



Simulation of Heat Transfer in Multilayer Structure

Saffa Issam Mohamad Ali^{1*}  , Haidar J. Mohamad²  , and

Mohammed Jassim Mohammed Ali³  

^{1,2,3} Department of Physics, College of Science, University of Mustansiriyah, Baghdad, Iraq

*Corresponding Author

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Abstract

Hard disk drives (HDDs) and recent data storage technologies are anticipated to play a transformative part in the development of information technology. Heat-assisted magnetic recording and its applications are one of the most significant technologies in this field, offering a pathway to noticeably higher storage densities. The thermal gradient in the tetralayer thin-film structure was generated by utilizing pulses of a femtosecond laser to produce a spin current. The tetralayer is made of an Al_2O_3 -Py (Ni81Fe19)-MgO-Copper-YIG ($\text{Y}_3\text{Fe}_5\text{O}_{12}$)-and $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ layers. To model the heat transfer and thermal gradients within this structure, COMSOL Multiphysics® software is used to conduct a detailed three-dimensional (3D) thermal simulation. Parameters such as thickness and time were shown to have a major effect on the generated spin current. In addition to that, the temperature gradients within the tetralayer are crucial indication for generating the spin current. The findings reveal that using MgO in the adjacent metallic layers did not provide sufficient thermal gradient, which is required to generate the spin current.

Keywords: Thermal Gradient, Multilayer Thin Films, Spin current, Ultrafast laser, Heat-assisted magnetic recording, COMSOL Multi physics.

1. Introduction

The continuous rise in data technology among various fields has highlighted the necessity to expand the storage capacity of hard disk drives. Using higher-capacity HDDs allows for efficient management and storage of big volumes of data, for example applications, multimedia files, and operating systems, thereby meeting the increasing demands of modern computing environments¹. This development is mostly critical in different fields that require processing and storing large datasets frequently, such as computational intelligence, large-scale data analysis, and utility computing. Higher HDD capacity allows efficient data backup and long-term archiving, which will help in reducing the need for regular hardware upgrades and contributing to overall system consistency and cost effectiveness². Spintronics is a topic that takes benefit the spin of electron for information storage, transport, and processing³.

Spintronics is a rapidly developing area in the science of electronics which are based mainly on optical and electrical control of magnetism as well as the spin control of electronics, despite the importance of this subject, semiconductor spintronics haven't reached its maximum potential until now^{4,5}.

The consistently rising tendency of device multifunctionality and miniaturization exerts substantial pressure on existing manufacturing technologies therefore, Heat-assisted magnetic recording can be utilized where the demands for precision, throughput, and expenses become more challenging to achieve with minimal room for compromises are needed^{6,7}.

Energy-assisted magnetic recording is generally recognized main tool to further enhance the areal density evolution of hard disk drives and its enhancement in comparison with the present perpendicular magnetic recording⁸.

HAMR technology raises the media temperature during writing. Higher temperatures reduce media coercivity, solving the “thermal stability against writability” problem. As grain size scales drop, magnetic recording density should rise once the “thermal stability against writability” barrier is solved^{9, 10}.

The laser is utilized to briefly heat the medium, enhancing its sensitivity and susceptibility to magnetic effects. This enables writing in extremely small areas while saving substantially larger volumes of data on a disk¹¹.

The relationship between ultrafast laser excitation and spin transport in multilayer thin films has been the topic of extensive research over the last decades some of those researches are:

A pulsed laser, rather than a continuous one, was simulated. The results indicated that synchronizing the laser pulses with the applied magnetic fields significantly improves the thermal gradients within the material¹². A study was presented that illustrated ultrafast spin and charge dynamics in thin ferromagnetic films using a semi-classical phase space model. The application of a femtosecond laser pulse in the visible range has been demonstrated to create an oscillating spin current in the film¹³.

Another study used COMSOL software to understand the temperature behavior of the laser pulse on the suggested sample FePt (8 nm) /MgO (8 nm) /SiO₂ (58 nm) /Si (9.32 E-7 m) • in which HAMR use was the focus of this study. The result showed that the laser power depends on the layer’s thickness, which gives a high temperature gradient within the sample layers and leads to saving energy¹⁴.

