Temperature Profile in the Presence of Hotspots in Heat Assisted Magnetic Recording

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Recently, the demands for increasing memory capacities in hard disk drives (HDDs) has resulted in state-of-the-art technologies including heat assisted magnetic recording (HAMR) with significantly higher operating temperatures. HAMR results in swift degradation of current lubricant and carbon overcoat (COC) materials, leading to magnetic media corrosion which is detrimental to HDD operation. In addition, the lack of thorough understanding of the temperature profiles arising from the hotspot and energy management throughout these materials also exacerbates the problem. To address this issue, in this paper we will focus on the COC and investigate the transient heat transfer in various examples of nanoscale thin films when a hot spot is created via lattice Boltzmann method (LBM) since traditional conduction models like Fourier law are not accurate due to dominant sub-continuum effects. LBM originates from the Boltzmann transport equations (BTEs) and is computationally efficient due to easy parallelization with convenient handling of complex geometries. Our results of the heat transfer mechanism and temperature profiles show that Fourier equation under-predicts the peak temperature rise at the center of the hot-spot as the system size approaches the nanoscale domain. Applying LBM to a multilayered system, we observe a temperature slip along the interface of two materials indicated by the broken isothermal contours, as the heat is confined to a single layer. Using LBM, we then explore a novel graphene overcoat which has outstanding thermo-mechanical properties, and thereby extremely compatible in HAMR applications.

***Index Terms*—Overcoat, Fourier law, graphene, heat assisted magnetic recording (HAMR), hotspot, lattice Boltzmann method (LBM).**

I. INTRODUCTION

THE relentless surge in higher recording density hard disk drives (HDDs) has resulted in smaller dimensions in head disk interface components including lubricant, carbon overcoat (COC), and the media layers. Novel technologies such as heat assisted magnetic recording (HAMR) have been proposed to further increase the areal density by operating at much higher temperatures than conventional recording (Fig. 1).

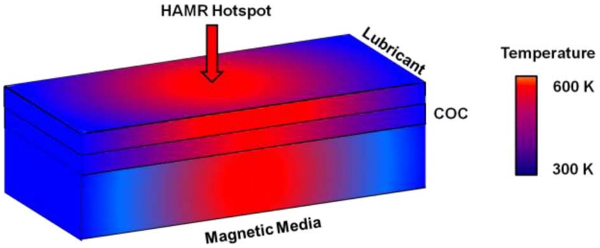

Fig. 1. Temperature variation in HDI components for HAMR.

As the lubricant layer approaches a monolayer thickness, the focus is now geared towards reduction in the COC thickness. However, industry standard overcoat material, known as diamond like carbon (DLC) fails at thicknesses less than 2 nm due to high tensile stresses, which adversely affect the mechanical integrity due to high surface tensile stresses [1]. This results in delamination and breakup of the COC surface and exposes the media to the environment, while severely reducing the lubricant adhesion, thus defeating the primary function of COC. It is obvious that HAMR induces further significant thermo-mechanical issues on all the head disk interface (HDI) components, especially the COC, which has to cope with changes in properties to avoid poor corrosion protection and tribology performance. Furthermore, COC has to manage the heat transfer so that the media temperature does not wastefully exceed the necessary thermal demagnetization temperature in order to avoid depositing excess energy, which can damage medium materials.

In essence, an accurate knowledge of the thermal management properties at nanoscale COC apart from introduction of novel materials which can withstand such conditions is urgently required. In this study, we have developed a transient mesoscale model to investigate the heat transfer mechanism in nanoscale films when a hotspot is created. Traditional conduction models like Fourier law are not suitable due to dominant sub-continuum effects such as ballistic thermal transport and temperature slip at the boundaries. Here, we utilize a lattice Boltzmann method (LBM) for phonons, which are primary carriers of energy at this scale, for the nano-scale thermal modeling. LBM originates from the Boltzmann transport equations (BTEs) and is computationally efficient due to easy parallelization with capabilities of handling complex geometries. The parameters in LBM are determined such that the macro-scale conservation laws are obeyed [2].

