Molecular Fan: A Heat Sink for Nanoelectronic Devices

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ABSTRACT

An innovative heat-dissipation surface containing active functional groups (CH, methyl, phenyl, and cyclohexyl) is designed to act as a molecular cooling fan, termed "molecular fan". Two different types of coatings are used to prepare molecular fan; the first is a thin (~ 1 μm) optically transparent sol-gel based coating; and the second is a 5-10 μm thick polymer emulsion. Use of this "molecular fan" coating on one-side of test panel lowers the equilibrium temperature of heat sinks by 5-12 ^{o}C. The efficiency of "molecular fan" coating is shown to depend on the active vibrational modes, heat sink substrates, coating adhesion and film thickness, and conductive property of coatings.

Keywords: molecular fan, nanocoating, molecular vibrations, heat sink, radiative cooling

1. INTRODUCTION

Currently, electrical components are cooled by conduction of heat to a heat sink, which is cooled by convection in air. The warm air is removed from the system using a mechanical fan. For future nanoelectronic (or optoelectronic) devices, simple convection and mechanical fan will not be able to keep up with the increased heat density. In molecular fan, the densely oriented molecular functional groups are prepared on the coated heat sink surface that absorbs the energy from heat source and leads to fast vibrations. The vibrating part of the molecule then effectively releases the heat via radiative/nonradiative processes, greatly reducing or eliminating the need for cooling by convection and mechanical fans.

All machines, including computers, produce heat that usually must be dissipated in order to prevent overheating. This heat usually comes from friction (in mechanical systems) or ohmic heating (in electronic systems). In electronic applications, excess heat reduces efficiency and can eventually cause total failure of the device [1]. As technology progresses and silicon chips have more components in a smaller area, the heat produced by the chips per volume will increase [2]. An innovative device and/or mechanism is critical for dissipating the heat and effectively lowering the temperature of the system.

There are three common mechanisms by which an object can release heat energy: conduction, convection, and radiation. The best way to draw heat away from a component is conduction, as is done in the regular heat-sink-and-fan arrangement. In convection, a hot region of a gas or liquid moves away from the source of heat. The hot fluid is replaced by cool fluid, which is then heated. In electronic instrument, such as computer, mechanical fans are positioned near these heat sinks to draw the warm air away from the heat sink by convection. This cyclical method of cooling is the common way for a modern machine to disperse heat [3-6].

There are several problems with the current heat release arrangement. One is that of the space required to add more fans. As the components become more powerful, they tend to release more heat and require more circulation to cool. Eventually the number of fans in the computer becomes cumbersome. Because of this, when the heat is to be transferred to the surroundings and away from the computer, convection is not the best solution. Another problem is present in miniaturization. As components, and therefore the computers and machines themselves, get smaller and smaller, they will have less room for fans while concentrating heat production into a smaller area [7-8]. This will result in a small center for a great deal of heat, and will require more efficient cooling than modern machines. Eventually machines would have fans as their largest components. Finally, mechanical fans create their own heat when they convert magnetic potential into kinetic energy. This amount of heat is small, and is almost immediately dispersed by the action of the fan itself. With many fans in a small area, however, this heat can actually cause an increase in temperature over time, reducing the rate of cooling of heat sinks and components.

Radiation is the best and most efficient way to transfer heat energy [9]. Conduction of heat away from the component to the surface of the coating is still necessary, whether by a heat sink or by simply coating the component itself. Once a coating molecule has absorbed the energy, it becomes excited and vibrates rapidly. This excess energy can be released by the emission of a photon of infrared light by the surface molecule. This process is more or less independent of many of the variables that limit the ability of mechanical fans to disperse heat, such as ambient temperature, air pressure and circulation, and humidity; however, good conditions will still benefit the molecular fan, since a portion of thermal energy will still be dispersed by convection.

In this paper, we describe the design of an innovative heat-dissipation surface that acts as a molecular cooling fan. The coated heat-sink surface is selected to display active CH, methyl, phenyl, and cyclohexyl functional groups

which are monitored by Raman spectroscopy. The cooling efficiency of molecular fan is investigated in relation to the active vibrational modes, heat sink substrates, coating adhesion and film thickness, and conductive property of coatings. The colored molecular fan is also fabricated and its cooling efficiency is also evaluated.

