Materials Selection for a Heat Sink

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Summary

This case study is designed to tackle the heat dissipation problems of multifarious microchip-based appliances by choosing and suggesting optimal materials for heat sinks.

A systematic material selection methodology has been applied through Ansys Granta EduPack and Ansys Granta Research Selector to visualize material properties and to select a proper material candidate for a heat sink with multiple software tools.

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1. Microchip heat dissipation challenges in multifarious microchip-based appliances

Since the invention of hybrid Integrated Circuits (ICs) by Jack S. Kilby in 1959 [1], modern ICs or microchips have become ubiquitous across different industries and within our daily lives. State-of-the-art microchips are at the heart of a microprocessor or multi-core processor and control everything from digital microwave ovens to cell phones to high-performance computers. In a word, modern computing, communication, manufacturing, and transportation systems all depend on the existence of microchips.

Over the years, microchips have continued to evolve and allow more circuits to be packaged per chip. This increases the capacity per unit area, which leads to reduced costs and increased functionalities. As a result, electronic components used in modern day electronics are becoming smaller, thinner, faster, lighter and more powerful [2].

However, opportunities and challenges always come hand in hand: due to the integration of the larger number of transistors into a single unit, heat dissipation becomes a significant issue when applying microchips into varied applications. Microchips only consume milliwatts of power, but due to their minuscule dimensions, the power-density is high enough to generate adequate heat energy to put the whole system at risk if not well controlled. Consequently, as microchips shrink and processing speeds grow, heat dissipation in multifarious microchip-based appliances becomes a problem [3].

2. How to tackle this heat dissipation problem?

The use of heat sinks has become one of the viable alternatives for heat control of the electronic devices. A heat sink (Figure 1), which is a passive heat exchanger, transfers the heat generated by an electronic device to via some coolant, usually air. In this way, the generated heat is dissipated away from the device, thereby avoiding overheating and failure of the device [2].

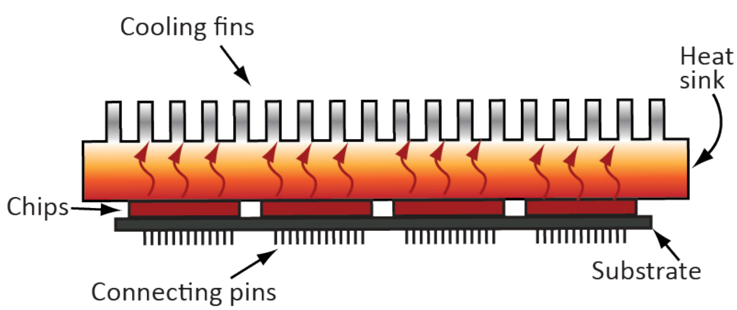

Figure 1: An illustration of a heat sink for an electronic device [3]

The performance of a heat sink is affected by air velocity, choice of material, protrusion design, and surface treatment [4]. One can conduct a thermal analysis of the heat sink in a device for to investigate the impact of the air velocity, protrusion design, and surface treatment using both simulation and experimental techniques Choosing a material that maximizes the performance of the heat sink is an essential prerequisite.

A stable heat sink absorbs more heat energy without shifting towards a high temperature, therefore materials with high heat capacity will be targeted. Since the purpose of a heat sink is to move heat away from the microchips as fast as possible, materials with high thermal conductivity are considered. In addition, materials that have a thermal expansion coefficient close to that of the microchip itself are desired, otherwise thermal stress caused by relative expansion will damage the electronics. The heat sink must also be a good electrical insulator with high electrical resistivity to prevent electrical coupling and stray capacitance between the microchip and the heat sink. Weight is considered, for example, in advanced aerospace appliances using microchips, light weighting is counted as one of the key design goals. Although cost is not a primary consideration for high-end applications of the microchips, it cannot be overlooked entirely and will bring economic perspectives in finalizing the promising candidates.

All these parameters have a combined influence on how effective a heat sink can drain heat away from microchips, which can be translated into measurable material property combinations.

