THz permeability of FePt nanowire

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Abstract

Compared with the GHz permeability of single Fe nanowires, we performed micromagnetic simulations on the terahertz permeability of FePt nanowires with L10-type crystal structure in the remanent magnetization state (Mr/Ms=1.0). Due to the strong magnetocrystalline anisotropy field of FePt nanowires, our study demonstrates that they can exhibit strong terahertz permeability at 0.348 THz, which was previously thought to be achievable only through artificial metamaterials. The THz magnetic spectrum of L10-FePt nanowires is distinctly different from the GHz magnetic spectrum of Fe nanowires, exhibiting an unusual negative imaginary part of permeability ($\mu'' < 0$). We believe this is related to the effective negative damping coefficient resulting from its unusual precession process under natural resonance.

Full Text

Preamble

Author Contribution Statements

(1) HAN proposed the entire research framework, provided simulation parameters, and designed the simulation procedures.

(2) MENG conducted the simulations under HAN' s guidance and prepared the figures.

(3) HAN analyzed the data.

(4) HAN prepared the complete manuscript in English.

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Abstract

The terahertz (THz) permeability of a single $L1_0$-FePt nanowire at its remanent state (Mr/Ms = 1.0) has been simulated using a micromagnetics approach and compared with the gigahertz (GHz) permeability of a single Fe nanowire. Due to its exceptionally large magnetocrystalline anisotropy field, it is feasible to obtain strong THz permeability at 0.348 THz—a capability previously thought possible only in metamaterials. The THz permeability spectra of $L1_0$-FePt differ markedly from those of Fe nanowires at GHz frequencies. An unusual negative imaginary part of permeability (' ' < 0) is observed, which is related to an equivalent negative damping constant and explained from the perspective of abnormal precession during natural resonance at THz frequencies for the FePt nanowire.

Keywords: Terahertz; permeability; FePt nanowires; natural resonance; micromagnetics

1. Introduction

Magnetic permeability characterizes the response of magnetic moments in magnetic materials to external magnetic fields. For electromagnetic applications, it is crucial to understand how the complex permeability values (real and imaginary parts) vary with frequency [1]. The resonance frequency (fr) of the permeability spectrum governs the operational range of magnetic materials. For applications requiring low magnetic loss, the resonance frequency should be far from the working frequency, as in magnetic transformer cores and microwave magnetic devices (e.g., circulators). Conversely, for applications requiring large magnetic loss, the resonance frequency should fall within the operational range to dissipate electromagnetic wave energy via magnetic resonance phenomena, such as in electromagnetic interference suppression or stealth technology.

To date, the highest operating frequencies achieved for electromagnetic devices employing naturally synthesized magnetic materials have been in the W-band (75–100 GHz), realized by using BaM-type ($BaFe_{12}O_{19}$) hexaferrites in which Fe cations are appropriately substituted by Al and Ga [2,3]. With rapid technological advances, researchers have begun developing devices that operate in the terahertz (THz) spectrum (0.1–10 THz) of electromagnetic waves. It is widely accepted that most naturally synthesized magnetic materials cannot function in the THz domain due to their inherently low resonance frequencies, which is why metamaterials are frequently designed to obtain THz permeability [4–6].

Is it truly impossible to employ naturally synthesized materials for THz applications? This paper demonstrates how a strongly hard ferromagnetic $L1_0$-FePt nanowire (hereinafter referred to as FePt) can exhibit pronounced THz permeability spectra. FePt with a tetragonal structure is among the most promising materials for achieving ultra-large areal storage densities (>400 Gb/cm^2) in next-generation perpendicular magnetic recording media [7]. $L1_0$-FePt possesses very large magnetocrystalline anisotropy constants (K) and a very small criti-

cal diameter for forming single-domain structures without superparamagnetic effects [8–10].

To elevate the natural resonance frequency into the THz range, a strong shape anisotropy field can be added to the magnetocrystalline anisotropy field (Hk). Nanowires represent a typical geometry that provides strong shape anisotropy. The following table gives the K values and coercivity values (Hc) for several typical hard magnetic materials, along with the ease of fabricating them in nanowire form via electrochemical deposition techniques.

