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Optical, magneto-optical and magnetic properties of CoPt alloy films

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The electronic structures of various phases of CoPt alloy were calculated using the linearized-muffin-tin-orbitals (LMTO) methods within the local spin density approximation (LSDA) to understand the optical, magneto-optical and magnetic properties of CoPt alloy film, especially, the temperature dependence of magneto-optical properties.

Bulk Co-Pt alloy is known to form a stable $L1_0$ structure in a wide range of composition. In this structure the alloy has a layered structure along (001) direction, with alternating layers of square lattice of Co and Pt. However, the $L1_1$ structure also has a layered structure along (111) direction. Therefore we calculated total energy of both structures to find the minimum total energy and the equilibrium lattice constants. We also calculated the same thing for B2 structure. The calculations were spin-polarized ones and the spin-orbit coupling was included in calculating the magneto-optical spectra.

We found that the $L1_1$ structure has a slightly lower total energy than the $L1_0$ structure (0.19 mRyd) and the B2 structure (46 mRyd). The equilibrium lattice constants were 7.072 a. u. and 7.063 a. u. for the $L1_0$ and $L1_1$ structures, respectively. The calculated magnetic moment

increases as the lattice constant decreases for all structures. The magnetic moments at the equilibrium lattice spacing were 2.058 μ_B/f.u. and 1.911 μ_B/f.u. for the $L1_0$ and $L1_1$ structures, respectively. By comparing the total energy and equilibrium lattice spacing to the calculated magnetic moments we can realize that the difference in the magnetic moments is rather large. This difference can explain the temperature dependence of the magneto-optical measurements of CoPt alloy films. We interpret the temperature dependence by the structural phase transition from the $L1_0$ to the $L1_1$ structure as the temperature decreases.

The other experimental results, such as photoemission spectra and optical conductivity spectra, are also explained by this structural phase transition.