

Nanotechnology and mathematical methods for high-performance thermal interface materials

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Higher power chips have resulted from a variety of new developments in the electronics industry. While these state-of-the-art devices offer the benefit of more power, more heat is typically produced. Using a dense particle packing theory, a variety of thermal management materials have been introduced to the marketplace that exceed the performance of current commercially available greases, gels and adhesives to meet the new heat requirements. As compared to more traditional empirical scattershot approaches, this new method uses a mathematical tool to optimize formulations. The result of integrating this theory has not only helped produce new thermal materials, but it has dramatically reduced developmental time.

Thermal Interface Materials, Nanotechnology, Thermal Management, Automotive Thermal Management, Bi-Modal Filler Systems, Filler Packing, Viscosity Optimization

Advances in the manufacture of silicon devices for the automotive industry have resulted in electronics with reduced feature size and higher operating speeds. While these attributes are beneficial, these new developments have resulted in increased power densities. As chips are running at these break-through power levels, the heat produced dramatically increases and it must be removed in order to ensure operating efficiency or prevent thermal destruction of the component¹⁻⁴. The automotive industry is strongly affected because of the demand by consumers for more and more components, as well as improved safety, all in smaller tightly defined areas. In addition, the automotive industry requires materials and components that survive harsher environments at higher temperatures. High performance thermal interface materials (TIM) have proven to be a solution for the transmission of heat from the silicon die to the heat sink in high power applications by connecting the silicon die and heat sink (and/or lid) using the TIM. But, in addition to transferring heat, TIMs must possess the appropriate mechanical, adhesive and rheological properties to ensure reliability of the device², which can be particularly challenging in places such as in the transmission or exhaust gas recirculation systems. A new theoretical approach that takes advantage of nanoparticle technology has proven successful in the creation of TIMs that possess the right combination of properties that are required for state-of-the-art devices in automotive and other applications.

The basics

The role of a thermally conductive material is to transmit heat generated from an integrated circuit away from the device. However, it is not enough for the heat to simply be moved from the surface of the die to a larger surface area. Rather, this heat must be moved out

of the package. In automotive applications (Figure 1), especially ones where the components are in a harsh environment, the thermal material must be stable to these high temperature conditions while still performing its function. Figure 2 shows a schematic diagram of the stack of parts typically used in a high power flip chip device.

The type and loading of the fillers in the polymer matrix also impact the thermal conductivity in TIMs since polymers often have very low thermal conductivity. Recognizing this to be true and in order to optimize thermal conductivity, the loading of these filler particles must be as high as possible. These juxtaposing factors create the challenge of maintaining low dispense viscosities despite the higher filler loadings.



Figure 1. Automotive electronics example.

Mathematical theory

An empirical, time-intensive approach is typically used for the development of TIMs. In such a scenario, fillers of different types, sizes and shapes are blended with resins at various ratios until a formulation is made that has the highest thermal conductivity (TC), while retaining the necessary rheological properties. In order to increase thermal conductivity, filler loading is typically increased.

Unfortunately, the trade-off here is an increase in formulation viscosity. For example, in order to develop a TIM for a power converter module, an exercise in balancing the properties of viscosity, filler selection and filler loading would occur. As one might imagine, this exhaustive approach often leads to longer than expected development cycles. Using mathematically developed formulations in tandem with nanoparticle technology as a starting point for the material development process, however, can dramatically reduce overall developmental time. The addition of nanoparticle technology to the blend predicted by optimal packing theory allows us to reach very high filler loadings while retaining low viscosity. Recent developments by LORD Corporation—a leading supplier of thermal management materials, adhesives, coatings and encapsulants—have proven the viability of using theoretical approaches in concert with nanotechnology to speed the development of new materials in the laboratory⁵.

The advantage of adding nanoparticles to thermal materials to increased filler loading is typically offset by the dramatic increase in viscosity. This is because of the large increase in the surface area due to the nanoparticles. The relative amounts of fillers can be determined using previously calculated ratios that help determine the lowest viscosity at a given loading⁶. Such an approach reduces the number of experiments needed and also limits the risk of missing the global minimum for viscosity.

Low viscosity at relatively high filler loadings is an ideal starting point for new material development. For example, LORD used the semi-empirical theory for dense particle mixtures⁶ to develop highly conductive TIMs possessing excellent rheology for insulated-gate bipolar transistor (IGBT) baseplates. In order to demonstrate the validity of the mathematical method, three types of TIM materials—all of which showed excellent thermal and material properties—were evaluated. The properties of the four example materials, two greases, one gel and one adhesive are listed in Table 1.

