Rarefied gas heat transfer between a nanometric tip and a sample

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RAREFIED GAS HEAT TRANSFER BETWEEN A NANOMETRIC TIP AND A SAMPLE

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ABSTRACT

We study the heat transfer through air between a nanometric tip and a sample. Using a Monte-Carlo simulation, we show that heat flux densities reach 40 $MW.m^{-2}$ on the surface under the tip. The modeling shows a spatial resolution of 40 nm for a tip size of the same order. This proves the relevance of using quasi-ballistic conduction through air as heat transfer channel in applications such as thermally assisted data storage, scanning thermal microscopy and any temperature control techniques out of contact where a good heat localization is needed.

1. INTRODUCTION

Understanding the heat transfer between a hot tip and a substrate is a key issue in data storage [1], scanning thermal microscopy (SThM) [2][3] and any nanometer scale temperature control. It involves heat conduction at mechanical contact, in the water meniscus as well as in air [4]. For tip temperatures higher than 100°C, the water film contribution disappears and recent works prove that conduction in air becomes predominant [4][5] in comparison to the heat transfer through the constrictions of the mechanical contact. The tip-sample contact creates a high local flux density just below the tip but the air conduction over microns around the contact point [5] spreads the heat flux reducing the expected resolution.
The scanning thermal profiler invented by Williams and Wickramasinghe [2] consists in a hot tip at a nanometric distance of the sample. The size of the tips used in scanning thermal microscopy was quite large until now, as for instance the Wollaston wire tip, which is micrometric [3]. But now true nanometer-scale resolved heat sources are realistic [6]. As we will see, the heat flux transferred through air from the tip to the sample then depends on the sample temperature on a small nanoscale area.

2. GOAL

We will show that a 40 nm thermal probe can efficiently exchange heat with a sample with a spatial resolution on the order of 40 nm. Different methods as Joule [8] or Peltier heating [4] are possible to heat such a probe. The spatial resolution then depends on the heat spreading in air. The phenomenon cannot be modeled by classical Fourier diffusion because the air mean free path (MFP) is on the order of the average distance between the tip and the sample. It follows that the Fourier's law is not valid.
Pure ballistic transfer is neither valid because of the extension of the heat flux on the sample surface: this problem has to be solved in the intermediate regime. 3D effects have also to be included if we want to see the effects of heating a non-symmetric tip. We therefore use a Monte-Carlo approach associated with the linear response theory in order to directly solve space and time dependent problems.

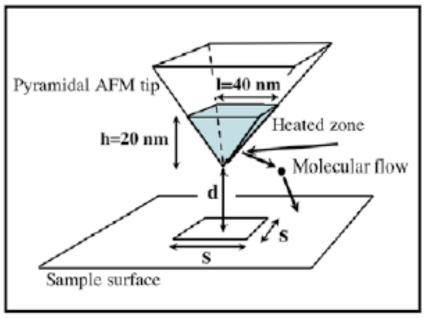

Figure 1. A skip of the tip. Typical lengths used are l=40 nm and h=20 nm. The distance d is in the nanometric range.

2. MODELING

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2.1. Geometry

We consider the extremity of a pyramidal AFM tip with a square base of l x l with l=40 nm and a height h=20 nm as shown by Figure 1. Heat confinement remains realistic since heat diffusion in the tip generates rapid temperature decay over a few tens of nanometers. Note that the use of specially designed materials such as insulators would be necessary. The distance d between the tip and the surface is in the nanometric range.

2.2. Linear response theory

The basis of our model consists in calculating the time evolution of the local heat flux on the sample $\left\langle q_{th}^{R}\left(r,t,T_{tip}\right)\right\rangle$ due to an impulse of molecular flux leaving the tip. The heat flux response $q_{th}^{R}\left(r,t,T_{tip}\right)$ to a given molecular flux excitation $q_{m}^{tip}\left(\tau\right)$ is then given by

$$q_{th}\left(r,t\right)=\int_{0}^{t}\left\langle q_{th}^{R}\left(r,t-\tau,T_{tip}\left(\tau\right)\right)\right\rangle \bullet S_{tip}q_{m}^{tip}\left(\tau\right)d\tau$$

where $\left\langle q_{th}^{R}\right\rangle$ can be assimilated to a susceptibility. S_{tip} is the area of the heated part of the tip. It is important to see that this model allows us to calculate the heat flux received by the sample when the tip temperature is modified. A realistic case where the tip temperature raises can as a consequence be simulated.

