

Magnetic Properties of Thin Films of a Magnetocaloric Material FeRh

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Abstract

A FeRh alloy is a well-known efficient magnetocaloric material and some experimental and theoretical studies of bulk FeRh have been reported already by several groups. In this study we report first-principles calculations on magnetic properties of different thickness FeRh thin films in order to investigate the possibility to enhance further the magnetocaloric efficiency. We used Vienna Ab-initio Simulation Package (VASP) code. We found that the FeRh thin films have quite different magnetic properties from the bulk when the thickness is thinner than 6-atomic-layers. While bulk FeRh has a G-type antiferromagnetic (AFM) state, thin films which are thinner than 6-atomic-layers have an A-type AFM state or a ferromagnetic(FM) state. We will discuss possibility of magnetic phase transitions of the FeRh thin films in the view point of a magnetocaloric effect. And we found 4-, 5-, 6-layers films with Fe surface and 7-layers film with Rh surface are FM and they have dozens eV magnetocrystalline anisotropy (MCA) energy. MCA energy leads to determine energy barrier when magnetic states are changed by external magnetic field.