2. EXPERIMENTAL DESIGN

Two major types of coatings were investigated. One is a transparent, durable coating formed using sol-gel techniques. The other is an organic/inorganic hybrid coating formed using one of two organic aqueous emulsions, an acrylate and a urethane. The sol-gel coatings were formed using silanes, alcohols, water, and potentially, acid catalysts, rheological agents, and/or wetting agents. Formulation was similar to other sol-gel coatings that show good adhesion (surface bonding), hardness (crosslinking), and transparency. Sol-gels were made of 20 wt% silane (Aldrich, Gelest), 60 wt% ethanol, and 20 wt% water, with small amounts (1 wt% or less) of any other additives. Four different combinations of silane precursors were tested, all including 3-glycidoxypropyltrimethoxy silane at 15 wt% of the total formulation. Each of the four sol-gels also contained 5 wt% of one of the following: tetraethylorthosilicate ("TEOS", Aldrich), methyltrimethoxysilane ("MTMOS", Aldrich), phenyltriethoxysilane (Gelest), and cyclohexyltrimethoxysilane (Gelest). The dry film thickness of sol-gel coating is less than 1.0 m.

The organic/inorganic hybrid coatings were made using an organic aqueous emulsion in conjunction with water and a small amount of co-solvent to enhance drying/curing. The coating solution consisted of 22 wt% organic oligomers (acrylic/styrene or urethane, Alberdingk, NeoCryl), ~63 wt% water, and ~15 wt% propylene glycol butyl ether ("PnB", Aldrich). A wetting agent was added (less than 1 wt%) to improve the appearance of the coating by removing fisheyes and other defects. In some cases, other conductive particles such as carbon black (Akzo Nobel) or titanium oxide (Ishihara Sangyo Kaisha, Ltd.) were used in an attempt to increase the surface conductivity of the coating. Some color molecular fans of the urethane coating were also made by adding a very small amount (0.05 wt%) of pH indicators or fluorescent dye. Two dry film thicknesses of the organic/inorganic coatings were applied on aluminum, copper, and cold-rolled steel heat sink coupons: one is about 4.5-5.0 mm and the other is about 9.5-10.5 mm.

The main type of testing was done by measuring temperature as a function of time. An aluminum (or other metal alloy) block was cut to have the same cross-section area as our test substrates (panels). The substrate was placed on the aluminum block with good thermal contact between the block and the panel. The outer part (one-side only) of the panel had been previously coated with the coating to be tested. A very small part (about 4 cm^2) of the coated side was left uncoated so that a temperature transducer could be placed, in good thermal contact, on the panel. The potential of the transducer was measured with a multi-meter that was interfaced with a PC to record data. To account for potential problems with ambient temperature fluctuation, an uncoated control panel was run every day that coated panels were measured. The surface vibrations of molecular fan were characterized by a microfocus Renishaw laser Raman imaging microscope.

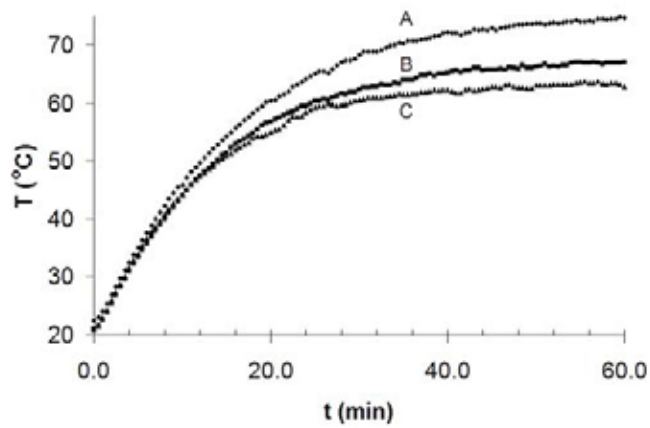

Figure 1. Cooling temperature vs, time of molecular fan made of AE coating with and without conductive carbon black

3. RESULTS AND DISCUSSION

Most of the molecular fan coatings showed the ability to cool heat sink (aluminum, copper, steel, or plastic) substrates, with a cooling temperature ΔT = 7-12 ^oC for a

Table 1. Molecular fan based on acrylic emulsion (AE),urethane emulsion (UE), and sol-gel (SL) coatings.