In the present study, COMSOL Multiphysics (v 6.1) was used to simulate the results, in which an ultrafast (fs) laser is used to induce a thermal behavior inside the nano-sized tetralayer Ni₈₁Fe₁₉(Py)/MgO/Cu/Y₃Fe₅O₁₂(YIG).

The primary problem involves studying the effect of heating the medium using ultrafast laser and examining the temperature differential generate inside the tetralayer as a function of both layers thickness and time This research holds significant importance as it contributes to the growing field of heat-assisted magnetic recording (HAMR) and spintronic device engineering, where understanding ultrafast thermal transport is essential for next-generation data storage technologies. By employing COMSOL Multiphysics simulations to analyze the heat transfer and temperature gradients within multilayer thin films under femtosecond laser excitation, this study provides critical insights into how material selection and layer configuration affect spin current generation. Such findings are vital for optimizing the design of nanoscale multilayer structures that enable higher storage densities, faster data processing, and improved energy efficiency in magnetic recording systems.

2. Materials and Methods

2.1 . Theoretical Consideration

Ultrafast laser pulses, with durations on the femtosecond timescale, induce rapid temperature rises within multilayered sample structures¹³. The thermal response can be correctly modeled by using the equation of three-dimensional heat diffusion, which integrates both of the spatial and temporal distribution of the absorbed laser energy as a heat source term.

This equation can be written as¹⁵:

$$\frac{1}{D} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{g(x,y,z)}{k} \quad (1)$$

Where D is the thermal diffusivity ($D = k / \rho C_p$), k is the thermal conductivity, ρ is the density of the material, C_p is the heat capacity per unit mass, and $g(x, y, z, t)$ is the absorbed power density within the sample¹⁵.

This equation is derived directly from Fourier's law of heat conduction, which was first formulated by Joseph Fourier in 1822¹⁶.

In systems with a multilayer structure, such as ferromagnetic/spacer/magnetic insulator, the local absorption in each active layer is ruled by the spatial profile of the electric field, thereby defining the distribution of the heat source. This approach is essential for understanding phenomena (such as spin current generation in the magnetic insulator under ultrafast optical excitation) by allowing the calculation of the temperature evolution in each layer^{17, 18}.

As detailed in recent studies^{19, 20}

The electron subsystem energy is mostly heated up through the initial laser absorption, which then transfers energy to the lattice via electron-lattice interactions, resulting in a rapid rise in lattice temperature.

The temperature gradients across the multilayer stack play a vital role in driving spintronic effects and are accurately shown by solving the heat diffusion equation with a suitable heat source profile^{17, 21}.

Recent developments in ultrafast spintronics have focused on the use of multilayer structures consisting of ferromagnetic metals, nonmagnetic spacers, and magnetic insulators to help in the producing and manipulation of spin currents on femtosecond timescales^{13,17}.

A tetralayer made up of Al_2O_3 / $\text{Ni}_{81}\text{Fe}_{19}$ (Py)/ MgO /Cu/ $\text{Y}_3\text{Fe}_5\text{O}_{12}$ (YIG)/GGG is observed for ultrafast spin current, which is generated via femtosecond laser excitation. Theoretical and simulation studies, notably using COMSOL Multiphysics, were demonstrated.

2.2 . Materials Used in the Simulation

In the current study, a three-dimensional were simulation by utilizing COMSOL Multiphysics version 6.1 software® to examine the thermal effects induced within a tetralayer as a result of heating by ultrafast laser optical, MATLAB coding were also used to improve the simulation accuracy.

The simulation is constructed for a time dependent study, as illustrated in **Figure 1**.

