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The First Principles Study on Two Alloys of Cr2ZnAl and Cr2AgAl

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Abstract: The Heusler alloy is with a ordered structure, in which the atoms are in specific location, and the alloy usually shows special character. The Co Mn Ni based Heusler alloys are all studied in many literature, but there is little study of the Cr based Heusler alloys. In order to find new Heusler alloys, Cr2AgAl and Cr2ZnAl are studied by first principles. Using the CALYPSO software, the crystal structure of Cr2AgAl is found to be F-43m, the lattice parameter is a=6.1100 Å, it is a Heusler alloy, and the density of states and the bands structure have been studied, showing it is a metal conductor and not a magnet. The X-ray diffraction result of the alloy was also obtained by calculating, the two peaks at 25 degree and 29 degree, represent the (111) and (200), and the existence of these two peaks implies an ordered atom structure formed. This X-ray result can be used to guide the experimental synthesis of this alloy material.The crystal structure of Cr2ZnAl is P4mm, the lattice parameter is a=b=2.97300 Å, c= 6.02320 Å, it is not a Heusler alloy, and it is also a metal conductor and not a magnet from the results of its density of states and the bands structure.

Keywords: Heusler Alloy, Band Structure, CALYPSO, Density of States

1. Introduction

The level of development of materials science is an important measure of the progress of human civilization. The discovery of new functional materials with special properties often leads to a major revolution in the field of science and technology. The advancement of new materials is driving the rapid development of high-tech industries such as the energy industry, communications, high-performance computing, and aerospace. In recent years, a new material Heusler alloy with highly ordered atomic structure has attracted the interest of condensed matter physics and metal materials science. This material system has very rich physical properties and contains a variety of application functions and is one of the hot material systems for the development of new metal functional materials. In 1903, F. Heusler first reported Cu2MnSn and Cu2MnAl materials, and found that the atomic arrangement of these two materials is highly ordered [1]. In 1969, P. Webster published a comprehensive paper on the crystal structure and physical properties of Heusler alloy materials [2]. Because Heusler alloy has a highly ordered atomic arrangement of crystal structure, it has rich physicochemical properties and has many potential application values. It is a hot material system for exploring and developing new materials in the field of condensed matter physics and functional materials. In this material system, the non-ferromagnetic element composition has been found to exhibit ferromagnetism [3], completely single spin orientation properties of half-metal [4], magnetoresistance effect [5], superconductivity [6], large magnetic field induced strain effect, both magnetically controlled shape memory effect of ferromagnetic and thermoelastic martensitic transformation [7-9].

The main series of Heusler alloys are as follows. Cu2YZ series (Y = Mn, Cr, etc., Z = Al, Si, Sn, etc.) [5]. This type of material is a typical representation of non-ferromagnetic combination of elements and exhibits ferromagnetic after high ordering. Magnetic originates from the indirect coupling of the spin polarization of conduction electrons

between the cesium atoms (such as manganese Mn). Co2YZ series (Y = Ti, Cr, Zr, etc., Z = Al, Sn, etc.) [3]. This type of material is usually a magnetic material, and the magnetic properties are derived from direct mutual exchange between Co-Co atoms, some of which exhibit semimetal characteristics. Co2MnZ, Ni2YZ series (Z = Al, Si, Sb, etc.) [4]. This type of material usually has ferromagnetism, its main magnetic property is derived from the contribution of Mn, and Co, Ni, etc. do not exhibit significant magnetic properties. In addition, theoretical calculations indicate that such materials may have semi-metallic properties with 100% spin rate of conductive electron. Ni2MnZ (Z = Al, Ga, In, Sb, Sn), Co2NiGa and Ni2FeGa series [7-9]. These materials usually combine two physical properties of ferromagnetism and thermoelastic martensitic transformation, and based on this, exhibit magnetic induction strain, shape memory effect, magnetoresistance effect and the like. It is an important material system for exploring new magnetic field controlled shape memory and large magnetic induced strain materials. Recently, MTiSb (M = Fe, Co, and Ni) [10], Rh 2 FeZ (Z = Ga and In) [11], Fe2CrX (X = Al, Ga) [12], Ti2FeZ (Z = Al, Ga, and In) [13], NbVMnAl and NbFeCrAl [14], and CrZrZ (Z = In, Sn, Sb, and Te) [15] Heusler alloys have been studied, so it makes sense to study other new Heusler alloys.