ΔT in ^oC				
	AE		AE with conductive carbon black	
	4.5 – 5.0 μm	9.5-10.0 μm	4.5 μm	10.0-10.5μm
Al coupon	6.6	7.3	7.5	11.1
Cu coupon	-	-	9.6	-
Steel coupon	-	-	11.8	11.8
UE on Al coupon (dry film thickness, DFT = 4.5 – 5.0 μm)				
UE transparent (clear fan)				7.7
UE with conductive TiO_2 (silver-white fan)				9.4
UE with aniline green (blue-green fan)				8.3
UE with fluorescein (light green fan)				8.1
UE with methyl red (orange red fan)				7.1
UE with bromomethyl blue (yellow fan)				7.8
UE with rhodamine B (pink fan)				6.7
SL on Al coupon (transparent, DFT less than 1.0 μm)				
Tetraethylorthosilicate				7.5
Methyltrimethoxysilane				4.8
Phenyltriethoxysilane				4.0
Cyclohexyltrimethoxysilane				4.0

single-side coating. Figure 1 shows the results of two of these coatings, acrylic emulsion formulations with and without conductive carbon black nanoparticles. Curve 1A shows the temperature as time progresses of a bare aluminum panel. It heats up from room temperature rapidly for the first twenty minutes and then begins to stabilize as the panel equilibrates with its surroundings, the equilibrated temperature is 74.5 ^{o}C. Curve 1B shows the same experiment with a heat-sink panel that was coated with a 9.5-10.0 mm thin layer of acrylate-based molecular fan with no conductive carbon black. It follows the same general pattern, but equilibrates at a temperature of 67.2 ^{o}C that is 7.3 ^{o}C cooler than that of the uncoated panel. Curve 1C shows the results of one of the best molecular fan coatings, an acrylate-based film of 10.0-10.5 mm thick with a small amount of added conductive carbon black. The coating equilibrates at a temperature of 63.4 ^{o}C which is 11.1 ^{o}C cooler than the uncoated aluminum control (curve 1A). It is suggested that a conductive molecular fan gives higher cooling efficiency of heat sink.

The results of the cooling experiments for molecular fan based on acrylic emulsion (AE), urethane emulsion (UE), and sol-gel (SL) coatings are summarized in Table 1; the numbers (ΔT in ^{o}C) are the differences between the "average equilibrium temperature" (average of last ten temperatures measured) of the molecular fan sample and the bare aluminum control. The top portion of Table 1 is the results for AE molecular fan, the cooling efficiency is enhanced for coating with conductive carbon black as also show in Figure 1. There is a slight enhancement in cooling efficiency for AE coating on steel and copper coupons as compared to aluminum coupon. The middle portion of Table 1 shows the results for UE molecular fan. Similar to AE molecular fan, UE coating with conductive TiO_2 particles gives a higher cooling efficiency than that of UE transparent clear fan. The molecular fan made of UE coating and organic dyes (aniline green, fluorescein, methyl red, bromomethyl blue, and rhodamine B) gives a bright color coating and good cooling efficiency. The bottom portion of Table 1 gives the results of sol-gel molecular fan. The coating is less than 1 mm thick and optically transparent. The cooling efficiency is sensitive to the molecular functional groups, following the order CH > CH_3 > phenyl ≈ cyclohexyl. The lighter functional group can vibrate faster upon heating, thus provides a higher efficiency radiative cooling.

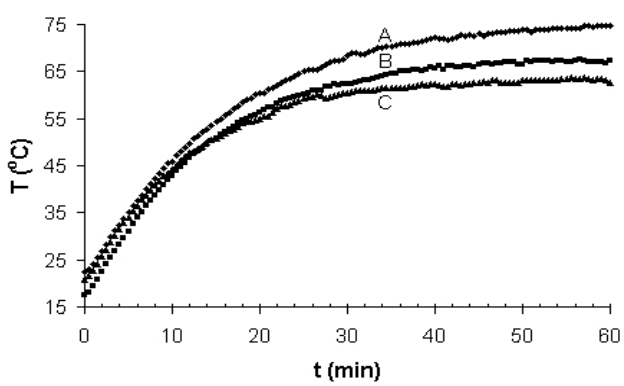

Figure 2. Cooling temperature vs. time of molecular fan for two thickness of AE coating with and without conductive carbon black.