2. Micromagnetics Theory and Simulations

The micromagnetics approach employs a continuum approximation to analyze magnetization behaviors (hysteresis loops), domain structures, and dynamic responses of magnetization. Micromagnetics describes magnetization on a length scale that is large enough to replace atomic magnetic moments with a continuous function of position, yet small enough to reveal transitions between magnetic domains. The micromagnetics simulations were performed using a three-dimensional object-oriented micromagnetics framework (OOMMF) by solving the Landau-Lifshitz-Gilbert (LLG) equation as a function of time [15]:

$$\frac{d\mathbf{M}}{dt} = -\gamma(\mathbf{M} \times \mathbf{H}_{\text{eff}}) + \frac{\alpha}{M_s}(\mathbf{M} \times \frac{d\mathbf{M}}{dt})$$

where M_s is the saturation magnetization and $\mathbf{H}_{\text{eff}}$ is the effective field that accounts for exchange, demagnetization, anisotropy, and applied field terms. γ is the Gilbert gyromagnetic ratio (2.21×10^5 m/(A $\cdot$ s)), and α is the damping constant. In this paper, α is set to 0.02 for permeability simulations and to 0.5 for hysteresis loop simulations to reduce computational time.

The default parameters in OOMMF for an isolated FePt nanowire were adopted in our simulations: saturation magnetization $M_s = 1.14 \times 10^6$ A/m, exchange stiffness constant $A = 1 \times 10^{-11}$ J/m, and magnetocrystalline anisotropy constant $K_1 = 6.6 \times 10^6$ J/m^3 [15]. The magnetocrystalline anisotropy easy axis is along the [001] direction, which is set parallel to the wire length. The initial magnetization is aligned along the nanowire length direction. The shape anisotropy constant K_s can be expressed as:

$$K_s = \frac{1}{2}\mu_0(N_{d\perp} - N_{d\parallel})M_s^2$$

where $N_{d\parallel} = 0.5$ for a long cylindrical nanowire and represents the demagnetization factor difference between the hard axis and the easy axis. The anisotropy field due to K_1 or K_s can be calculated as:

$$H_k = \frac{2K}{\mu_0 M_s}$$

A cubic cell size of 2 nm × 2 nm × 2 nm was adopted for all simulations. For comparison, an isolated Fe nanowire was also simulated with the following physical parameters: $M_s = 1.7 \times 10^6$ A/m, $A = 2.1 \times 10^{-11}$ J/m, $K_1 = 4.8 \times 10^4$ J/m^3. Both FePt and Fe nanowires are 100 nm long with a diameter of 10 nm to ensure strong shape anisotropy.

To obtain the permeability spectra, we adopted the following procedure. First, a remanent state was selected as the equilibrium magnetization configuration, obtained by reducing the applied saturation magnetic field to zero. Second, a weak pulsed magnetic field ($h(t) = 50\exp(-10^{11}t)$, where t is in seconds and h is in A/m) was applied as a small perturbation to the equilibrium state, with $h(t)$ oriented perpendicular to the nanowire length direction. The dynamic magnetization responses in the time domain were recorded under this perturbation. Finally, the fast Fourier transform (FFT) method was used to convert the recorded data into the frequency domain, from which the permeability spectra were derived. For hysteresis loop simulations, the magnetic field (H) was applied along the length direction and varied between -200 kOe and +200 kOe for the FePt nanowire, and between -40 kOe and +40 kOe for the Fe nanowire, with a field step size of 0.1 kOe.