Assuming the microchip operates continuously and the finned face of the heat sink is cooled by a fan or by water-cooling which keeps its temperature at T_0. The power which is drained from the microchip can be estimated by:

$$Q = A\lambda\frac{\Delta T}{X} \tag{1}$$

where *A* is the contact area between the microchip and the heat sink, *λ* is the thermal conductivity of the heat sink and it is assumed to be constant, *ΔT* represents the temperature difference across the heat sink with *X* as the heat sink thickness. Since the rate of heat transfer is directly proportional to the area of contact, a large chip will require a large heat sink. The total area of microchip contact can be described as:

$$CA \tag{2}$$

where *C* is a constant. Therefore, the mass of the sink, *m*, is given as:

$$m = CAX\rho \tag{3}$$

where *ρ* is the density of the sink material. Combining equations (1) and (3), the power drained per unit weight is thus:

$$\frac{Q}{m} = \frac{\Delta T}{CX^2}\left[\frac{\lambda}{\rho}\right] \tag{4}$$

Considering the thermal expansion difference between the microchip and the heat sink, *Δε*, it must be kept below the damaging value *Δε**:

$$\Delta\varepsilon = \Delta\alpha\Delta T \leq \Delta\varepsilon^* \tag{5}$$

where *Δα* is the difference in coefficient of thermal expansion between sink and microchip.
Using equation (5) to eliminate ΔT in equation (4) gives:

$$\frac{Q}{m} = \frac{\Delta\varepsilon^*}{CX^2}\left[\frac{\lambda}{\rho\Delta\alpha}\right] \tag{6}$$

A combination of material properties including the difference in thermal expansion coefficient, density and the thermal conductivity is derived as:

$$\boxed{\boldsymbol{M_1} = \frac{\lambda}{\rho\Delta\alpha}} \tag{7}$$

$\mathbf{M_1}$ can be used to measure material performance in heat sink, by maximizing this group of material properties, candidates with maximized performance will be found.

3. What can Ansys selection software do to select a proper material for a heat sink?

Ansys Granta EduPack and Ansys Granta Research Selector will be used to conduct materials selection for a heat sink. Both tools follow the rational materials selection methodology by Ashby *et al.* [3], illustrated schematically in the diagram below.

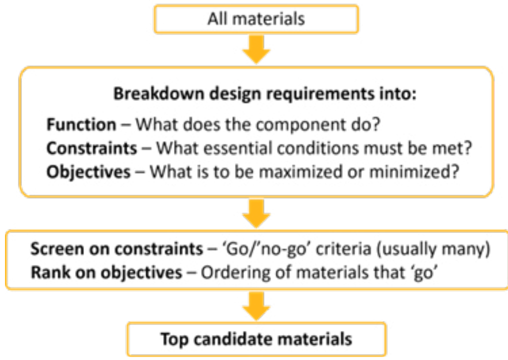

Figure 2: Systematic Materials Selection Methodology - a rational strategy for materials selection

To fulfill the function of a heat sink to regulate the microchip temperature, our key objective is to maximize heat flux per unit weight and it would be ideal if the material could be light and at a reasonable cost. As a result, the following constraints are considered in the case study:

a. A good insulator with high electrical resistivity, $\rho_e \geq 1018$ µΩ.cm
b. Maximum service temperature higher than 150 °C
c. Good thermal conductivity larger than 20 W/m.K
d. Similar thermal expansion relative to silicon, the common material for microchips (*i.e.* $\Delta\alpha \leq 10$ μstrain/°C)
e. All design dimensions are specified

Utilizing our performance index M_1 (Eq. 7), a chart (Figure 3) with λ/ρ on y-axis and α on x-axis can be plotted in Ansys Granta EduPack to visualize materials properties to conduct materials selection. In this case study, Level 3 database in MaterialUniverse is used and the selection is started by clicking Chart/Select in the main toolbar choosing 'All bulk materials' subset. This results in an initial subset of more than 3000 grades of engineering materials in various materials families. The combined material properties, λ/ρ, can be added through the advanced option in the Chart/Index Stage.