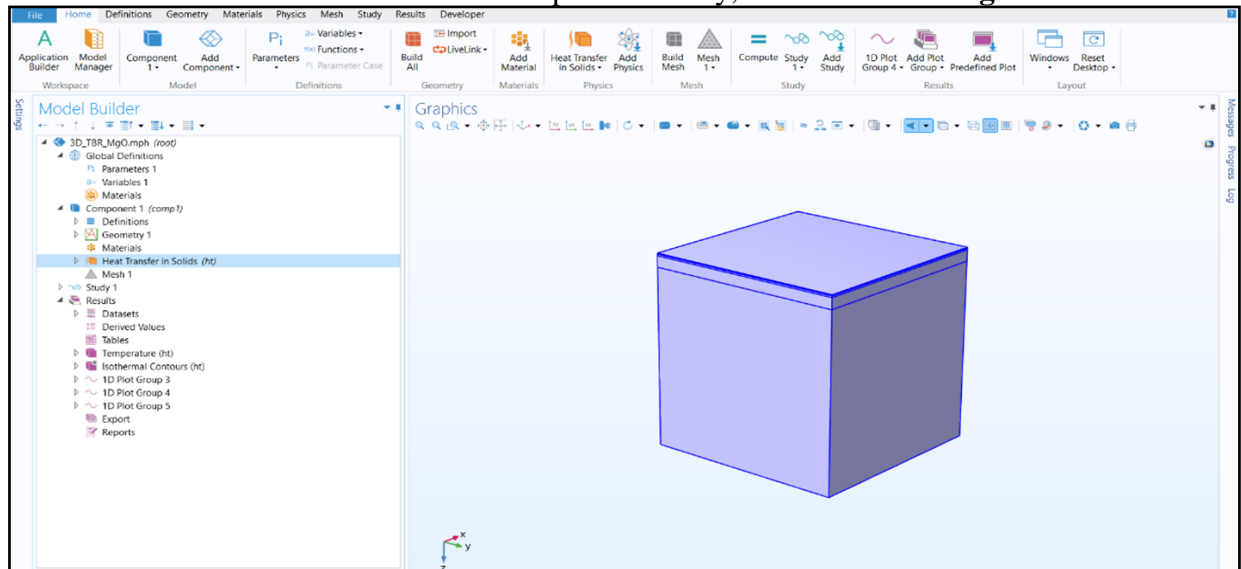


Figure 1. COMSOL Multiphysics of the 3-D model interface.

Optical and the thermal parameters employed in the calculation of thermal flow and optical absorption. those Properties can be chosen from COMSOL's built-in material library, which provides access to standard material properties from reputable sources²² or it can be manually inputted based on empirical data. All material parameters are considered temperature-independent and are assumed not to vary due to optical excitation throughout the simulation as in **Table 1**.

The parameters listed in **Table 1** are essential for performing the numerical simulations in COMSOL Multiphysics. These material properties serve as fundamental input data that define the thermal and physical behavior of the multilayer structure under optical excitation. Accurate specification of these parameters ensures the reliability and precision of the simulation results. Thermal boundary layer was included in the calculations and was obtained from previous study²³.

Table 1. properties of the materials at an ambient temperature of 300K which were used in the calculation.

Material properties.	Al ₂ O ₃	Py	MgO	Cu	YIG	GGG
Mass density. (kg/m ³)	3890	8700	3580	8930	5170	7080
Heat conduction coefficients. (W.m-1K-1)	1 - 4.5 ²⁸	46.4 ²⁷	30 ²⁶	150 ²⁵	6.63 ²⁴	7.94 ²⁴
refractive index n (800 nm)	1.759	2.2+j3.6 ³⁰	1.7+j0.2	0.2499+j5.0337	2.19+j2.48*10 ⁻⁶²⁹	1.95
Specific heat (J.kg-1K-1)	880	430	880	385	578	400

The modeled sample comprises a multilayer 3D cubic structure. where the width and depth are each 2 nm, and the height is 2 nm for the Al₂O₃ layer, followed by Py (8 nm), MgO (8 nm), Cu (8 nm), YIG (58 nm), and Gd₃Ga₅O₁₂ (GGG) (0.9325 μm) layers as shown in **Figure 2**. The selection of materials and layer thicknesses in this study was guided by several previous works^{14, 23, 31} that investigated ultrafast thermal transport and spin current generation in multilayer thin-film structures.

Earlier studies primarily focused was on trilayer configurations, such as Py/Cu/YIG systems. In contrast, the present research extends these investigations by employing a tetralayer configuration that includes an additional MgO layer between the ferromagnetic (Py) and nonmagnetic (Cu) layers. This modification allows for a more comprehensive understanding of how an insulating interface influences the temperature gradient and heat flow across the structure and therefore the generation of spin current.

