Molybdenum-copper-composites for the advanced thermal management of modern electronics

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Abstract

Molybdenum-copper-composites are interesting materials in the field of thermal management of gallium nitride based electronic devices. Depending on the application and packaging requirements, the coefficient of thermal expansion and thermal conductivity can be tailored for these composites by varying structure and composition. This work gives an overview on thermophysical properties, electrical resistivity as well as interface reliability and stability.

Keywords

CMC, SCMC, composites, multilayer, CTE, thermal conductivity, thermal management, heat spreader, heat sink, molybdenum, copper

Introduction

With the increasing success of gallium nitride (GaN) based radio-frequency devices, the thermal management of these devices is gaining more and more attention. The existing thermal management solutions for silicon are limiting the potential of GaN. Actually, the smaller footprint and higher operating temperature of GaN devices is resulting in higher heat flux densities compared to silicon. Thermal management materials not adapted to the GaN requirements may cause heat damage to chip or induce thermo-mechanical stresses which both lead to failure of the device (Figure 1).

The coefficient of thermal expansion (CTE) of heat spreaders for GaN chips should be slightly higher than the CTE of GaN and other materials used for packaging like Kovar or ceramics in order to have these materials under compression. This restricts the acceptable CTE of the heat spreader to 6–12 ppm/K. Typically, the highest thermal conductivity is demanded in order to avoid any heat accumaltion at the die. However, thermal conductivity requirements vary widley depending on the application.

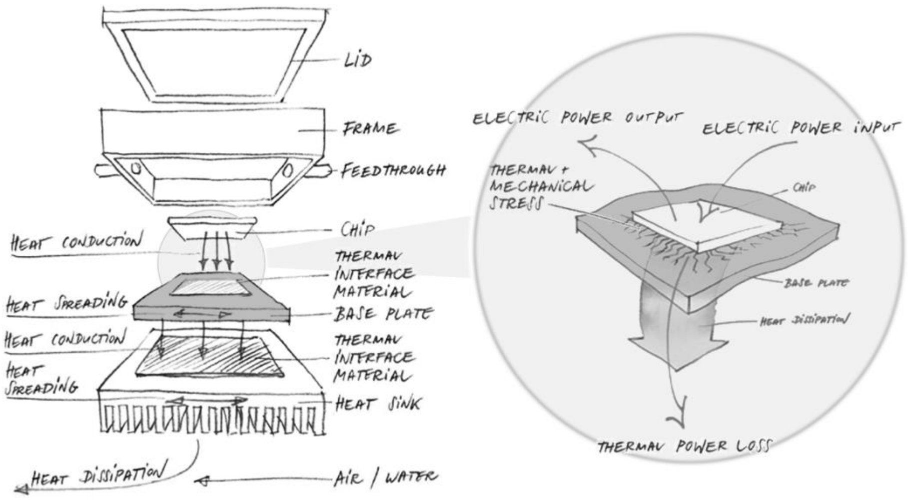

Figure 1: Illustration of a package (left) and detailed view on heat spreader and die (right). Heat spreaders with inappropriate thermophysical properties may induce thermal and mechanical stresses into the chip.

Pure copper shows a high thermal conductivity (397 W/m/K at room temperature) but its CTE (16.5 ppm/K) prohibits the use as heat spreader for GaN chips. Contrary to copper, the CTE of molybdenum is significantly lower (5.35 ppm/K) but its thermal conductivity is also lower (138 W/m/K) [1]. Both metals can be combined to a composite in order to achieve a low CTE and a high thermal conductivity.

The scope of this work is to give an overview on material properties of molybdenum-copper-composites. First of all, typical structures and compositions of multilayered composites are introduced. Then, thermal conductivity and CTE data of several composites is shown. It is demonstrated how the thermal conductivity can be estimated for any kind of molybdenum-copper-multilayer based on existing data. Furthermore, the electrical resistivity is derived from thermal conductivity measurements using the Wiedemann-Franz law. Results on interface stability and reliability complete this review on the molybdenum-copper-composites.