2.3. Kinetic Monte-Carlo approach

The susceptibility is computed using a Monte-Carlo approach. The heat transfer is due to air molecules, which are in first approximation nitrogen molecules. A molecule is considered to carry the translational and rotational energy $\frac{5}{2}k_{B}T$ where k_B is the Boltzmann's constant (reference [10]). Thus, we do not consider the degree of freedom due to internal vibrations of the diatomic molecule at our temperatures. A cold molecule is heated when impacting the hot tip and then flies with a velocity chosen according to a Boltzmann's law at T_{tip}. The emission laws for velocity v and direction described by the cylindrical angles θ and φ are derived from the equilibrium molecular flux leaving the probe at T_{tip}:

$$q_{m}^{tip}=n_{tip}\left(\frac{m}{2\pi k_{B}T_{tip}}\right)^{3/2}\int_{v=0}^{\infty}v^{3}e^{\frac{-mv^{2}}{2k_{B}T_{tip}}}dv$$
$$\times\int_{\theta=0}^{\pi/2}\cos\theta\sin\theta d\theta\int_{\varphi=0}^{2\pi}d\varphi$$

where m is the diatomic molecular mass. n_{tip} is the number of molecules per unit volume derived from the condition of null molecular flux at the tip surface.

2.4. Shock computation

The gas is at the ambient temperature T_a. We neglect the increase of T_a due to the presence of the tip. Thus, we consider that the incident molecules meet molecules coming from the sample surface at T_{sample} or molecules of the gas coming from a far area. Note that T_a is here equal to T_{sample}. A molecule leaving the tip flies until undergoing a collision with another molecule or with the sample surface. The path length between two collisions is computed according to an exponential law with a characteristic decay length given by the MFP

$$\Lambda=\frac{1}{\pi\sqrt{2}\left(2R_{pot}\right)^{2}n}$$

which is 55 nm at atmospheric pressure for nitrogen. R_{pot}=0.2075 nm [9] denotes its molecular radius.

The velocities of the collision partners are computed with Boltzmann's law taken at ambient temperature T_a. It allows us to define a new velocity and a new direction after the collision for the test-molecule according to the Very Hard Sphere model [9]. A molecule may undergo several collisions before it reaches the sample surface. Hot molecules that remain in the gas are discarded and the contribution of collision partners to the tip-sample heat flux is neglected. Finally, the thermal flux received by an element $\delta x.\delta y$ of the surface is:

$$\left\langle q_{th}^{R}\left(r,t,T_{tip}\right)\right\rangle=\frac{E\left(r,t\right)}{\delta x\delta y\delta tN}$$

where N is the number of emitted molecules and *E(r,t)* is the net energy transferred by the molecules emitted by the tip and falling in the area δx .δy during the time interval δt. Each molecule arrives with an energy determined by the Monte-Carlo simulation and leaves the sample area with the sample energy depending on T_{sample}. This energy is the one of a molecule in the air taken at equilibrium at temperature $T_{sample.}$. Thus:

$$E\left(r,t\right)=\sum_{i\in\delta x\delta y}\left[\frac{mv_{i}^{2}}{2}-2k_{B}T_{sample}\right]$$

where the index i denotes the incident molecules falling in the δx .δy area. We therefore assume in the calculations that the kinetic energy is fully absorbed at the air-sample interface. Those molecules are considered to leave the tip at the same initial time and the arrival time t is given by their flight time. The calculated susceptibility is a statistical average over N= 10^8 molecules. What is important to notice here is that the heat flux depends on the fixed sample surface T_{sample}.