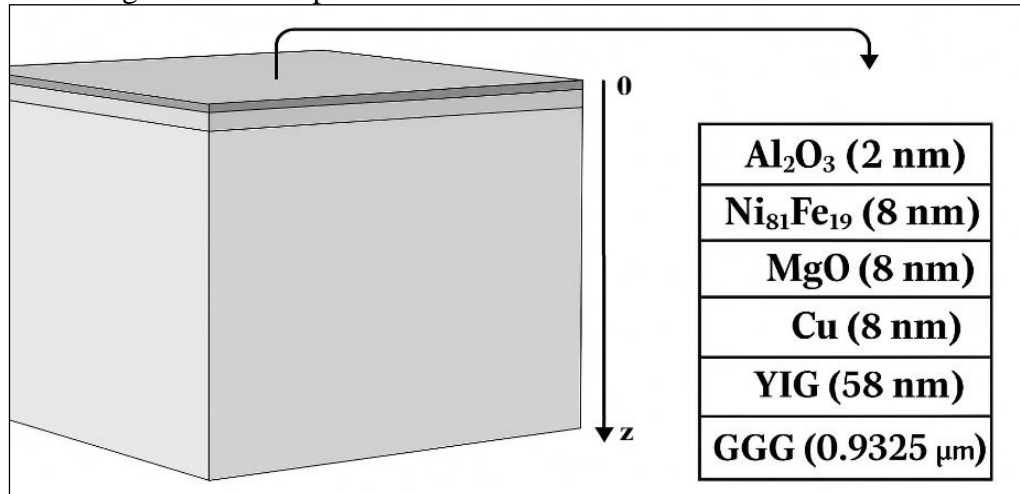


Figure 2. Illustration of the layers and their thicknesses used in this simulation.

The study's results rely on measurements performed on the tetralayer (Py/MgO/Cu/YIG) heated by an ultrafast laser in which Al₂O₃ (cup layer) and GGG (substrate layer) wasn't taken in consideration during the calculations because of their insignificant effect. Several studies have been carried out to examine the temperature variations in the tetralayer sample.

3.Results

A time-based study in a Heat Transfer in Solids interface were used to generate A 3-D model by using COMSOL Multiphysics to examine the effect of using MgO in tetralayer on the generated of the spin current.

The modeled sample consists of a multilayer 3D cubic where several investigations have been carried out to examine the temperature distribution within the sample, as shown in **Figure 3** (The color legend denotes the temperature). Thermal modeling in **Figure 4** represents the temperature evolution along the depth of the tetralayer sample due to femtosecond laser pulse excitation at chosen time intervals. **Figure 5** depicts how temperature varies over time at specific depths inside the sample with the incorporation of TBR.