In almost all cases, the thinner coatings showed less cooling than their thicker counterparts, as can be seen in Figure 2. Curve 2A shows the temperature as time progresses of a bare aluminum panel, with an equilibrated temperature at 74.5 ^{o}C. Curves 2B and 2C are molecular fan made of two film thickness of AE coating with conductive carbon black particles, where curve 2B is 4.5 mm and curve 2C is 10.0-10.5 mm thick. We believe that the thicker coatings offer better coverage of the substrate, filling the microscopic pores that a thinner film might leave and increasing the amount of fans available to dissipate heat.

The intention of using organofunctionalized silanes was to introduce groups with different vibrational frequencies into the coating to increase infrared emission, thereby releasing more energy over time and increasing cooling power. The radiative cooling (ΔT) is 7.5 ^{o}C for tetraethylorthosilicate coating, 4.8 ^{o}C for methyltrimethoxylsilane, and 4.0 ^{o}C for both phenyltriethoxysilane and cyclohexyltrimethoxysilane coatings. The Raman spectra of four sol-gel coatings are displayed in the bottom portion of Figure 3. The most intense (Raman active) vibrations are the carbon-hydrogen

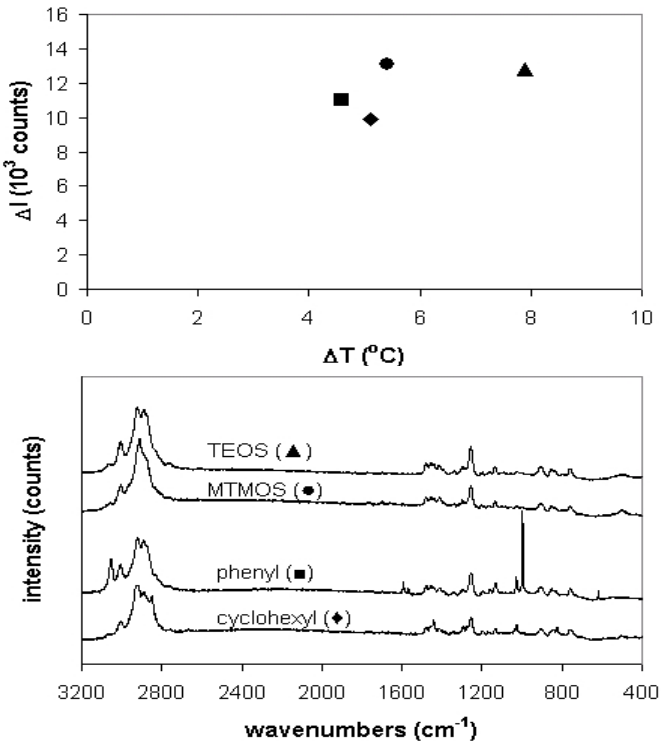

Figure 3. Four sol-gel fans with different molecular functional groups: Top – Raman intensity of CH vibrational mode vs. cooling temperature; Bottom: Raman spectra

stretches at 2930, and 2890 cm^{-1}. The top portion of Figure 3 is a plot of the integrated Raman intensity in the spectral range of 2930-2890 cm^{-1} vs. cooling efficiency (ΔT in ^oC) for four sol-gel molecular fans. The correlation is good that the lighter functional group has a higher efficiency radiative cooling

4. CONCLUSIONS

A set of molecular fan has been fabricated by using acrylic emulsion, urethane emulsion, and sol-gel coatings. The molecular fan has a coating layer of less than 1 mm or thicker layer 10 mm, and can be an optical transparent layer, a conductive black layer, a conductive silver-white layer or a bright color layer. With only single-side coating, the cooling efficiency of molecular fan is excellent at ΔT = 10-12 ^oC. The molecular fan can be fabricated on metal (such as aluminum, copper, steel, etc) and plastic (such as PC, PMMA, PET, etc.). The molecular fan with a lighter functional group gives a higher efficiency radiative cooling, due to a faster vibration upon heating.

5. REFERENCES

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