Determining the proper filler ratio is the first step to improving packing. The importance of mathematically calculated

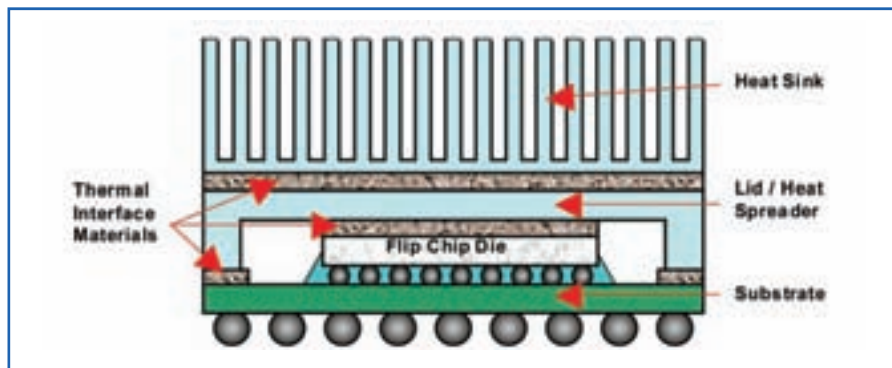


Figure 2. Chip module showing location of thermal interface materials.

TIM	Type	TC (W/mK)	Viscosity (cP)	Density (g/cc)
A-1	Grease	5.2	212,000	2.9
A-2	Grease	6.0	248,000	2.9
B-1	Gel	3.5	128,000	2.7
C-1	Adhesive	2.4	60,000	3.1

Table 1. Properties of newly developed, high thermal conductivity TIM materials.

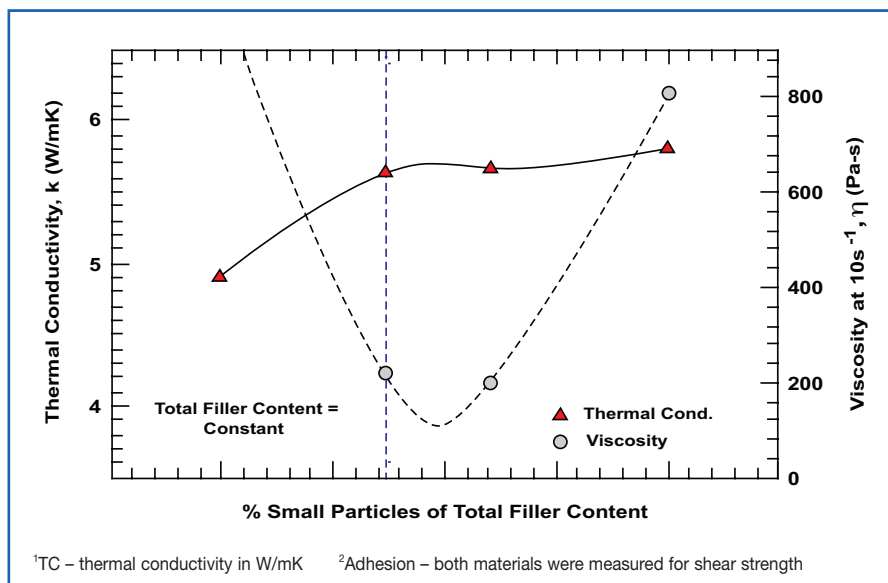


Figure 3. Plot shows a minimum in viscosity of a high thermal conductivity material demonstrating the importance of mathematically derived optimal packing levels. Open circles show experimental viscosity data and the dotted line shows mathematical calculations. The vertical dotted line represents the mathematically calculated viscosity minimum.

optimal packing levels is demonstrated in the plot in Figure 2, which shows the minimum in viscosity at high thermal conductivity. Interestingly, the calculated minimum is very close to the empirically measured minimum viscosity. Although there are differences in the values—likely caused by the fact that actual formulations containing fillers have particle size distributions and the mathematical calculations assume a mono-disperse filler particle size—the theory is able to closely predict the expected minimum viscosity because of the optimal filler packing.

Although it is possible that conventional methods would have resulted in determining the right combination of fillers with minimal viscosity, mathematical modeling allowed for a close approximation of the minimum before laboratory work, resulting in shorter development time for new materials.

Once the mathematical best packing ratio of nano- and micron-sized filler particles is obtained (as in the example in Figure 3), additives and processing technology can then be used to optimize other variables. The four sample materials discussed below, greases A-1

and A-2, gel B-1, and adhesive C-1, were all developed with the aid of the packing theory.

Thermal materials

Thermal greases are an important class of TIMs. They are used in a variety of applications, including IGBT base modules, electric car power converter modules, and engine control modules, because of extremely low thermal resistance and reworkability. The two greases derived with the aid of the mathematical theory were compared to a known thermal grease developed in the traditional manner.