Structure and Composition

Multilayered composites with alternating copper and molybdenum layers allow the adjustment of CTE and thermal conductivity by varying the number of layers and their thickness. Typically, those multilayers consist of three or five layers with a symmetric structure. Asymmetric structures would cause bending due to the different CTE of the layers. The outer layers are usually copper in order to achieve an appropriate heat spreading. Examples of common structures are shown in Figure 2.

Figure 2: Polished cross sections of (a) a three and (b) five layered molybdenum-copper-composite.

Commercially the names CMC and SCMC ((**s**uper) **c**opper **m**olybdenum **c**opper) are established, which should not be confused with the material class *ceramic matrix composite* using the same abbreviation. The molybdenum-copper-composites are not forming alloys and can hence rather be assigned to the *metal matrix composite* (MMC) category.

Thermophysical Properties

Compared to high-end thermal management materials, such as metal-diamond-composites, molybdenum-copper-composites show a lower thermal conductivity and cover a wider CTE range (Figure 3). The main advantage of molybdenum-copper-composites is their machinability which allows both low volume and cost-efficient mass production.

Material properties are easy to adapt to application demands due to the variable layer structure. Depending on the structure, through-plane thermal conductivities are ranging from 220 W/m/K to 270 W/m/K and the CTE between 6 ppm/K to 13 ppm/K (Figure 4). Due to the high thermal conductivity of the copper layer (397 W/m/K) next to the die, the generated heat is efficiently spread.

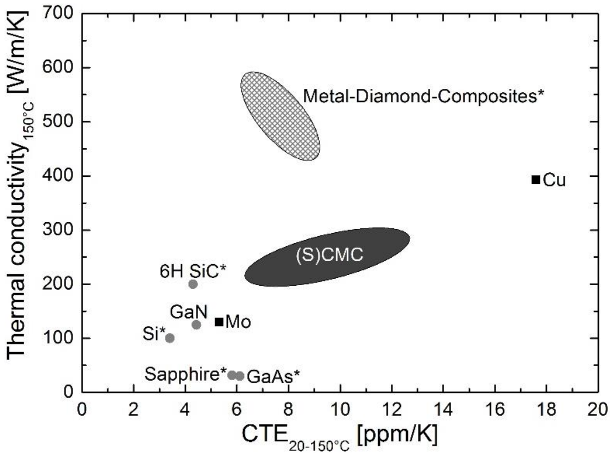

Figure 3: Through-plane thermal conductivity of molybdenum-copper-multilayers ((S)CMC) as a function of the CTE. For comparison, data of semiconductors and metal-diamond-composites is plotted. Data points marked with an asterisk are taken from literature [1–4].

