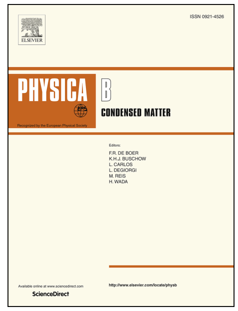

Monte Carlo simulation study for hysteresis properties of a Prussian blue analog nanowire

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Monte Carlo simulation study for hysteresis properties of a Prussian blue analog nanowire

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Abstract

We have studied the hysteresis loops and hysteresis related properties (like coercivity, remanence and saturation magnetization) of a cylindrical ternary alloy Prussian blue analog nanowire of the type AB_xC_{1-x} by means of Monte Carlo simulations. We consider a ferromagnetic coupling between type-A and type-B magnetic components ($J_{AB} > 0$) and an antiferromagnetic coupling between type-A and and type-C magnetic components ($J_{AC} < 0$). By defining exchange interaction ratio, $R = |J_{AC}|/J_{AB}$, we have shown that for special values of R and concentration x, nanowire displays a minimum value of coercive field which is attributed to the existence of compensation behavior in the system. Moreover, minimum values of remanent magnetization are observed for x values at which the positive and negative magnetization components are about to balance each other. Finally, temperature dependence of coercivity and remanence are investigated in a wide temperature range.

Keywords: Ternary alloy, Magnetic nanowire, Monte Carlo simulation.

1. Introduction

A special type of molecular based magnets, the Prussian blue analogues (PBAs) [1, 2], have attracted the interest of researchers because of their functional and considerably controllable properties. Besides, PBAs have diverse possible technological applications including hydrogen storage, [3, 4], battery materials [5, 6, 7] and biomedical applications [8]. In the last decades, thanks to the recent experimental developments, nano-structured materials, for instance, nanoparticles [4, 9, 10, 11], nanowire arrays [12, 13] and nanotubes [14], comprised of PBAs have been synthesized. In order to make PBAs practicable for technological applications, one of the aim of the the studies is to enhance the magnetic ordering temperature of the system [10, 15, 16].

Okhoshi et al. [17, 18, 19] have focused on ternary metal PBAs, $(\mathrm{Ni_x^{II}Mn_{1-x}^{II}})_{1.5}\mathrm{Cr^{III}(CN)_6}$, which includes both ferromagnetic ($J_{\mathrm{Ni-Cr}} > 0$) and antiferromagnetic ($J_{\mathrm{Mn-Cr}} < 0$) exchange interactions for the first time in their series of studies. They have demonstrated that ternary metal PBAs show interesting properties, for instance, magnetic pole inversion [20], two compensation temperatures [21, 22] and inverted magnetic hysteresis loop [23]. Moreover, ternary alloy PBAs become very important due to their adjustable hysteresis properties (such as saturation magnetization and coercivity) which can be enhanced by tuning the concentration of magnetic components [21]. The numerous interesting and tunable features of ternary alloy PBAs have stimulated the researchers to model and investigate them by several techniques. Furthermore, ternary alloy PBAs become excellent candidates for testing the efficiency of numerical methods since they can include both ferromagnetic and antiferromagnetic interactions. Thus, bulk ternary alloy systems have been investigated by, for instance, mean field theory (MFT) [24, 25, 26, 27, 28, 29, 30, 31], effective field theory (EFT) [32, 33, 34, 35] and Monte Carlo (MC) simulation method [36, 37, 38, 39, 40, 41]. In these works, the authors have mainly concentrated on the magnetic properties of the ternary alloy PBAs in the absence of magnetic field. Also, in some recent studies, a ternary alloy PBA nanoparticle [42], nanowire [43] and **a nano-ferrimagnetic surface–bulk PBA** [44] have been studied in detail by MC simulation technique.

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