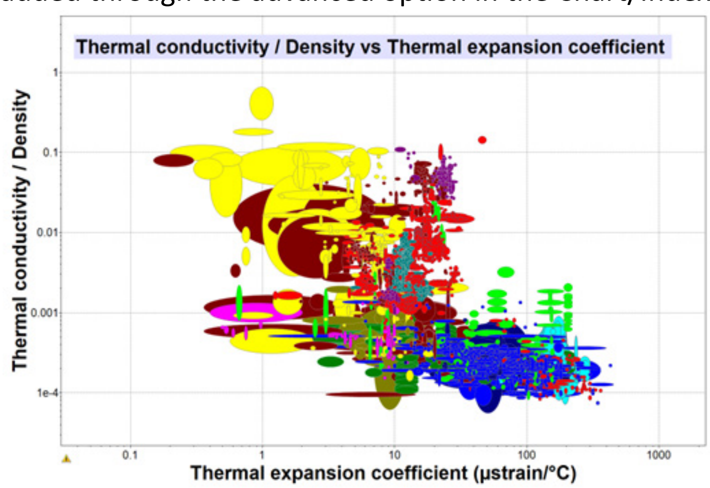

Figure 3: Chart of thermal conductivity per unit weight, λ/ρ, against thermal expansion coefficient α, with 'All bulk materials' subset

Continuing to apply other constraints, first of all, when comparing with microchip made from silicon, materials with a thermal expansion coefficient difference less than 10 µstrain/°C are targeted. In the material data sheet of silicon, as shown in Figure 4, silicon has a thermal expansion coefficient around 2.53 µstrain/°C.

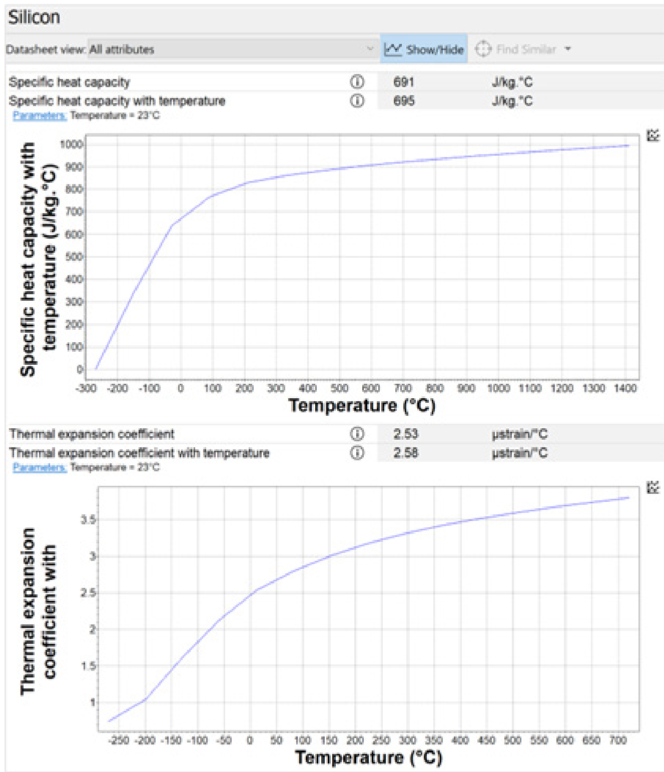

Figure 4: Excerpt from Silicon material record in Level 3 database

Therefore, materials with a thermal expansion coefficient between -7.47 and 12.53 (in reality, this means from 0 to 12.53) will be our target. Labeling silicon in Figure 3, a box selection tool is used to screen some materials out. At the same time, the failed materials grayed out, as shown in Figure 5, which leaves over 1200 materials before applying other constraints.