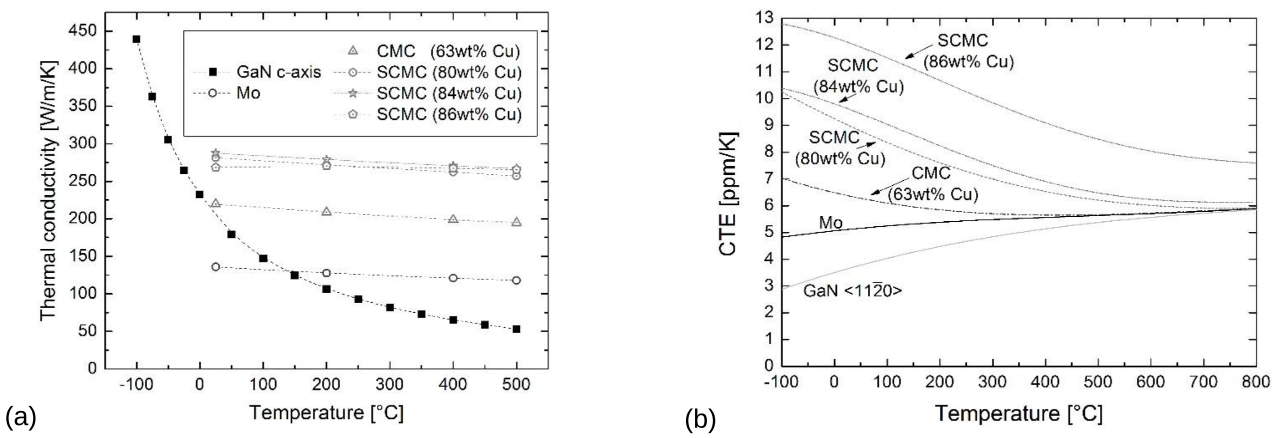

Figure 4: (a) Thermal conductivity and (b) linear coefficient of thermal expansion of molybdenum-copper-composites and monocrystalline GaN.

Figure 4 (b) indicates that molybdenum is dominating the CTE almost throughout the whole temperature range for multilayered composites with 63 wt.% copper. Higher copper contents result in higher CTE up to 300°C, but above that temperature the low CTE of the moylbdenum layers significantly lowers the overall CTE of all composites. This is probably related to the softening of copper.

While there is no simple model to approach the CTE of multilayered composites, the inverse rule of mixture can be used to estimate the thermal conductivity of a layered material [5]:

$$\lambda = \left(\frac{\Sigma x_i}{\lambda_i} + n * R_{th}\right) \tag{1}$$

In this equation, λ is the thermal conductivity, x_t the total thickness of the composite, n the number of interfaces, R_{th} the thermal contact resistance, x_i the thickness and λ_i the thermal conductivity of layer i.

If the thermal contact resistance is known, the thermal conductivity of any multilayered composites can be estimated using literature data for the thermal conductivities of the single layers. In previous work we have shown, that the thermal contact resistance between molybdenum and copper can be determined with the Netzsch LFA 457 LaserFlash [6]. For this, we prepared molybdenum and copper discs with a diameter of 12.7 mm and thicknesses of 3 mm and 3.2 mm respectively. Prior bonding to bilayered samples, the thermal diffusivities of the pure metals were measured since it is needed as input parameter for the LaserFlash software. Then, the thermal diffusivities of the bilayered samples were measured and the provided software was used to calculate the thermal contact resistances following the approach of Hartmann *et al.* [7].

Figure 5 shows the thermal contact resistance of a two-layered molybdenum-copper-composite. Four similar samples were measured in total and an average contact resistance of 4.2×10^{-7} m²K/W at room temperature was determined.

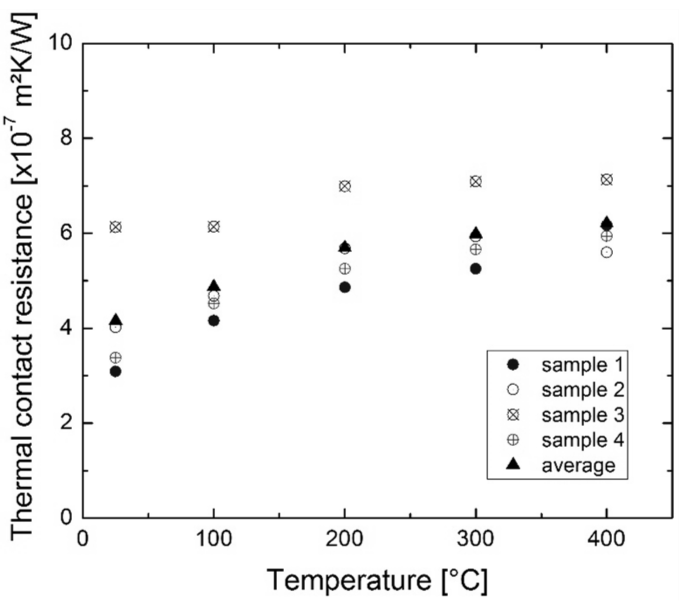

Figure 5: Thermal contact resistance between molybdenum and copper.