The CALYPSO (Crystal Structure Analysis by Particle Swarm Optimization) is a crystal structure seek software, which developed by professor Ma' team in Jilin university of China. It is developed to search crystal structures of materials [10-12]. The Particle Swarm Optimization (PSO) algorithm is employed, which is inspired by team organization pattern of a bird flock [13]. The CALYPSO software combines with Vasp, Pwscf, Castep, Gaussian, etc to carry out the structure relaxation. For one material, the CALYPSO can generate kinds of structures, then, the geometry optimization will be done, the fair structures will be made further optimization to get the lowest energy, the final result is a list of the structures according their energy.

In this paper, using the CALYPSO software, Cr2AgAl and Cr2ZnAl are studied to seek possible Heusler alloys, which are not mentioned in any other literature.

2. Computational Methods

The CALYPSO software is installed on a computing workstation which is with a linux system. First, there should be a input file for the calculation target, then, the number of element specie, name of the element Cr, Ag, Zn, Al, the atom numbers in one formula, the number of formula, a estimate volume of the structure and the distance of the atoms are all supplied to the CALYPSO software, the maximum step of the revolution in the procedure is 25. In one loop, the algorithm is set as local particle swarm optimization, the number of species is set to 30, the number of local optimization is set to 3. The reasonable structures are reserved, and the others will be given up in one loop. Finally, we will obtain a number of structures which are listed according their energy.

3. Results and Discussions

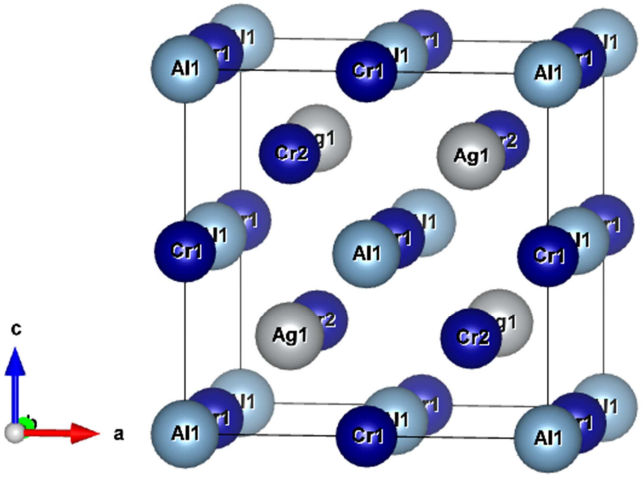

Figure 1. *The structure of the Cr2AgAl alloy.*

Table 1. *The site positions of the atoms in Cr2AgAl crystal structure.*

Site	Site symmetry	*x/a*	*y/b*	*z/c*	*sym*
Cr1	4b	0.5	0	0	-43m
Cr2	4d	0.75	0.25	0.25	-43m
Ag	4c	0.75	0.25	0.75	-43m
Al	4a	0	0	0	-43m

According the calculated result, the crystal structure of Cr2AgAl is F-43m, the space group is number 216, which is as figure 1. It belongs to the cubic system, the lattice parameter being a=6.1100 Å, and the site positions of the atoms is as table 1. It is a new Heusler alloy. There are two kinds of Cr atoms, one is Cr1, locates at 4b (0.5, 0, 0), the other is Cr2, locates at 4b (0.75, 0.25, 0.25). Though as same atom, these two kinds Cr atoms has different properties, because they have different coordination in the structure.