3. RESULTS

Levels of heat flux on the sample depend on one hand on the tip-sample distance and on the other hand on heat losses during the molecules collisions. We have tried here to consider the consequences of these two different effects. As shown in Figure 2, the collisions are responsible for the loss of 70 % of the power of the pure ballistic case when the height *d* is equal to the mean free path of our simulation (near 60 nm).

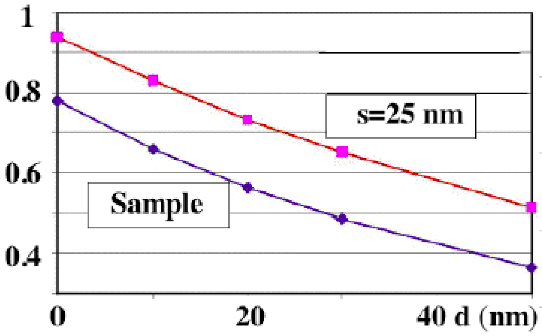

Figure 2. Full power on the sample normalized by the pure ballistic flux when the tip is retracted. This illustrates the decay of the flux due to collisions.

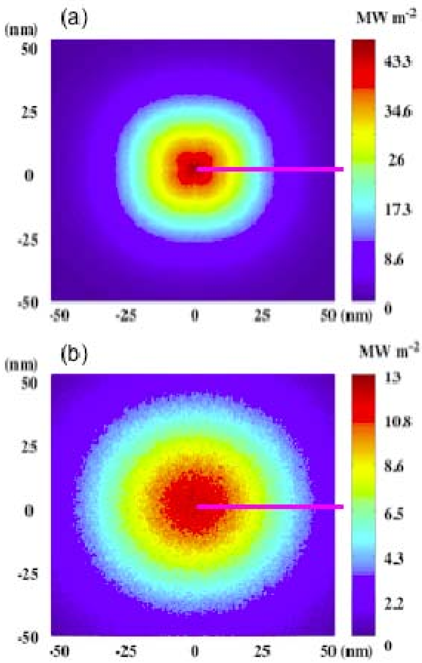

Figure 3. Heat flux density on the substrate.
(a) d=0 nm
(b) d=10 nm

Results for a tip temperature of 800 K and a sample at $T_{sample}=T_a=300$ K show that heat flux densities reach 40 MW.m^{-2} on the surface under the tip (see Figure 3). Taking into account that the energy is not completely fully absorbed [10] does not change the results significantly. The imprint of the tip geometry is lost on the heat flux mapping when the height *h* is higher then 10 nm (case (b)). The decrease of the heat flux density along a section is also less strong when the tip is retracting as shown on Figure 4. The results confirm a spatial resolution on the order of 35 nm when the tip is really close to the sample (insert of Figure 4). This spatial resolution is linked to the size of the hot part of the tip. It should be in consequence the best resolution that an SThM with such a tip could reach.

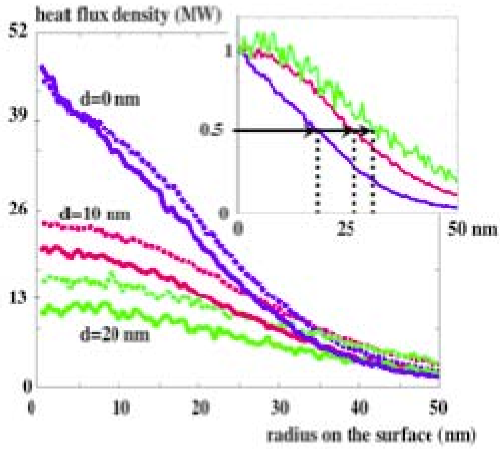

Figure 4. Heat flux density along the section shown in figure 3. Dashed lines show results when collisions are not taken into account. The inset shows the normalized heat flux density.

4. CONCLUSIONS

Finally, it seems that heat transfer through the air at distances on the order of 10 nm is sufficient to allow non-contact scanning thermal microscopy. We have found the relation between the heat flux transferred by a nanometer-scale hot tip and the temperature of the sample that it is thermally probing. A first step in the description of nanometer-scale resolved thermal probes has been achieved. The detection of hot spots in electronic devices would be surely improved if such probes were used.

5. ACKNOWLEDGEMENTS

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