$L1_0$ FeNi and $L1_0$ FePt ultra-thin films with in-plane and tilted magnetic anisotropy: density functional theory calculations

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The increasing miniaturization of electronic devices, evident in today's processors, and the growth of recording density in memories are directing researchers' attention to structures on the order of nanometers in size, whose properties can differ significantly from those of bulk macroscopic materials. Also, the growth of demand for hard magnetic materials without rare-earth elements was observed. In connection with the mentioned issues, many systems are considered, such as $Fe_{1-x}Co_x$ alloys, iron-based $L1_0$ phases: FePt and FeNi, or $L1_0$ CoPt [1,2].

$L1_0$ FePt phase, especially thin films, is considered for applications in heat-assisted magnetic recording, which allows reducing of switching magnetic fields without decreasing its stability after the recording process [3]. An experiment has shown that a tilted magnetization direction characterizes $L1_0$ FeNi slabs. Tilted magnetization direction allows such films to reduce the necessary switching magnetic field while maintaining the temperature stability of the systems' magnetic properties [4]. Considering the above, we decided to research further slabs of $L1_0$ phases: FePt and FeNi, with (010) and (111) surfaces.

For this purpose, we performed quantum calculations based on the full-potential local-orbital (FPLO) method using the density functional theory (DFT) implemented in the FPLO18 code. Our research allowed us to determine the preferred direction of the easy magnetization axis and changes in this direction as a function of film thickness in the considered systems. It confirmed the experimentally observed tilt of the easy magnetization axis from the out-of-plane direction in the case of both viewed materials, with it being greater for FeNi $L1_0$. In addition, we determined changes in magnetic moments and magnetic anisotropy energy of systems with magnetization consistent with particular crystallographic directions as a function of layer thickness.

References:

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