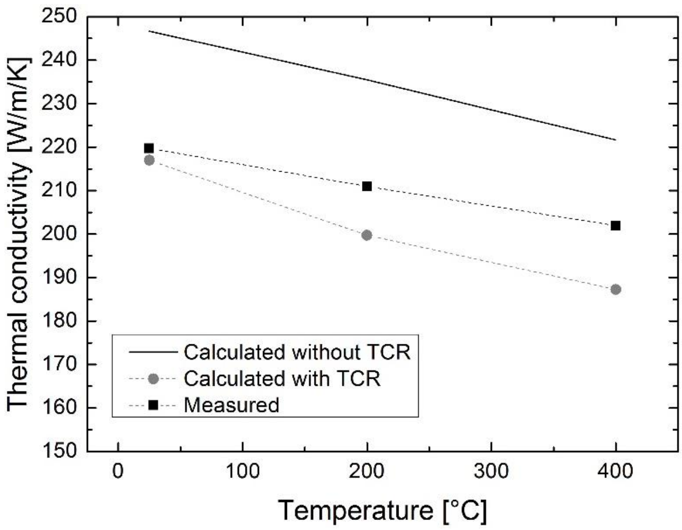

Figure 6: Thermal conductivity calculated according to inverse rule of mixture, with and without thermal contact resistance (TCR), in comparison to measured data.

Eq. 1 was used to estimate the thermal conductivity of a three layered copper-molybdenum-copper composite with a thickness of 0.5 mm per layer, inserting literature data for the thermal conductivites of copper and molybdenum and the average contact resistance from Figure 5. This estimated thermal conductivity is compared to actual measured data and to calculated values neglecting the contact resistance (Figure 9). At room temperature, calculated data with thermal contact resistance coincide with actual measured data. The gap between measured and calculated data is increasing with temperature and reaches ~7 % at 400 °C. Bearing in mind that the accuracy of the thermal conductivity data is +/-5 %, one can conclude, that there is a good agreement between measured and calculated data.

Electrical Resisitivity

The measurement of the electrical resistivity is due to the limited thickness of the composites a challanging task. In the ideal case, the thickness of a sample should be ten times larger than the length and width in order to avoid inhomogeneous potential and current within the sample which would lead in turn to erroneous results. Since the typical material thickness is 0.5 mm to 1.5 mm, an edge width of 50 µm to 150 µm would be required for reliable measurements. However, not only the preparation of such samples is challenging but also the measurements itself. In addition, even minor defects in the material would drastically affect the measurement results.

Due to the challenges and uncertainties related to the measurement of the electrical resistivity, we decided to follow a different approach. According to the Wiedemann-Franz law, the ratio of thermal conductivity λ to electrical conductivity σ is proportional to temperature T [9]

$$\frac{\lambda}{\sigma} = L * T \tag{2}$$

In metals, both electrical and thermal conductivity are dominated by electron transport, which explains the validity of the Wiedemann-Franz law. The Lorenz number L can be derived from the free electron model and it follows that it is 2.45×10^{-8} WΩ/K² for any kind of metal [9]. Experimentally, the Lorenz number is actually different for each metal and its value can be determined by measuring the thermal and electrical conductivity. Since measured data for the electrical resisitivity is lacking in our case, we will use the Wiedemann-Franz law to estimate the electrical resisitivity of the composites based on thermal conductivity measurements. Inserting Eq. 1 in Eq. 2 and replacing the electrical conductivity by Ohm's law gives, after rearranging,

$$L = \frac{1}{T} * \frac{1}{\frac{x_{Cu}}{\lambda_{Cu}} + \frac{x_{Mo}}{\lambda_{Mo}}} * (\rho_{Cu} * x_{Cu} + \rho_{Mo} * x_{Mo}) \tag{3}$$

where ρ is the electrical resistivity.

The ideal Lorenz number can be calculated with literature data from Table 1 and the known layer thicknesses. For instance, for three layered structure (x_{Cu1} = 0.5 mm, x_{Mo} = 0.5 mm, x_{Cu2} = 0.5 mm) it follows that L = 2.49 × 10^{-8} WΩ/K², which is a typical value for metals.