Table 2 lists selected properties for three different thermal interface greases. The A-3 grease—which has a similar viscosity to A-2 but slightly higher viscosity than A-1—was developed over months in the laboratory using traditional methods. In contrast, using the mathematical theory, LORD was able to develop improved thermal conductivity materials such as A-1 and A-2 with lower viscosities in weeks. This new method, combined with proprietary additive and processing technology, led to dramatic reductions in the amount of time needed to deliver new customized formulations. Further, since the mathematical calculations can be used to determine filler ratios at any total filler loading, the A-2 grease, which has substantially higher total filler loading than the A-1, could be developed using this proprietary method to achieve lower viscosity despite the increased loading. This allows for materials with workable viscosities at extremely high loadings, without the need for solvent addition to allow syringe dispensing.

One obvious concern relates to whether or not material properties are sacrificed in the process despite the speed at which formulations are developed. To ascertain the validity of using the mathematical model, the thermal greases were tested in a humidity chamber at 85°C and 85 percent relative humidity. Figure 3 shows X-ray photographs of 12.6 mm x 12.6 mm TIM sandwiches. After 150 hours, the A-1 material showed no change. A visual inspection using an X-ray revealed that the surface was quite smooth and no voiding or cracking was apparent. The A-2 grease also showed no changes after the humidity testing, validating that the A-2 grease is also a robust material.

Stencil printability was also tested, and the A-1 material was found to stencil print well at various thicknesses. As can be seen in Figure 4, this material shows very clean edges and adhesion to the printing surface for this sample board.

A second area of interest is thermal gels, which are often used in applications in which low thermal resistance is required and

TIM	TC ¹	Viscosity (cP)	Density (g/cc)	BLT ²
A-1	5.2	212,000	2.9	25
A-2	6.0	248,000	2.9	45
A-3	4	250,000	2.8	50

¹ TC - thermal conductivity in W/mK ² BLT – thinnest measured bondline thickness in microns

Table 2. Comparison of mathematically derived thermal greases (A-1 and A-2) to material developed using traditional methods (A-3).

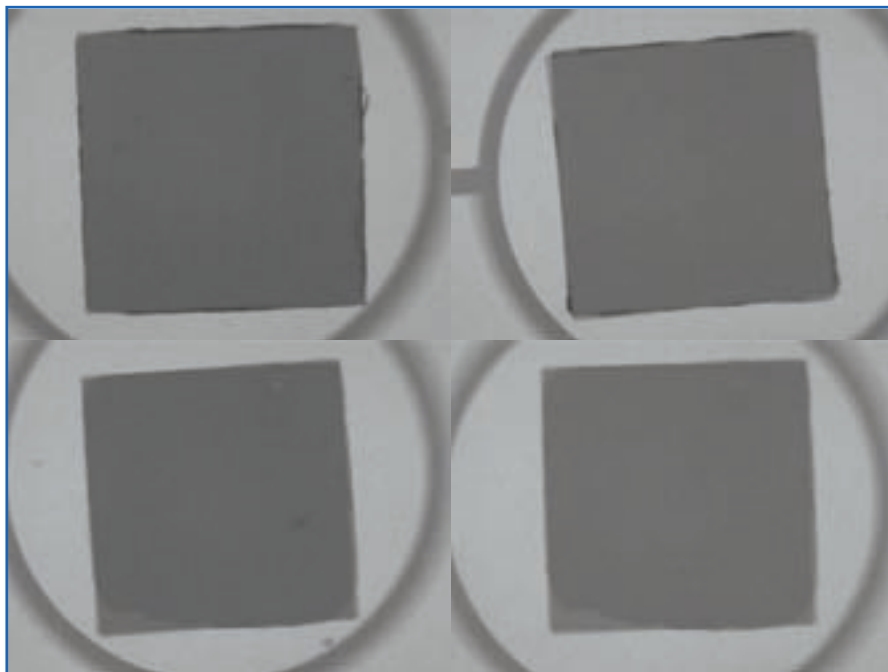


Figure 4. X-ray images after humidity testing of A-1 and A-2. The images (a) and (c) are from before starting the test (i.e. t=0 hrs) and (b) and (d) are of after 150 hrs.

material movement due to either pump-out or separation would cause problems. Typically, gels are a lightly cross-linked system that retain quite low modulus, which allows for rework. Table 3 lists select properties of two thermal gel materials. The B-2 formulation allows for both increased thermal conductivity as well as reduced modulus. In many cases, reducing the modulus can reduce stress-induced delamination that rigid TIM materials can cause. Once again, the use of mathematical theory helps speed the process as global minima can be discovered in weeks rather than the months required via empirical testing.