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We develop, validate, and compare the LBM models for various geometries including monolayer to multilayered films under hotspots. Once this is complete, we apply this method for analyzing the temperature profile in a novel graphene overcoat, especially for HAMR application.

II. THEORETICAL METHODS

The BTE [3] with the single relaxation time approximation is used to accurately simulate energy transport as long as the particle assumption for the heat carriers is valid. The BTE, however, is difficult to solve and, in general, a large computational effort is required for the solution for even simple geometries. Thus, we developed a novel LBM scheme [4], which, in essence, discretizes the BTE, while maintaining its accuracy while reducing the computational requirement, described by the following equation:

$$\frac{\mathrm{df}}{\mathrm{dt}} + \mathrm{v} \cdot \nabla \mathrm{f} = -\frac{\mathrm{f} - \mathrm{f}^0}{\tau} + \mathrm{g}, \tag{1}$$

where f, $\mathbf{v}$, t, and f^0 are the carrier distribution function, group velocity, relaxation time, and equilibrium distribution function, respectively. f^0 is given by the Bose-Einstein distribution for phonons and Fermi-Dirac distribution for electrons. The term g is the phonon generation rate due to external sources such as laser heating hotspot. Equation (1) can be transformed to a similar BTE for carrier energy density e:

$$\frac{\mathrm{de}}{\mathrm{dt}} + \mathbf{v} \cdot \nabla \mathrm{e} = -\frac{\mathrm{e} - \mathrm{e}^0}{\tau} + \mathrm{Q}, \tag{2}$$

here, Q is the energy source, which arises due to the hotspot and the electron-phonon interactions. These cross carrier interactions will be examined in future communications. In this study, we examine only a phonon LBM, where energy of the phonons is given as:

$$\mathrm{e}(\mathrm{T}) = \frac{1}{2\pi} \sum_{\mathrm{p}} \int \mathrm{f} \hbar\omega \, \mathrm{D}_{\mathrm{p}}(\omega) \, \mathrm{d}\omega, \tag{3}$$

here h is the Planck constant, ω is the frequency, and $\mathrm{D}_{\mathrm{p}}(\omega)$ is the density of states for carriers with polarization p.

In order to translate the above variables to physical quantities, one must consider the temperature. However, the conventional definition of temperature is not valid under non-equilibrium conditions, therefore, an equivalent temperature term needs to be defined, where the total energy of carriers is equal to the total energy of the equilibrium carrier distribution at the equivalent temperature. The phonon energy densities $(\mathrm{e}_{\mathrm{ph}})$ at their equivalent non-equilibrium temperatures $(\mathrm{T}_{\mathrm{ph}})$ are given by [4]:

$$\mathrm{e}_{\mathrm{ph}}(\mathrm{T}_{\mathrm{ph}}) = \frac{9\eta_{\mathrm{ph}} \mathrm{k}_{\mathrm{B}} \mathrm{T}_{\mathrm{ph}}^4}{\theta_{\mathrm{D}}^3} \int_0^{(\theta_{\mathrm{D}}/\mathrm{T}_{\mathrm{ph}})} \frac{\mathrm{z}^3}{\mathrm{e}^{\mathrm{z}} - 1} \mathrm{dz}, \tag{4}$$

here, k_{B} is the Boltzmann constant, θ_{D} is the Debye temperature, η_{ph} is the number density of phonons.

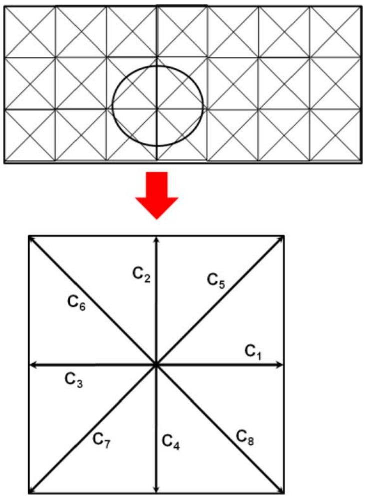

Fig. 2. Two dimensional LBM lattice with the corresponding velocity vectors.