3. Results and Discussions

We first simulated the hysteresis loops of single FePt and Fe nanowires, as shown in Fig. 1 [Figure 1: see original paper], with the external magnetic field applied along the longitudinal direction. Both nanowires exhibit perfectly rectangular loops, indicating strong shape anisotropy fields. The easy magnetization direction is along the nanowire length. The remanence ratio (M_r/M_s) equals 1.0 (see point "A"), providing an excellent equilibrium state for dynamic simulations (i.e., $\mu \sim f$) because nearly all magnetic moments are aligned in the same direction, yielding a strong response. The simulated coercivity is 122.51 kOe for the FePt nanowire, which is larger than the reported value (23 kOe) for bulk materials containing multiple magnetic domains with very weak shape anisotropy fields [16]. A similar trend is observed for the Fe nanowire: the simulated H_c is 10.65 kOe, much larger than the measured value (356 Oe) for arrays containing millions of Fe nanowires. Detailed explanations for these differences were provided in our previous work [17,18].

The remanent states of the FePt and Fe nanowires are illustrated in Fig. 2 [Figure 2: see original paper]. Clearly, each magnetization vector points along the longitudinal direction, with no domain walls present. For magnetic materials containing multiple domains, the frequency dependence of permeability is dominated by the domain wall resonance frequency, which is far below the natural resonance frequency. For instance, we previously studied the domain wall resonance frequency (f_{DW}) and natural resonance frequency (f_r) for NiZn spinel ferrite, revealing that f_{DW} is lower than f_r by an order of magnitude [19]. Therefore, we can infer that a single magnetic domain structure is a prerequisite for obtaining obvious THz permeability in naturally synthesized magnetic

materials with extremely large K values, as shown in Table 1.

When the remanent state (an equilibrium state) shown in Fig. 2 is used to study dynamic magnetic responses, the complex susceptibility ($\chi = \chi' - j\chi''$) can be defined as:

$$\chi(\omega) = ---(4)$$

Accordingly, the respective expressions for the real ($\mu' = 1 + \chi'$) and imaginary ($\mu'' = \chi''$) parts of permeability are given below [20]:

$$---(5)$$
$$---(6)$$
$$---(7)$$

When the following condition is satisfied, the imaginary part of permeability (μ'') reaches a maximum value. This physical phenomenon is termed "natural resonance" :

$$\omega_r = ---(8)$$

The natural resonance frequency (f_r) can be calculated according to Eq. (8), in which H_0 is expressed as follows [20]:

$$---(9)$$

Since the damping constant (α) is extremely small compared to the product of γ and M_s (see Eqs. 9 above), H_0 can be approximately represented by H_{eff}. In other words, the natural resonance frequency (f_r) and the permeability spectrum cannot be adjusted by controlling the damping constant; they can only be modified by controlling the effective anisotropy field (H_{eff}), which may arise from H_k, H_{shape}, and/or other sources such as stress-induced anisotropy fields.

The frequency-dependent permeability spectra for both nanowires are compared in Fig. 3a. Obviously, the natural resonance frequency of the Fe nanowire is about 31 GHz, much smaller than that of the FePt nanowire (348 GHz = 0.348 THz). According to Eqs. (2), (8), and (9), the calculated f_r values are 31.49 GHz and 0.344 THz for Fe and FePt nanowires, respectively, which agree very well with the simulated values and corroborate that these observed peaks originate from natural resonance phenomena related to their effective fields. However, the shape anisotropy field (H_{sh}) plays an important role in enhancing the f_r value of the Fe nanowire, while it can be neglected in the FePt nanowire because H_{sh} is much smaller than the magnetocrystalline anisotropy field (H_k).

Therefore, only one natural resonance frequency is observed in FePt. The other resonance peak found at 18 GHz is attributed to an "edge mode." As indicated in Eq. (7), D is always a positive value. Hence, μ'' is always positive (see Eq. 6) since the damping constant (α) is generally considered positive to represent energy dissipation during precession. This widely accepted fact ($\mu'' > 0$) is observed in the permeability spectrum of the Fe nanowire, as shown in the inset of Fig. 3a [Figure 3: see original paper].

