T = 0$ K temperature. The EMTO predicted WS radii of quaternary and quinary HEAs are very close to each other. The FM alloys have slightly larger WS than the PM ones, except for Mn-containing alloys, due to the magnetic order.

3.2. Curie temperature

Within the numerous successful applications, the EMTO-CPA method has been developed an attractive tool in materials science to predict finite temperature magnetic properties. Here we use Curie temperature T_C to describe the finite temperature

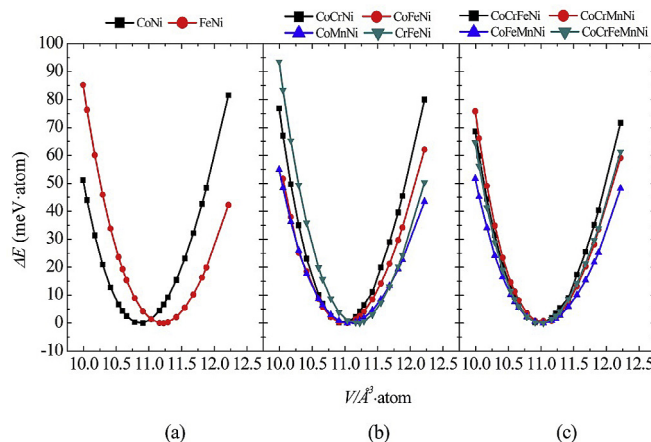


Fig. 1. Equation of states (energy (meV/atom) vs volume ($\text{\AA}^3/\text{atom}$)) for the at paramagnetic (PM) Cr-Mn-Fe-Co-Ni multi-principle element alloys. Left column (a) is for binary alloys, middle column (b) for ternary alloys, right column (c) for HEAs (quaternary and quinary alloys). All energies are relative to their corresponding total energy at the equilibrium volume.

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