Thermal gel formulations, as with other TIMs, are typically developed with higher filler loading in order to achieve the high thermal conductivity necessary for high power applications. However, such high filler loadings may result in increased viscosity and/or higher modulus. The TIM B-1 (Table 3), a thermal gel developed in a more traditional manner over the course of months, has a modulus of 350 KPa. In contrast, the new material B-2 has a measured modulus that is an order of magnitude lower, despite the



Figure 5. Demonstration of stencil printability of A-1 onto FR4 board.

additional filler loading. Mathematical modeling was used to optimize filler ratios in order to reduce viscosity. Then, proprietary chemical and processing technology was employed to dramatically reduce the modulus. The implementation of this technology has led to the new thermal gel, B-2, which shows both higher bulk TC and lower modulus. Once again, while the B-2 formulation could have been developed using traditional methods, the use of the mathematical method

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TIM	TC ¹	Viscosity (cP)	Modulus (KPa)	BLT ²
B-1	2.3	144,000	350	50
B-2	3.5	128,000	10	25

¹ TC - thermal conductivity in W/mK ² BLT - thinnest measured bondline thickness in microns

Table 3. Comparison of mathematically derived thermal gel (B-1) to material developed using traditional methods (B-2).

TIM	TC ¹	Viscosity (cP)	Density (g/cc)	Adhesion (MPa) ²
C-1	2.4	60,000	3.1	19.6
C-2	1.7	65,000	2.6	2.1

¹ TC - thermal conductivity in W/mK ² BLT - thinnest measured bondline thickness in microns

Table 4. Comparison of mathematically derived thermal adhesives (C-1) to material developed using traditional methods (C-2).

allowed for the development of this material in weeks rather than months. This material property improvement was achieved by mathematically calculating the new local (or global) minimum for viscosity, achieved by ideal packing, to dramatically reduce the number of experiments that were necessary.

Since thermal gels can also be used in stencil printing applications, B-2 was printed using a stencil mask with an aperture of approximately 50 microns. As can be observed in *Figure 4*, this material adheres well to a FR4 board surface. Tests performed on various lead frames show excellent adhesion and stencil printability as well.

For thermal adhesives, increased filler loadings usually lead to a reduction in adhesive properties. With this mathematical method, new adhesive formulations with lower viscosities can be developed to which newer resins and additives can be added. This can lead to higher thermally conductive thermal adhesives with improved adhesion (*Table 4*).

Summary and conclusions

The development of new electronic packages that are running at ever-increasing speeds and at increased power levels is driving the development of new thermal interface material. The heat produced by these packages requires thermal interface materials with improved thermal conductivity while retaining rheological and other properties. Key to success for the automotive and electronics industry is the rapid development of new materials to meet this need. One proven solution is the use of proprietary mathematical methods, used in concert with nanotechnology, chemical and processing technology for the development of thermal interface materials with improved properties to meet the requirements of the next generation of electronic packages and power modules.

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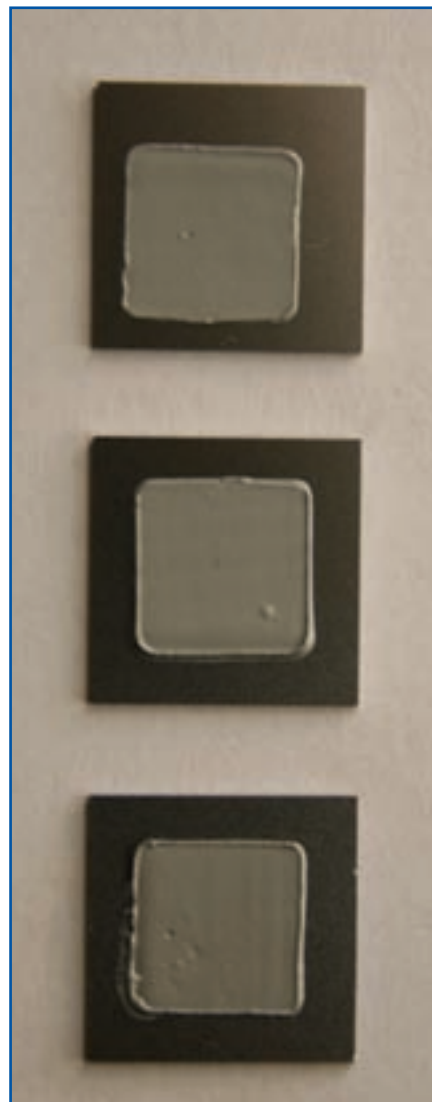


Figure 6. Sample images of B-2 thermal gel stencil printed onto FR4 board. The bondline thickness is approximately 50 microns.

SEMI-THERM Symposium, San Jose, CA, 2001, pp 64-71

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