However, the THz permeability of FePt shows different behavior: μ'' first reaches a negative dip ($\mu'' < 0$) and then jumps back to a normal positive peak at the resonance frequency (f_r). To interpret this abnormal behavior, we must compare the precession dynamics between Fe and FePt nanowires. As shown in Fig. 3b, the time-dependent M_z component of the Fe nanowire oscillates symmetrically around zero and finally reaches a static state ($M_z = 0$) when the precession of M_s completely stops. For the FePt nanowire, M_z first shows an asymmetrical oscillation above zero and then returns to normal symmetrical oscillation around zero. Examining the time dependence of both M_z and M_y together provides clearer evidence of the abnormal precession in the FePt nanowire, as shown in Fig. 4a. For the Fe nanowire, both $M_y(t)$ and $M_z(t)$ follow identical precession behavior, as demonstrated by their overlapped time-dependent curves in Fig. 4b. For the FePt nanowire, $M_y(t)$ and $M_z(t)$ are not overlapped at the beginning of precession.

By comparing these precession patterns, the THz permeability of the FePt nanowire is anticipated to differ from that of the Fe nanowire. Under excitation by an external pulsed magnetic field, the magnetization ($\mathbf{M}$) deflects from its equilibrium direction by an angle (termed the "precession angle") and begins to precess around this direction (called Larmor precession). In our case, the effective anisotropy field direction is along the x-axis. The other torque is termed "damping torque," which points toward the center of the precession circumference and reduces the precession angle as energy absorbed from the external field is dissipated. In other words, a gradually decreasing precession angle denotes a positive damping constant, and vice versa. The imaginary part (μ'') of permeability, representing energy loss, is therefore always positive for normal precession. From Eq. 6, a positive damping constant ensures positive μ'' values, which is widely accepted as a natural law that μ'' cannot be negative for general physical scenarios.

However, if the precession angle can be enlarged during abnormal THz precession, as observed in the FePt nanowire, this is equivalent to having a negative damping constant and will result in negative μ''. The negative μ'' phenomenon has also been proposed by us in another paper for normal precession where spin-transfer torque from spin-polarized current was used to enlarge the precession angle [21]. Furthermore, from the standpoint of energy dissipation, when external energy input (e.g., spin-transfer torque effect) exceeds dissipated energy, it leads to an enlarged precession angle and an effectively negative damping constant. Accordingly, negative μ'' will be observed as per Eq. 6. Additionally, it

should be noted that the damping time of magnetization, shown in Fig. 4, differs significantly between FePt and Fe nanowires, being almost ten times longer for the Fe nanowire.

The differences in precession between FePt and Fe nanowires can also be viewed from the perspective of Gibbs energy (E_{tot}), as shown in Fig. 5 [Figure 5: see original paper]. When normal natural resonance occurs, E_{tot} exhibits a sudden jump due to energy coupling from the pulsed magnetic field excitation, then dissipates through magnetic loss as the precession angle gradually decreases to zero, giving rise to positive μ'' values. However, multiple peaks in E_{tot} are observed for FePt, indicating that the precession angle does not decrease monotonically. At certain moments, the angle enlarges, as inferred from the sudden increases in E_{tot}. As stated previously, this is equivalent to having a negative damping constant (α), which results in negative μ'' values. Obviously, from point "D" to point "F" in Fig. 5a, E_{tot} dissipates normally, and therefore we observe normal positive μ'' values again.

4. Conclusions

At the remanent state ($M_r/M_s = 1.0$), $L1_0$-FePt nanowires with large H_k values and square M-H loops can exhibit pronounced THz permeability spectra ($\mu \sim f$) with a natural resonance frequency (f_r) of 0.348 THz. Surprisingly, μ'' is found to be negative below some frequency around f_r, which is attributed to abnormal precession behavior and has been compared with an isolated Fe nanowire showing normal precession. We believe that if the precession angle is enlarged during Larmor precession, it is equivalent to having a negative damping constant, which consequently results in negative μ'' values.

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Supplementary Information

FIGURES: (FIG. 1) (FIG. 2) (FIG. 3a) (FIG. 3b and 3c) (FIG. 4a [Figure 4: see original paper]) (FIG. 4b) (FIG. 5a) (FIG. 5b)

Note: Figure translations are in progress. See original paper for figures.