Unlike the BTE, which is a continuous equation in phase space, the LBM discretizes the space domain by defining a lattice network (Fig. 2) where the energy carriers reside. Carriers propagate ballistically to a neighboring lattice site and collide with carriers at that site.

Time domain is discretized by restricting the carriers to travel from a lattice site to the neighboring lattice site in a given time step. The velocity space is discretized in regular intervals and only a discrete set of c_{i} in the main lattice directions is allowed. Then, (2) is discretized using the forward Euler difference for the time derivative and first-order upwind scheme for the spatial derivative. The time step-lattice spacing relationship is incorporated by $\Delta \mathrm{x}_{\mathrm{i}} = \mathrm{c}_{\mathrm{i}} \Delta \mathrm{t}$. This leads to the LBE with heat generation:

$$\mathrm{e}_{\mathrm{i}}(\mathrm{x} + \Delta \mathrm{x}_{\mathrm{i}}, \mathrm{t} + \Delta \mathrm{t}) = (1 - \mathrm{W})\mathrm{e}_{\mathrm{i}}(\mathrm{x}, \mathrm{t}) + \mathrm{W}\mathrm{e}_{\mathrm{i}}^0(\mathrm{x}, \mathrm{t}) + \mathrm{Q}\Delta \mathrm{t} \tag{5}$$

where $\mathrm{W} = \Delta \mathrm{t}/\tau$ and $\mathrm{e}_{\mathrm{i}}(\mathbf{x}, \mathrm{t})$ is the discrete carrier energy distribution. Notice that the total carrier energy density is $\mathrm{e}(\mathrm{x}, \mathrm{t}) = \sum_{\mathrm{i}=1}^{\mathrm{D}} \mathrm{e}_{\mathrm{i}}(\mathrm{x}, \mathrm{t})$, where D is the number of propagation directions in the lattice. The equilibrium carrier energy distribution can be derived by assuming the isotropic distribution,$\mathrm{e}_{\mathrm{i}}^0(\mathrm{x}, \mathrm{t}) = \mathrm{e}_{\mathrm{i}}(\mathrm{x}, \mathrm{t})/\mathrm{D}$. This definition inherently guarantees energy conservation.

Due to the availability of abundant theoretical and experimental literature, our model was analyzed and validated by inducing a hotspot in a nano-scale silicon film and comparing the resultant transient temperature profile with Fourier equation for a system shown in Fig. 3, since the generalization for complex geometries in LBM is straightforward. All the side boundaries of the system were maintained at constant temperature of 300 K. The critical silicon parameters of group velocity and relaxation time are taken to be 6400 m/s and 6.53 ps, with bulk conductivity value taken as 148 W/m-K. A phonon scattering condition is used at the top and bottom system boundaries, where a novel specularity factor P is introduced, which represents the fraction of carriers undergoing diffusive scattering at the boundary accounting for the surface roughness. The dimensions of the film and hotspot are used such that a high Knudsen number

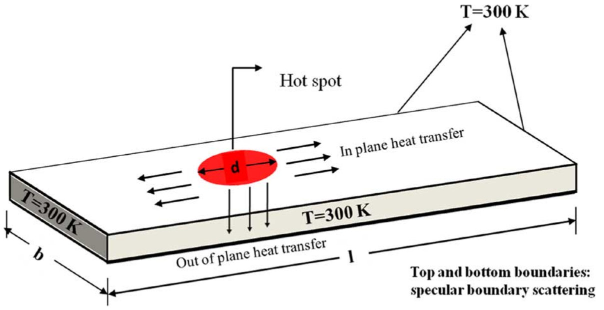

Fig. 3. Schematic of a nanoscale thin sheet with a hot spot. l is the length of the sheet and b is the thickness, and d is the width of the hot spot region.