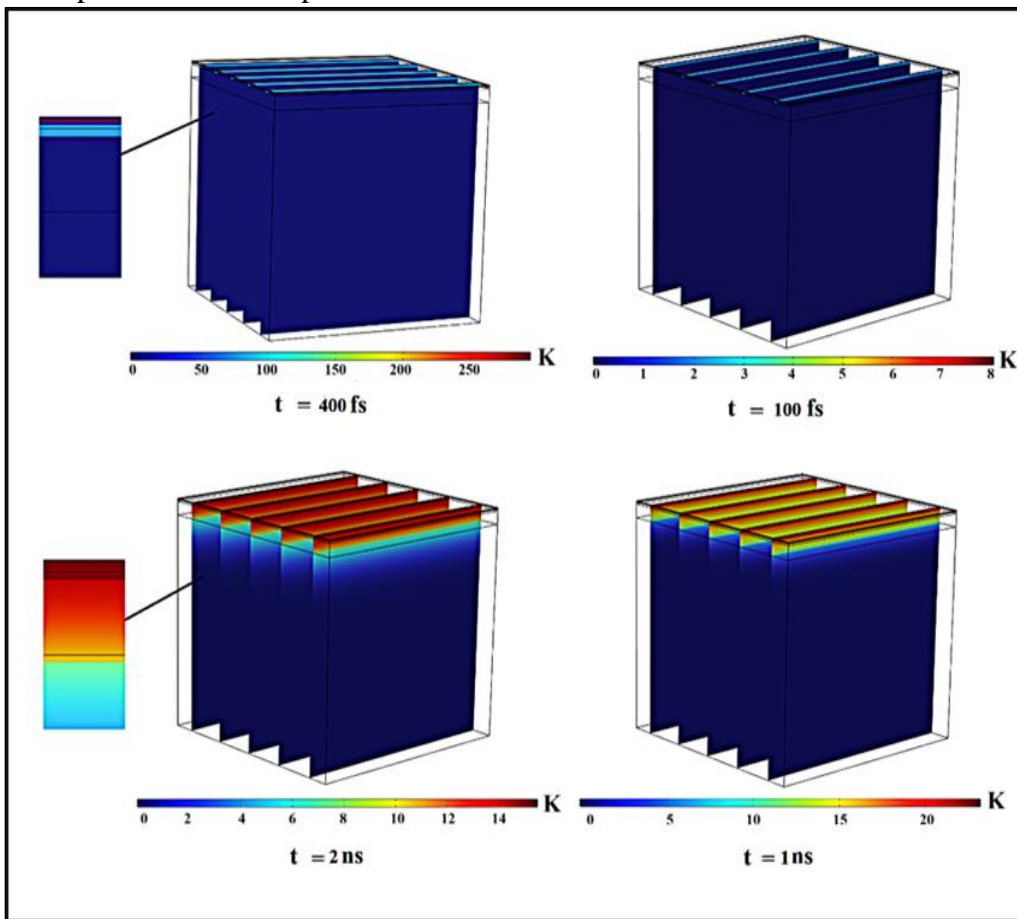


Figure 3. Temperature distribution within the trilayer specimen at specified time intervals.

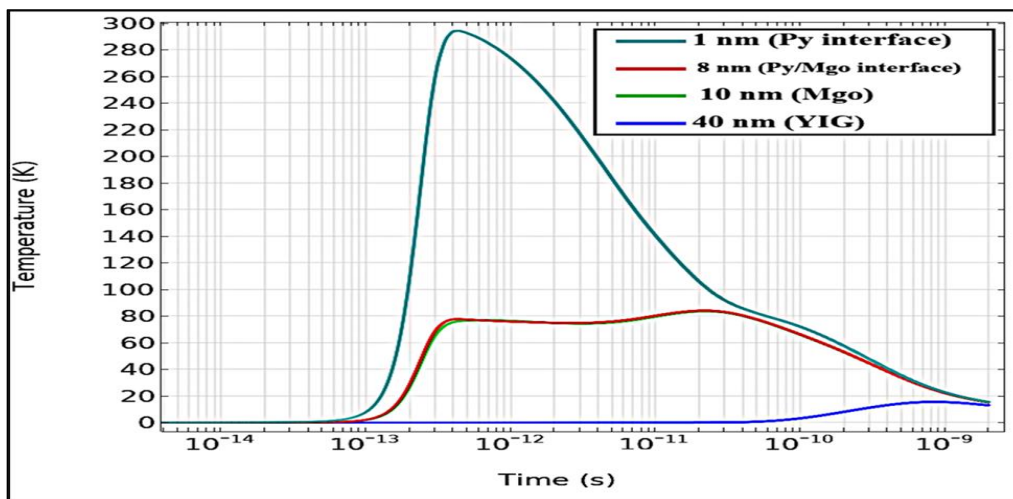


Figure 5. The temperature change as a function of time in the tetralayer sample at specific depths

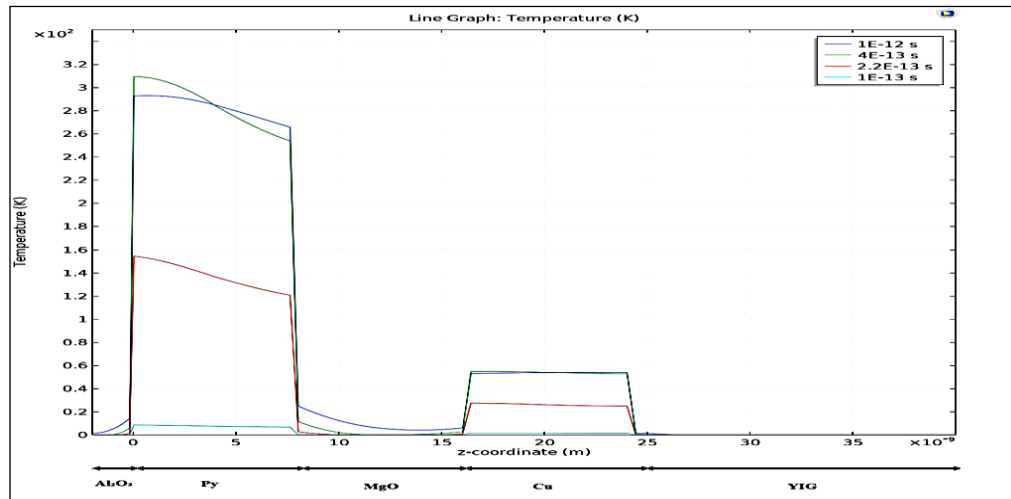


Figure 4. Variation in temperature at specified time intervals and as a function of depth within the tetralayer sample.