Table 1: Literature data for Lorenz number, thermal conductivity and electrical resistivity of copper and molybdenum [1,9]. In addition, measured (*λ*) and calculated data (*L*, *ρ*) for the molybdenum-copper-multilayers is shown.

	Copper	Molybdenum	CMC (63 wt.% Cu)	SCMC (80 wt.% Cu)	SCMC (86 wt.% Cu)
L [WΩ/K²]	2.23 × 10^{-8}	2.61 × 10^{-8}	2.49 × 10^{-8}	2.41 × 10^{-8}	2.35 × 10^{-8}
λ [W/m/K]	397	140	220	251	268
ρ [Ωm]	1.741 × 10^{-8}	5.7 × 10^{-8}	3.4 × 10^{-8}	2.9 × 10^{-8}	2.6 × 10^{-8}

The Lorenz number can now be used to calculate the electrical resistivity based on the measured thermal conductivity and Eq. 2. The results are summarized in Table 1. Figure 7 compares the ideal electrical resisitivity calculated according to Ohm's law and the electrical resisitivity estimated using the Wiedemann-Franz law. Considering this approach as a rough estimation, the obtained values are in good agreement with the ideal resistivity. Since actual measured data was used for the thermal conductivity, interface resistances are taken into consideration in this approach.

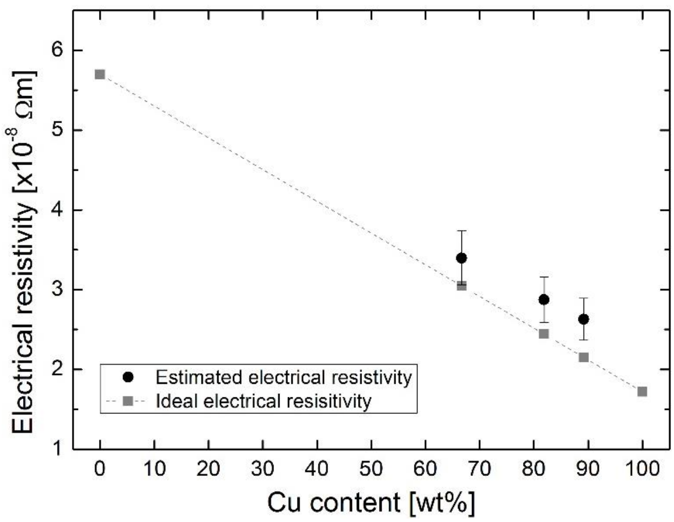

Figure 7: Ideal electrical resistivity calculated from Ohm's law and estimated electrical resisitivity based on thermal conductivity data.

Interface Stability and Reliability

One of the major concerns of package designers regarding the molybdenum-copper multilayers is their long term stability. The large difference in CTE between molybdenum (5.35 ppm/K [1]) and copper (16.5 ppm/K [1]) might induce stress at the interfaces during processing and operation of the device and might hence lead to delamination between the molybdenum and copper layers. In order to dispel doubts, not only thermal cycle tests were performed but also detailed interface studies.

Thermal cycling was performed according to EN 60068-2-14 in an ESPEC TSD 100 thermal shock tool. The three layered CMC samples were first transferred to a hot chamber at +125 °C and kept in this chamber for 30 minutes. Then, the samples were directly moved to a cold chamber at -40 °C and also kept at this temperature for 30 minutes. Figure 8 illustrates the temperature-time profile of the thermal cycling. Ten samples were taken each after 100, 500, 1000 and 2000 cycles.

The samples were analyzed for interface defects by a Winsam Vario III acoustic microscope operating at 150 MHz and 50 dB. Due to the limited penetration depth both sample surfaces were scanned. Thus the two molybdenum-copper-interfaces could be analyzed for defects. Polished cross sections were prepared for scanning electron microscopy and studied by a Carl Zeiss Ultra Plus Field Emission SEM.