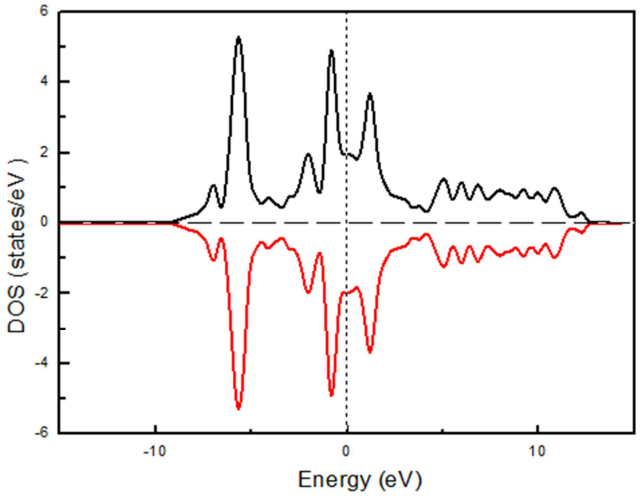

Figure 2. *The total density of states of Cr2AgAl with F-43m crystal structure.*

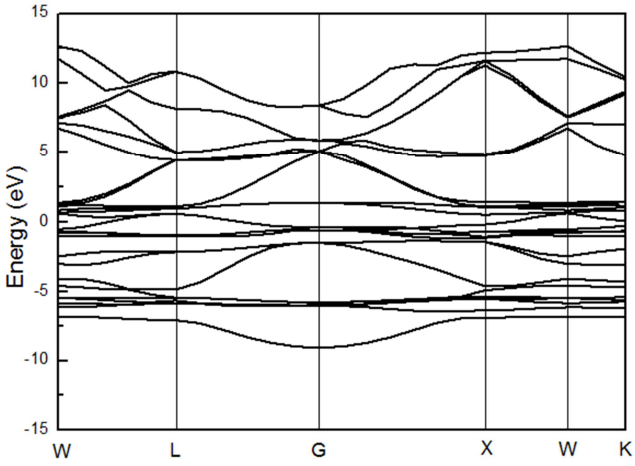

Figure 3. *The majority spin band structures of Cr2AgAl with F-43m crystal structure.*

The calculated total density of states (DOS) is shown in figure 2. The dot line is the Fermi level. The dash line divides the picture into two parts. The shape of the upper and lower parts is symmetrical, showing non-magnetic property. The DOS in the Fermi level is non-zero, so this alloy has metallic conductor property. The energy bands along high-symmetry directions in the Brillouin zone for Cr2AgAl are presented in figure 3. The conduction band and the valence band overlap, and the Fermi level passes through the overlapping area, also showing the nature of the conductor, which is consistent with the state density map results.

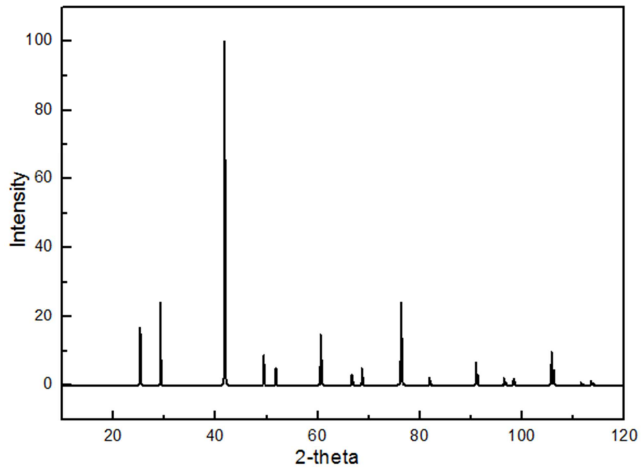

Figure 4. *The x-ray diffraction results of Cr2AgAl.*

The X-ray diffraction result was obtained by calculating, the data were plotted in the figure 4. The first peak at 25 degree represents the (111), and the second peak at 29 degree represents (200), the existence of these two peaks implies an ordered atom structure. The F-43m structure is just a ordered crystal structure. Anyone who is interested in it can synthesize this alloy according to this diffraction result.

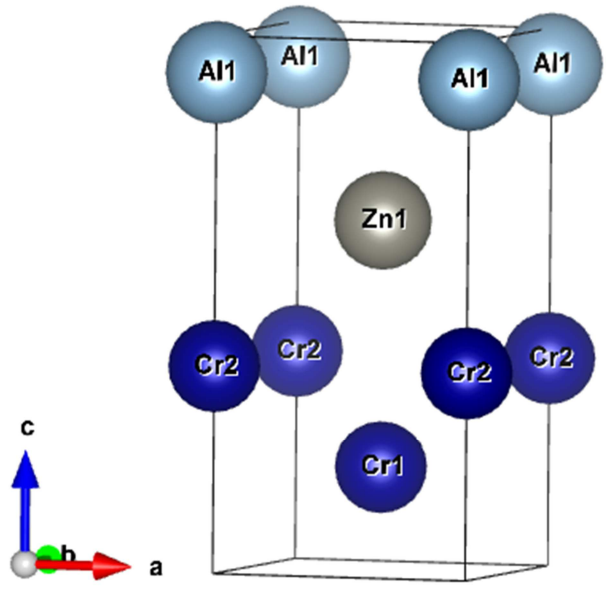

Figure 5. *The structure of the Cr2ZnAl alloy.*

Table 2. *The site positions of the atoms in Cr2ZnAl crystal structure.*

Site	Site symmetry	*x/a*	*y/b*	*z/c*	*sym*
Cr1	1b	0.5	0.5	0.1902	4mm
Zn	1b	0.5	0.5	0.6502	4mm
Cr2	1a	0	0	0.3859	4mm
Al	1a	0	0	0.9326	4mm

