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High spin polarization in ordered Cr_3Co with the DO_3 structure: A first-principles study

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Abstract

The electronic structure of the highly ordered alloy Cr_3Co with the DO_3 structure has been studied by FLAPW calculations. It is found that the ferrimagnetic state is stable and that the equilibrium lattice constant of Cr_3Co equals 5.77 Å. A large peak in majority spin density of states (DOS) and an energy gap in minority spin DOS are observed at the Fermi level, which results in a high spin polarization of 90% in the ordered alloy Cr_3Co. The total magnetic moment of Cr_3Co is $3.12\mu_B$, which is close to the ideal value of $3\mu_B$ derived from the Slater–Pauling curve. An antiparallel alignment between the moments on the Cr (A, C) sites and the Cr (B) sites is observed. Finally, the effect of lattice distortion on the electronic structure and on magnetic properties of Cr_3Co compound is studied. A spin polarization higher than 80% can be obtained between 5.55 and 5.90 Å. With increasing lattice constant, the magnetic moments on the (A, C) sites increase and the moments on the (B, D) sites decrease. They compensate each other and make the total magnetic moment change only slightly.
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1. Introduction

In recent years, one of the most active fields of research has been spin-electronics (spintronics) [1–3], in which it is the electron spin that carries information based on the alignment of a spin relative to a reference. This offers opportunities for a new generation of devices combining standard microelectronics with spin-dependent effects. In particular, most magnetoelectronic devices rely on an imbalance in the number of majority- and minority-spin carriers, so that a material with high spin polarization at the Fermi level E_F is preferred [3]. Ideal as a choice are the so-called half-metals, which have an energy gap in the minority-spin density of states (DOS) at E_F whereas the majority-spin DOS is strongly metallic, which results in a complete spin-polarization of the conduction electrons [4].

Within this framework, the first half-metal was predicted in 1983 by de Groot et al. [4], in the half-Heusler alloys. In succession, some Heusler alloys have been theoretically predicted to be half-metals and many experiments have been carried out to establish their magnetic and transport properties [5–9]. A high tunnel magnetoresistance (TMR) was also observed in some magnetic tunnel junctions (MTJs) based on Co_2FeSi [10] and on $Co_2Cr_{0.6}Fe_{0.4}Al$ [11] films.

However, the atomic disorder is always a problem in the practical application of half-metallic Heusler alloys. Raphael et al. [12] have successfully grown Co_2MnSi and Co_2MnGe films and have studied their saturation magnetization and spin polarization by SQUID magnetometry and Andreev reflection. However, they found that the films had a spin polarization of only 50–60%, which may be

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attributed to atomic disorder. It was found that the spin polarization may be affected by antisite disorder in Heusler alloys [13,14]. To reduce the disorder in this kind of material, a binary alloy with DO_3 structure may be a possible way. The DO_3 type of structure is a binary derivative of the $L2_1$ Heusler structure, which can be looked upon as four interpenetrating fcc lattices and which has four different crystal sites, namely: A (0, 0, 0), B (1/4, 1/4, 1/4), C (1/2, 1/2, 1/2) and D (3/4, 3/4, 3/4) in Wyckoff coordinates. In the DO_3 structure, the A, B and C sites are occupied by the same kind of atom. So the disorder between (A, C) and the B site in the $L2_1$ structure, which is found to decrease the spin polarization strongly [13], can be alleviated. Mn_3Al and Mn_3Ga are the only two binary alloys with the DO_3 structure reported to have high spin polarization [15]. In the present work, we studied the electronic structure of an ordered Cr_3Co alloy with the DO_3 structure by first-principles FLAPW (full-potential linearized-augmented planewave) calculations. An energy gap in the minority spin band and a spin polarization as high as 90% are observed at the equilibrium lattice constant. We also studied the effect of lattice constant on the spin polarization and on magnetic properties, and found that a high spin polarization can be obtained at a relatively large range of lattice distortion.

2. Computational method

We carried out the electronic-structure calculations using the self-consistent FLAPW method based on the local spin-density approximation within the density-functional theory [16,17], where the potential and/or the charge density in the crystal are treated with no shape approximation. A grid of 182 k points is employed in the irreducible Brillouin zone. The self-consistent calculation stops if the charge-density deviation is less than 0.01 me/a.u. and the total energy deviation is better than 0.1 mRy per cell. The density plane-wave cutoff is $Rk_{max} = 8.0$. The electron states were treated in a scalar relativistic approximation. Using the energy eigenvalues and eigenvectors at these points, the DOS was determined by the tetrahedral integration method [18]. The calculations were based on the theoretical equilibrium lattice parameters.