Acoustic microscopy was performed on all samples and none of them showed any defects at the molybdenum-copper-interfaces (Figure 9). However, this technique only allows detecting defects larger than approximately 0.3 mm. Hence, only the presence of large scale defects can be excluded by acoustic microscopy on the studied samples.

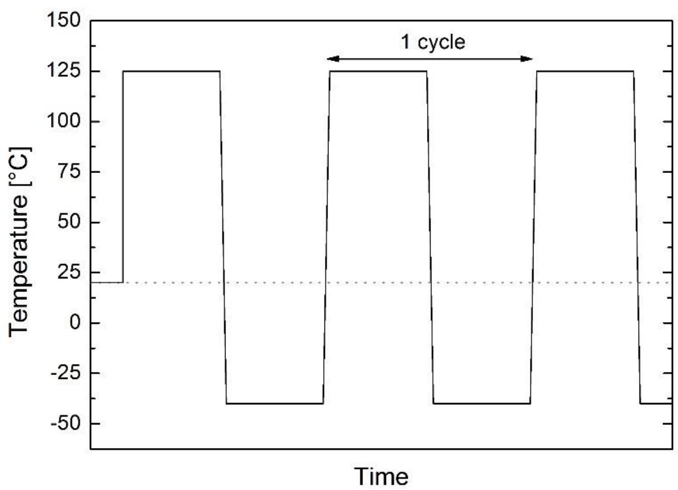

Figure 8: Temperature test profile for thermal cycling.

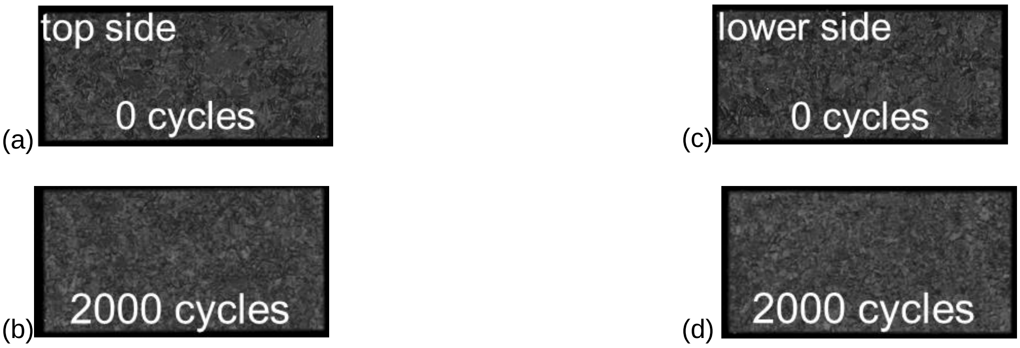

Figure 9: Top side (a, b) and lower side (c, d) acoustic microscopy images.