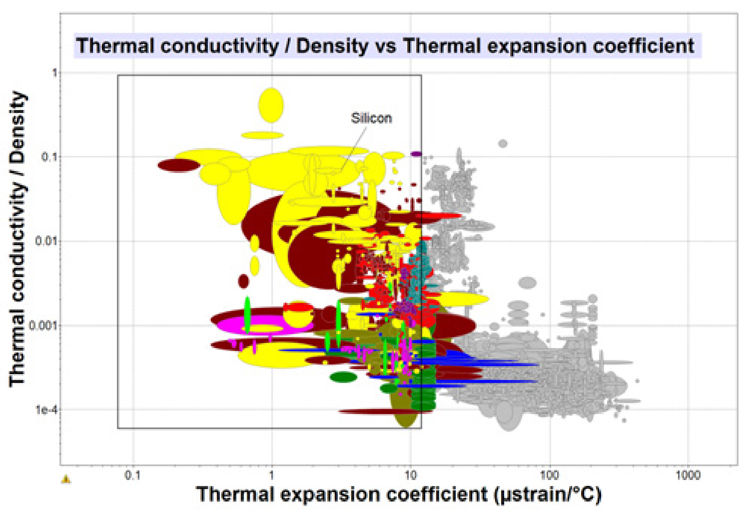

Figure 5: Materials with a thermal expansion coefficient difference less than 10 µstrain/°C when comparing with microchips made from silicon

Another way to achieve this is using the Limit Stage, under Thermal properties, find 'Thermal expansion coefficient', fill in with 0 and 12.53 under Minimum and Maximum, respectively.

Repeat this process for the other constraints – 'Maximum service temperature' and 'Thermal conductivity' under Thermal properties and 'Electrical resistivity' under Electrical properties with values shown in Figure 6.

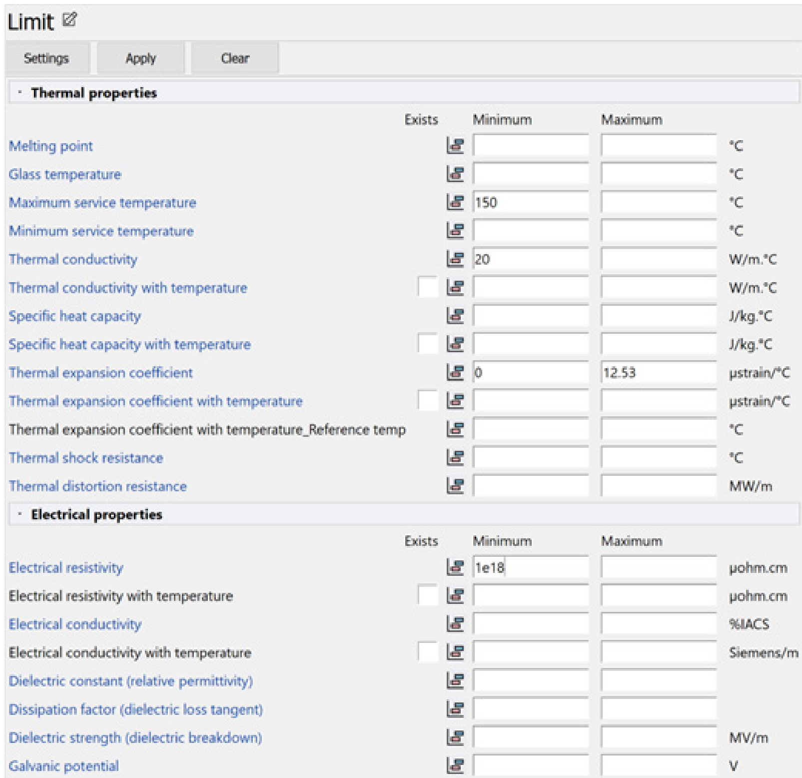

Figure 6 Applying all the constraints at the Limit Stage to find the material candidates for a heat sink

After applying, the number of the remaining candidates is reduced to 52, which is reflected in the chart with λ/ρ against α in Figure 7.