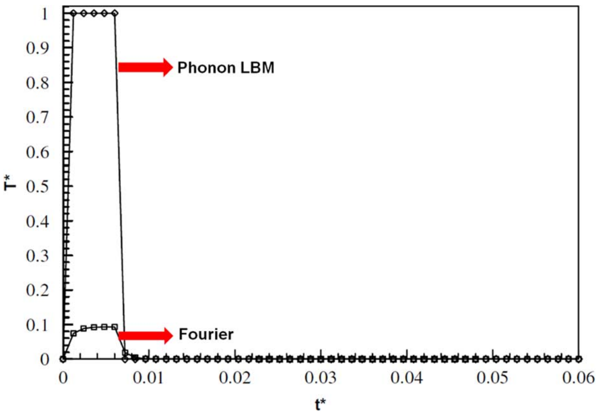

Fig. 4. Transient non-dimensionalized temperature profile at the center of the hotspot for Fourier equation and LBM solutions. $T^* = (T - T_{W1})/(T_{W2} - T_{W1})$, where T_{W1}, T_{W2} indicate initial film temperature and hot-spot temperature, respectively.

(Kn) regime is obtained, which occurs at operation conditions of HAMR in nano-scale thin films, which also results in temperature slip. Thus, here the advantage of LBM formulation which is the capability to accurately account for the temperature slip at the boundaries and interfaces is fully utilized.

III. Results and Discussion

Validation of LBM and Comparison With Continuum Heat Transfer Models

As shown in Fig. 4, in the ballistic transport regime of high Kn, a highly non-equilibrium behavior occurs in the temperature evolution at the center of the hotspot. As can be seen from the transient profiles of the non-dimensionalized temperature, the peak value of the curve predicted by the Fourier equation under predicts the value compared to the LBM result by a factor of 10. This result is consistent with the observations made previously that the Fourier equation underestimates the maximum temperature substantially as the we move towards sub-continuum (high Kn) regime and cannot adequately capture the highest temperature levels present in sub-continuum energy transport.

The next step is to analyze the capability of the phonon LBM model to observe the complex temperature slip at the interface of two multilayered films when a hotspot in focused on one of the films similar to HAMR process in HDI. Since the velocities of the carriers are different on either side of the interface, there is a mismatch of the lattice sites at the interface and additional physics is required to treat it accurately. Also, since there is a considerable difference in the thermal properties of the adjacent films and the interface also introduces non uniformities in the structure, all the carriers become diffusively scattered at the interface. This results in the interfacial resistance to heat transfer across the boundaries of the two materials, and there exist a number of models focusing on accurately capturing the behavior of the heat carriers at these interfaces [5]. In this work we use the diffusive mismatch model for the carrier scattering at the interface. However, our LBM can be modified to include a wide range of interface boundary conditions, and a robust sensitivity analysis of the best interface heat transfer models will be performed in the future communications. Here, a transmission coefficient α is defined which represents the total fraction of energy transmitted across the interface as: $\alpha = c_{3-i}^{-2}/\sum_i c_i^{-2}$. Here c_i is the phonon group velocity on the side i of the interface.

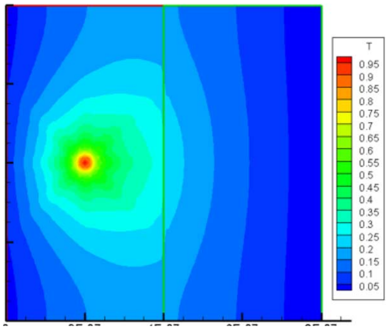

Fig. 5. Calculated non-dimensionalized temperature profile at the interface of two layers, with $P = 0.5$ and $\alpha = 0.5$.

Fig. 5 shows the temperature profile in a physically analogous system to HDI, consisting of an oxide layer attached to the silicon layer, with the hotspot focused on the latter. This double layer system clearly shows that the introduction of the interface not only introduces a temperature slip, shown as the broken isothermal contours at the interface, but also causes confinement of heat, illustrated by compression of contours near the interface.

Since the LBM successfully displays all the required physical phenomena occurring at sub-continuum scale heat transfer, it can now be applied accurately. In this regard, we introduce a novel graphene overcoat [6] whose exotic properties in its pristine form, including superior thermal conductivity and excellent mechanical response [7], will revolutionize many nano devices and potentially improve areal density in HDDs by as much as six times [8] by drastically reducing head media spacing. This is a significant improvement in HDD simply by reducing COC thickness alone. In addition, its properties also make it an ideal candidate for HAMR. Since molecular simulation methods such as non-equilibrium molecular dynamics are limited by the box size, LBM is more attractive in investigating full scale systems of graphene COC. In the next section, we describe a preliminary LBM scheme of analyzing the thermal response of graphene via in-plane and out of plane temperature distribution.