The crystal structure of the Cr_3Co alloy is shown in Fig. 1. It crystallizes in DO_3 structure and has space group $Fm\bar{3}m$. In Cr_3Co, the three Cr atoms occupy the (A, C) and B sites and the Co atom enters D site. So in the crystal, the atom at the A and the C site has four Co and four Cr as nearest neighbors, while atom at the B and the D site has eight Cr as nearest neighbors.

3. Results and discussion

To determine the theoretical lattice constant and investigate the most stable magnetic state, we performed calculations on Cr_3Co for three kinds of magnetic states, the paramagnetic (PM), ferromagnetic (FM) and antiferromagnetic (AF) state. The results are shown in Fig. 2. It is clear that the PM state has the highest total energy, which is about 0.73 eV above the curves of the FM and the AF state. But the energy difference between the FM and AF states is quite small and difficult to be distinguished, as shown in Fig. 2. In fact the energy difference at the equilibrium lattice constant is smaller than 1×10^{-4} eV. Meanwhile, the calculations in both the FM and the AF state give similar total and partial magnetic moments with ferrimagnetic alignment. The equilibrium lattice constant,

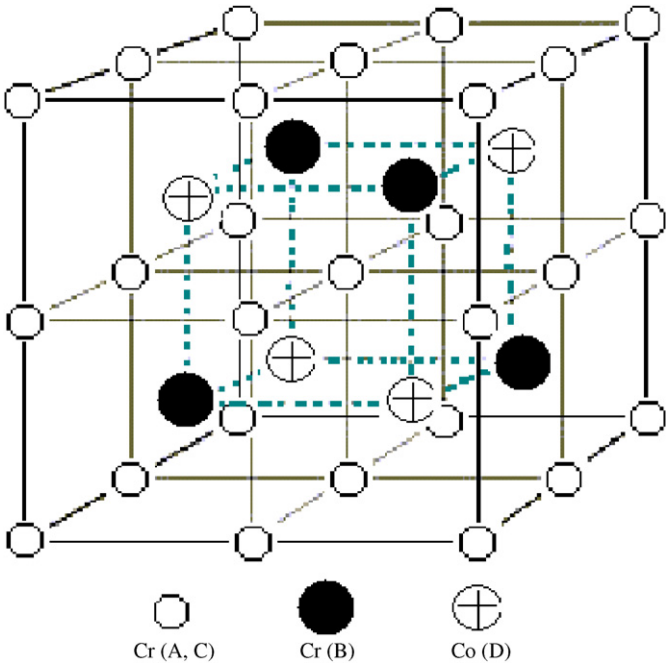

Fig. 1. Crystal structure of the alloy Cr_3Co. The DO_3 lattice consists of four fcc sublattices. The unit cell is that of a fcc lattice with four atoms as basis: A (0, 0, 0), B (1/4, 1/4, 1/4), C (1/2, 1/2, 1/2) and D (3/4, 3/4, 3/4) in Wyckoff coordinates, in which the Cr atoms occupy the A, B, C sites and Co enters the D site.

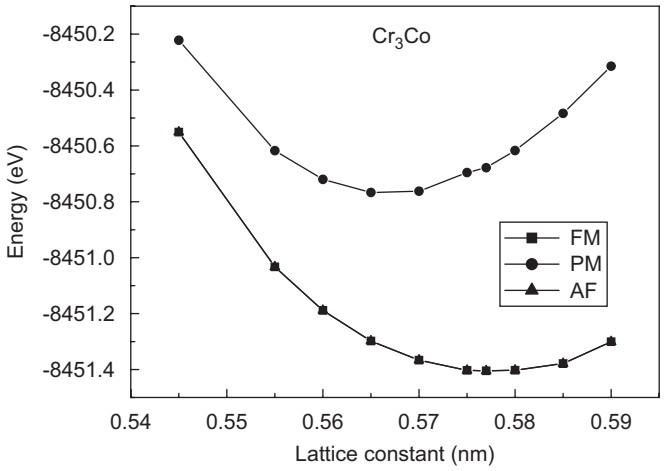

Fig. 2. Calculated total energy for Cr_3Co as a function of the lattice constant for the paramagnetic (PM), the ferrimagnetic (FM) and the antiferromagnetic (AF) state.

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