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Calculated structural and magnetic properties of artificially made $L1_0$ FeCu superlattice

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Abstract

The ordered $L1_0$ FeCu alloys were studied by the first-principle calculations. The FLAPW method was used for structural optimization while the anisotropy energy and magnetic properties were investigated by the LMTO method. The anisotropy of the system is found to be perpendicular to the FeCu layers, and an enhancement of the magnetic moments is also observed. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Anisotropy energy; Magnetic moment

Compared with bulk materials, artificially grown ultrathin magnetic multilayers exhibit a number of novel properties such as enhanced magnetization at surface/interface, perpendicular magnetic anisotropy and oscillatory exchange coupling. Of particular interest at the moment is the stability and the unusual properties of artificially made thin film magnetic structures which would otherwise not exist as bulk materials. For example, unstable BCC Co [1] and hcp $Ni_{1-x}Fe_x$ [2] have stabilized as a ultrathin film, respectively, on GaAs(1 1 0) and Cr(2 1 1). More recently, metastable FCC Fe–Cu alloys in the $L1_0$ phase have also been prepared on a Cu(0 0 1) substrate [3] and a number of interesting properties of these film systems have been reported [4]. In this work, we have carried out ab initio studies on the structural and magnetic properties of these systems.

We have performed first-principles spin-polarized electronic structure and total energy calculations for these ordered $L1_0$ FeCu alloys. Our calculations are based on the density functional theory with the standard local density approximation. We have used highly accurate full-potential linear augmented plane wave (FLAPW) method for structural optimization and the linear muffin-

tin orbital (LMTO) method for magnetic properties especially magnetic anisotropy. The magnetocrystalline anisotropy is obtained via the force-theorem [5], i.e., defined by the magnetocrystalline anisotropy energy as the difference in the eigenvalue sum between the spin-polarized relativistic band structures for the different magnetization directions considered.

Artificially ordered $L1_0$ FeCu alloys were found to grow pseudomorphically on a Cu(0 0 1) substrate up to 50 monolayers [3]. However, the interlayer spacings were not determined. As a result, in our calculations we assumed all the atomic layers to have the same two-dimensional square lattice, but the systems were separated into two cases. In case 1, the volume of a unit cell of bulk FCC Cu is kept constant, but the ratio of c/a is varied. However in case 2, the length a is fixed, only c is changed.

The total energy as a function of the Fe–Cu interlayer distance is calculated by using the FLAPW method, and we found that the ordered $L1_0$ FeCu lattice is a tetragonal structure rather than the ideal FCC structure. The ratio of c/a was predicted to be about 5% larger than the ideal FCC lattice in the first case. In case 2, on the contrary, the interlayer spacing was found to be 6% smaller than the ideal FCC Cu(0 0 1) interlayer distance.

In the LMTO calculations, the ordered $L1_0$ FeCu alloys are also divided into two cases as previously mentioned. Both the magnetic moments and magnetocrystalline anisotropy energies are studied. Experimentally the

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Fig. 1. The anisotropy energy of the ordered $L1_0$ FeCu alloys. The filled circles represent the case in which the volume of a unit cell is fixed, while the filled squares represent the case in which the length of a is fixed. The line is a guide to the eye only.

Fig. 2. The Fe spin moment (a) and orbital moment (b), as well as Cu spin moment (c) in the ordered $L1_0$ FeCu alloys. The moment is in unit of μ_B . The filled circles represent the case in which the volume of a unit cell is fixed, while the filled squares represent the case in which the length of a is fixed. The line is a guide to the eye only.

magnetization in the FeCu films was found to be in plane for any film thickness [3,4]. However, both previous experiments [6] and calculations [7,8] showed that the

magnetization direction of a single layer on or sandwiched in Cu(001) is perpendicular to the monolayer plane. In our calculations we also found a perpendicular anisotropy of the ordered $L1_0$ FeCu alloys for both cases. The anisotropy energy is defined as the difference of the eigenvalue sum between the (001) and (100) orientations of magnetizations. In particular, the largest anisotropy in both cases occur at $c/a = 1.02$ (Fig. 1). Compared with the FLAPW calculations, the most stable states, i.e., $c/a = 1.05$ in case 1 and $c/a = 0.94$ in case 2, have almost the same anisotropy energies in the LMTO calculations (Fig. 1).

The magnetic moments of the Fe atoms in the ordered $L1_0$ FeCu alloys also attract considerable interest. Based on the previous reports, Fe atoms in the magnetic ultrathin films with enhanced magnetic moments can be explained by the reduction of the coordination numbers [9]. However, recent experiments of ordered $L1_0$ FeCu alloys showed 1.8 and 0.26 μ_B of the Fe spin and orbital moments by using the X-ray magnetic circular dichroism (XMCD) technique [4]. The spin moment is reduced, but the orbital moment is significantly higher than the theoretical predictions [7]. Our calculations of this system showed that the spin moments of Fe are enhanced and increased with the increasing c/a ratio, which results from the reduction of the overlap of the wave functions (Fig. 2a). The orbital moments of Fe are also higher compared with bulk Fe, but the value is still much smaller than the experiments. We also found that the tendency of the orbital moments are quite different in the two cases of our calculation (Fig. 2b), and interestingly the spin moments of Cu have a completely opposite behavior (Fig. 2c). Although the magnetic moments of Fe are somewhat different between experiments and theories, the calculated spin moments of Cu are in reasonable agreement with experimental results.

Summarizing, we have performed all-electron self-consistent electronic structure calculations for the ordered $L1_0$ FeCu alloys. We determined the interlayer spacing of the system by the FLAPW method and found the magnetocrystalline anisotropy energy and magnetic moments by the LMTO method. The structure of the system is obtained to be tetragonal and the magnetization prefers the perpendicular direction which is consistent with the previous reports [7,8]. The magnetic moments of Fe are enhanced, and an interesting trend between the orbital moments of Fe and spin moments of Cu is found. In the calculations, the second case may be more realistic for the Cu substrate in the experiments. However, the discrepancies between experiments and calculations are outstanding. We may conclude that the strain-induced anisotropy should not be the critical factor of the in-plane anisotropy found in the experiments, and the unusual enhanced Fe orbital moment remains to be clarified.

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