LBM for Graphene COC in HAMR

Due to high conductivity in graphene films, phonons have much higher group velocities and consequently much shorter re-

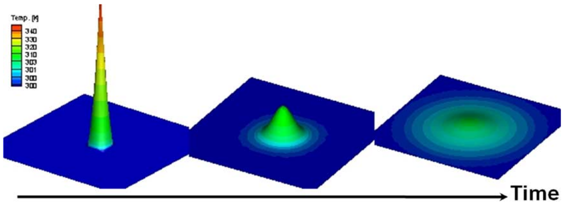

Fig. 6. Transient temperature variation for a single layered graphene sheet.

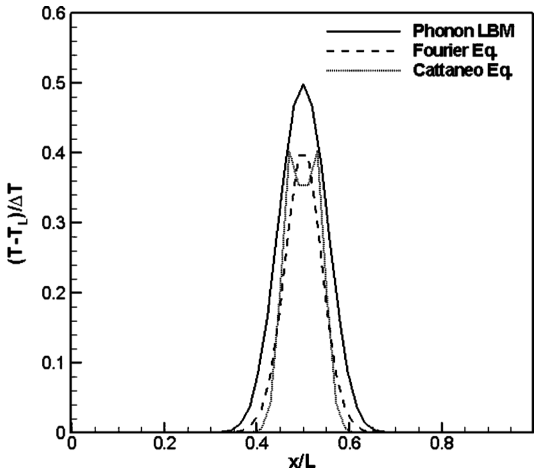

Fig. 7. Comparison of in-plane temperature profiles along the sheet via LBM, and Fourier and Cattaneo conduction equations, respectively.

laxation times between collisions. Thus, LBM is robust and accurate choice for thermal simulation in graphene. The graphene sheet we simulated was similar to Fig. 3, where the size of the sheet 2 nm × 2 nm and the conductivity, group velocity and relaxation time are 3 000 W/m-K, 24 000 m/s, and 33 ps, respectively and the hot spot was focused for 1 ns. The transient temperature distribution along a monolayered graphene sheet using LBM is given in Fig. 6, and our scheme accurately predicted the conductivity.

When compared with the steady state temperature distributions obtained from Fourier and Cattaneo conduction equations as shown in Fig. 7, our phonon LBM again displays higher temperature at the hotspot. The other approaches consistently under-predict the peak temperature at the center of the hotspot. Compared to the temperature profiles in silicon, we observe that the heat flux distributes much faster, resulting in a lower value of peak temperature at a much faster rate in the graphene sheet, thus, proving that graphene is valuable COC material for future HDI.

IV. CONCLUSION

In this study, we introduced a novel mesoscale level LBM to investigate the thermal properties in silicon nanoscale films, especially in HDI for HAMR with hotspots. Here, phonons are the dominant energy carriers. Our phonon LBM predicts the transient temperature at the hotspot better than Fourier conduction equation. In multilayered films, the efficient boundary and interface conditions makes LBM predict temperature slip accurately. We observe that hotspot in one domain interferes with the neighboring domains in a complex manner and the interfaces strongly affect the thermal profile of the system.

We then apply this methodology to the monolayer of novel graphene COC under a hotspot by analyzing in-plane heat transfer. The results show that the LBM is superior with other conduction models and predicts higher temperature at the center of hotspot and heat distributes much faster in graphene compared to silicon. Thus, our thermal model provides essential physics for the accurate thermal modeling of the complex data storage with multilayered thin films, thereby resulting in novel design criteria for thermal management in HAMR HDIs. Future extensions will be performed by incorporating electron carrier LBM schemes and realistic graphene sheets with defects (grain boundary) and integrated with LBM models for the remaining HDI components including media, lubricant layer, and air bearing for improved HDI design.

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