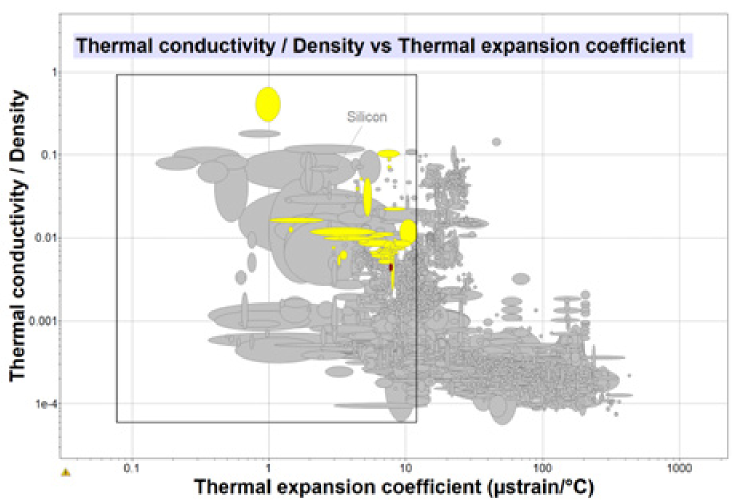

Figure 7: 52 material candidates left for a heat sink after applying all the constraints

Granta EduPack can be used to rank all these candidates by all the properties or properties combinations used in the materials selection as well. Taking 'Rank by Thermal conductivity' as an example, the Results panel will return with top candidates, such as diamond, beryllia, aluminum nitride, magnesia, boron nitride, silicon nitride, sapphire and alumina.

Another chart with Price against Density is created to gain extra insights to find the best candidates for a heat sink. In this chart shown in Figure 8, noting that it highlights all the 52 candidates only by hiding all the failed materials, we can see that diamond and sapphire are probably not practical for the reasons of their costs. While at the same time, compounds of beryllium are toxic, therefore, beryllia are not desirable candidates either.

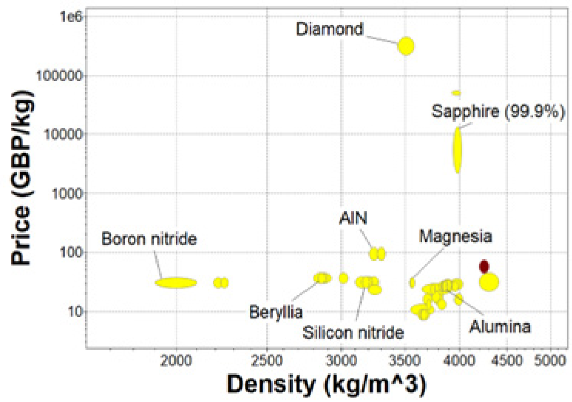

Figure 8 Price against Density with all 52 material candidates for a heat sink

Until this point, with Granta EduPack, aluminum nitride, magnesia, boron nitride, silicon nitride and alumina are top material candidates for a heat sink.

It is important to point out here that commercial heat sinks are commonly made from aluminum alloys or copper due to their high heat capacity and thermal conductivity. In addition, they are popular because they can be produced by common manufacturing methods with relatively low production costs. For example, one-piece aluminum heat sinks can be made by extrusion, casting, skiving or milling and one-piece copper heat sinks can be made by skiving or milling, which are standard manufacturing approaches [2]. However, this should not stop the research on finding more effective materials for heat sinks to come up with new candidates as mentioned above

Similar materials selection process can be carried out in Granta Research Selector, using MaterialUniverse with 'All bulk materials' subset', same list of material candidates for a heat sink can be confirmed.

At the same time, continuing to think about thermal analysis with modeling and simulation tools (more details can be found here: Thermal Analysis of Heat Sinks with Ansys Discovery), Granta Research Selector supports with extra temperature-dependent data in JAHM Curve Data database. It contains temperature-dependent curve data for: mechanical, thermal, physical and electrical properties, stress-strain curves, fatigue, creep and magnetic properties for over 11000+ materials across 27,000+ records, providing ready access to material property curve data and enables comparison of material performance at temperatures ranging from -270°C to over 5000°C. As an example, in Figure 9, there is a series of illustrations of thermal conductivity against density with temperature changing from 23 °C to over 800 °C.

