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Magnetic anisotropy of ultrathin Pd₄Co(111) film by first-principles calculations

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The Pd–Co alloy is a good candidate for the perpendicular magnetic recording and related applications. However, no research is available to clarify the influences of local structures on the magnetic anisotropy of the Pd–Co alloy. Therefore, in this work, we studied the effects of Co arrangement on the magnetic anisotropy of ultrathin $Pd_4Co(111)$ film with 20% Co content by using the density functional theory calculations. We found that a Co monolayer in the surface layer of the ultrathin film offers a large in-plane magnetic anisotropy while the Co atoms mixed inside the Pd matrix exhibit the perpendicular magnetic anisotropy. Notably, a Co monolayer beneath the surface layer of the Pd matrix maximizes the perpendicular magnetic anisotropy up to 1.85 erg/cm². Electronic properties were also analyzed to clarify the magnetic anisotropy of the ultrathin film.

Keywords: Magnetic Recording; Magnetic Anisotropy; Density Functional Theory; Electronic Structure Properties; Ultrathin film.

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