By calculating, the crystal structure of Cr2ZnAl is P4mm, the space group is number 99, which is as figure 1. It belongs to the tetragonal system, and it is not a Heusler alloy. the lattice parameter is a=b=2.97300 Å, c= 6.02320 Å, and the site positions of the atoms is as table 2. The Cr1 atoms locate at 1b (0.5, 0.5, 0.1902), the Cr2 atoms locate at 1a (0, 0, 0.3859). the Zn atoms locate at 1b (0.5, 0.5, 0.6502), and the Al atoms locate at 1a (0, 0, 0.9326).

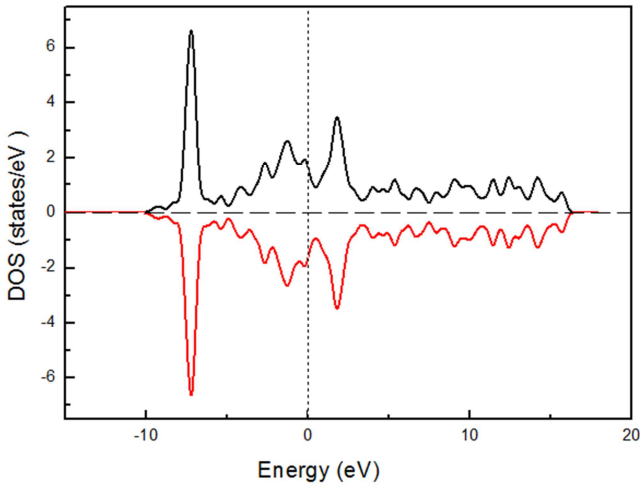

Figure 6. *The total density of states of Cr2ZnAl with C2/m crystal structure.*

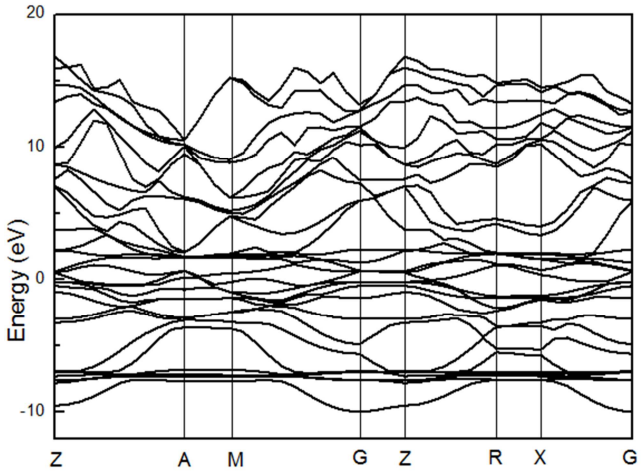

Figure 7. *The majority spin band structures of Cr2ZnAl.*

The calculated DOS of Cr2ZnAl is shown in figure 6. The bands are distributed in the range of -10eV to 15ev range. The shape of the upper and lower parts is symmetrical, so Cr2ZnAl is not a magnet. The DOS in the fermi level is non-zero, so the alloy is a metal conductor. The energy bands along high-symmetry directions in the Brillouin zone for Cr2ZnAl are presented in figure 7. The conduction band and the valence band overlap which is showing a conducting property.

4. Conclusion

The Cr2AgAl and Cr2ZnAl alloys are investigated for finding new Heusler alloys by the CALYPSO software. The Cr2AgAl has been found to be a new Heusler alloy with F-43m crystal structure, the electronic structure is studied, it is a metal conductor and not a magnet, and the X-ray diffraction result is obtained by calculating which can guide the experimental researcher to study it. The Cr2ZnAl alloy has a P4mm crystal structure, it is not a Heusler alloy, and it is also a metal conductor and not a magnet. The founding of new Heusler alloy of e Cr2AgAl is rewarding, this may point the way to exploring new Heusler alloys, the Cr based Heusler alloy may has special properties to make use of, and this alloy provides a certain reference. If anyone is interested, try synthesizing this new alloy. And it is to do it, because the xrd result is provided in the article.

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