4. Discussion

The temperature gradient arises from optical pumping using an ultrafast (fs) laser with set time delays. It is shown in **Figure 3** with the inclusion of thermal boundary resistance in the calculations. This sequence clearly visualizes the transition from highly localized, ultrafast surface heating immediately after the laser pulse hits the very top surface, to diffusive thermal spreading and cooling over the time scales through the multilayer stack.

Figure 4 illustrates the temperature profiles as a function of depth. Each material layer is annotated along the x-axis, delineating the regions corresponding to Al_2O_3 , Py, MgO, Cu, and YIG.

The thickness of each layer plays a crucial role in determining the overall heat transfer behavior within the multilayer structure²³. Thinner layers tend to facilitate faster heat diffusion and smaller temperature gradients, while thicker layers increase the thermal resistance and delay heat propagation. Therefore, specifying the layer thicknesses is essential for accurately modeling the temperature distribution and understanding how heat is transmitted across the interfaces. This parameter directly influences the temporal evolution of temperature and, consequently, the conditions required for spin current generation in HAMR systems.

The data reveal a pronounced temperature rise within the Py layer shortly after excitation (notably at 4×10^{-13} s and 1×10^{-12} s), followed by a rapid decrease in temperature within the MgO layer, then a small increase in temperature in the Cu layer and finally a thermal diffusion into adjacent layers. Over time as the temperature gradients diminish, which indicate the progression toward thermal equilibrium throughout the stack, the results were confirmed to have the same behavior as reported in previously published data^{14, 23}.

Distinct temperature steps at the interfaces reflect differences in thermal properties and heat transport across the multilayer structure and as can be shown and here the MgO layers acted as a thermal insulator layer which will not aid in generation of spin current. **Figure 5** shows the temporal evolution of temperature at various depths along the z-axis in a tetralayer structure, which is extremely affected depending on the sample's proximity to the surface.

Immediately after excitation by the ultrafast laser, the temperature rises abruptly, reaching a peak before decreasing over time as heat dissipates over the structure. The highest initial temperature is observed at the location near the surface which is the closest to the excitation source. This behavior is due to the strong localization of heat near the laser-irradiated region and the following spread determined by the thermal conductivities of the materials composing the tetralayer^{14, 31}.

5. Conclusion

The results of the simulation showed that the temperature distribution which is obtained by laser-induced is highly non-uniform along the multilayer stack, with a steep thermal gradient that can be detected immediately after excitation by the laser. The Py layer, being the primary

absorber of the ultrafast laser pulse, exhibited a significant rise in temperature trailed by a sharp drop across the MgO layer.

The MgO behavior as a thermal barrier rather than a conductive interface, hindering efficient heat transfer and thus limiting the conditions necessary for the generation of the spin current then there is small increase in temperature in the Cu layer before diffusing into the YIG layer and the underlying substrate layer (GGG).

This finding highlights the significant of proper selection of the materials in spintronic devices design that are based on HAMR technologies. the choice of spacer material must be reconsidered to enhance and improved the thermal transport and allow for the desired spin dynamics. The result also highlights the importance of precisely controlling layer thicknesses and thermal conductivity to improve ultrafast laser energy efficiently.

Future works and study should focus on experimental different simulation results by exploring more materials with improved thermal and spin transport properties to entirely show the interaction between heat and spin currents in these heterostructures. Replacing MgO with alternative materials such as aluminum nitride (AlN), silicon carbide (SiC), or diamond-like carbon (DLC) could enhance heat conduction across the multilayer.

These materials possess higher thermal conductivities while maintaining structural compatibility with the metallic and magnetic layers, thereby improving both thermal performance and spin transport efficiency in future HAMR-based device designs. Future studies may further investigate various simulation outcomes by examine different material thicknesses aiming to achieve enhanced thermal and spin transport properties. such investigation would provide a more understanding of the influence of material thickness on heat and spin currents within these models.

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Conflict of Interest

The authors declare that they have no conflicts of interest.

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