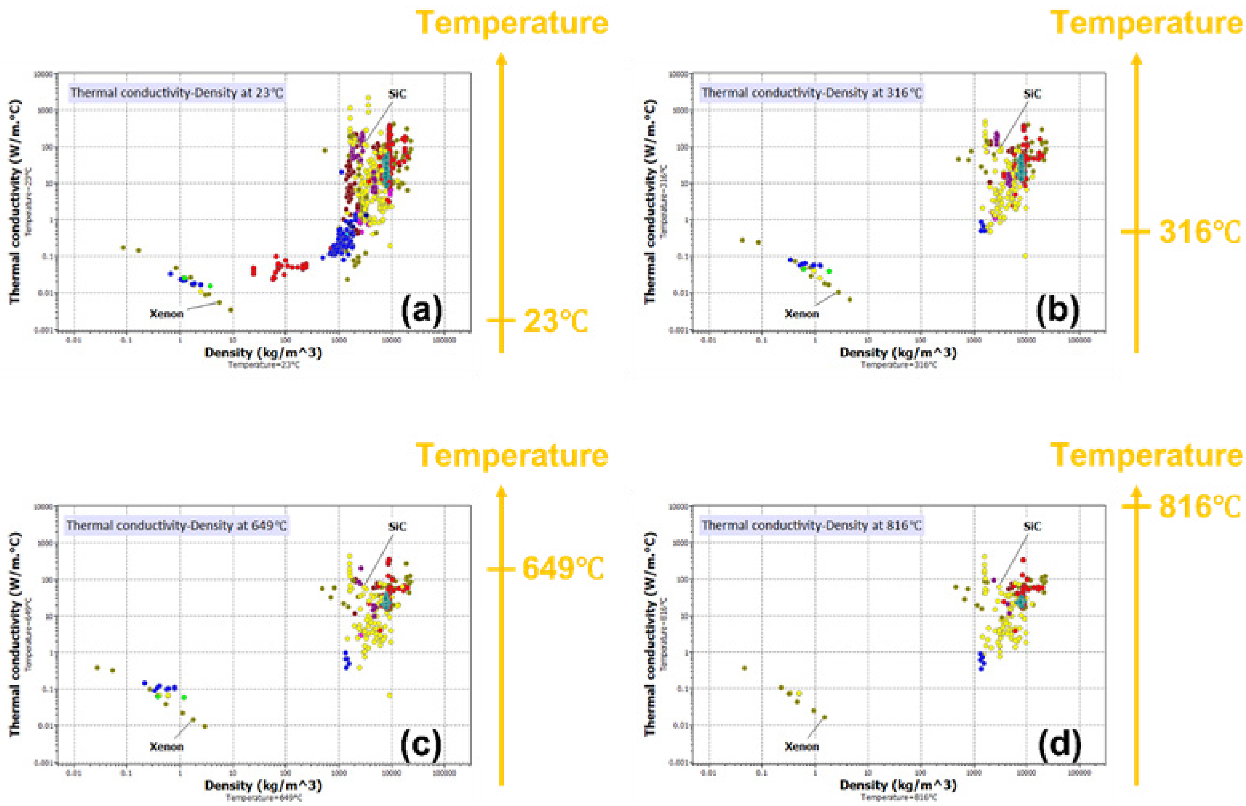

Figure 9 Illustrations of thermal conductivity against density at: (a) 23 °C; (b) 316 °C; (c) 649 °C; (d) 816 °C

4. Conclusions

In this case study, to tackle the heat dissipation problems in multifarious microchip-based appliances, Ansys Granta EduPack and Granta Research Selector are used to choose material candidates that maximize the performance of the heat sink with extra temperature-dependent data to further support a thermal analysis of the heat sink using numerical simulation methods.

5. References

[1] Jack S. Kilby. (1964). Miniaturized electronic circuits - US Patent No. US3138743A. United States Patent Office. https://patents.google.com/patent/US3138743

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