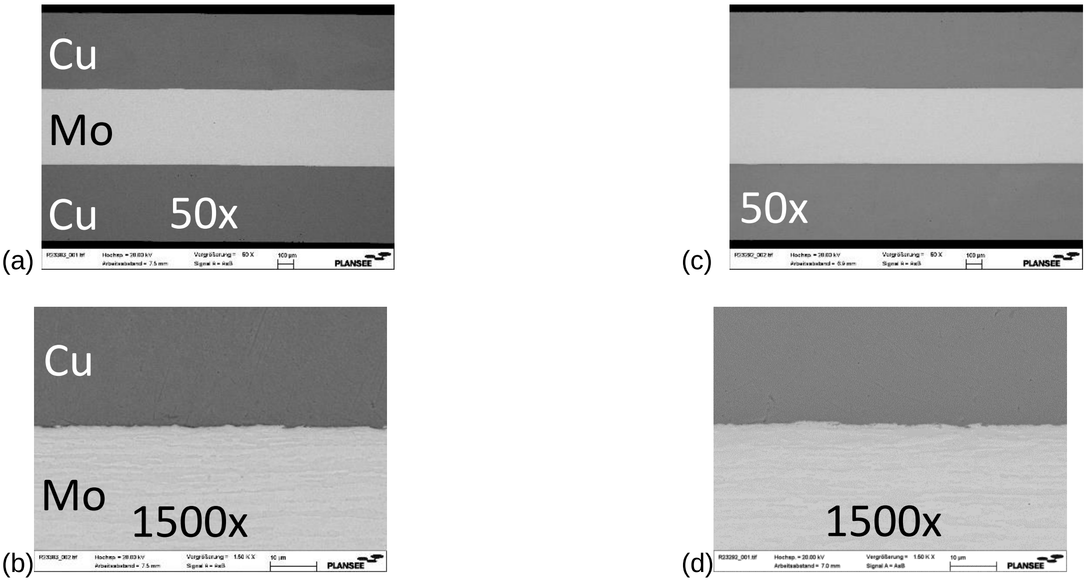

Figure 10: SEM images on polished samples of fresh samples (a and b) and samples with 2000 cycles (c and d).

SEM imaging was done on the polished cross sections to check for large scale cracks and small pores. The overview images in Figure 10 do not show any large scale defect at the interfaces. Even at higher magnifications no degradation of the interfaces was observed.

In addition, the thermal conductivity may indicate if interface defects are present. An increasing number of pores or cracks at the molybdenum-copper-interfaces should result in a lower thermal conductivity. The room temperature thermal conductivity of the cycled samples is plotted in Figure 11. These results illustrate that the thermal conductivity is not affected by thermal cycling. Hence, the generation of interface defects can be excluded confirming the previously mentioned investigation results.

Recent transmission electron microscopy (TEM) results indicate a sharp interface between the copper and molybdenum layers [6]. The interfacial orientation between molybdenum and copper observed by high resolution TEM probably allows the transmission of dislocations across that interface, explaining the mechanical stability upon thermal cycling. The sharp interface also explains the good thermal and electrical conductivity of the composite. A solid solution at the interface, caused by interdiffusion, would result in electron scattering at the interface which would drastically deacrease both electrical and thermal conductivity.

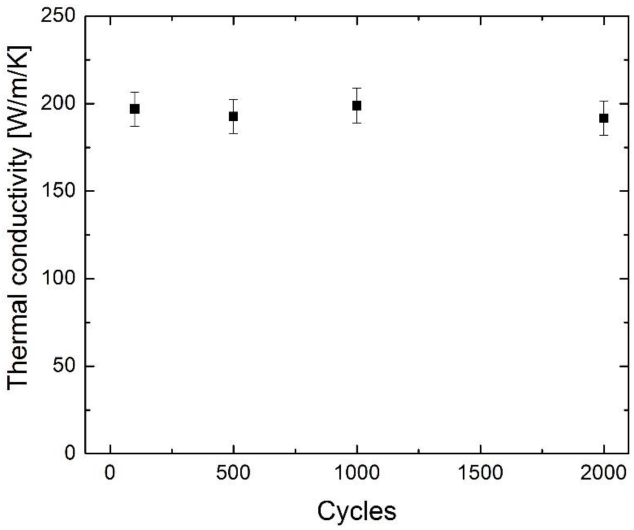

Figure 11: The thermal conductivity after different number of thermal cycles showing that this property is not degrading even after 2000 cycles.

Summary

Molybdenum-copper-composites are promising materials for the thermal management of GaAs and GaN based devices. The thermophysical properties can be tailored to application demands. The through-plane thermal conductivity is typically ranging from 220 W/m/K to 270 W/m/K whith a CTE between 6 ppm/K and 13 ppm/K. The electrical resistivity was estimated to be 2.6×10^{-8} Ωm – 3.4×10^{-8} Ωm for a composite with 86 wt.% and 63 wt.% copper respectively. The composite was shown to be stable even after 2000 temperature cycles between -40 °C and +125 °C.

References

1. W. Martienssen, H. Warlimont, Springer Handbook of Condensed Matter and Materials Data, Springer, Berlin Heidelberg, (2005)
2. R. Bollina, J. Landgraf, H. Wagner, R. Wilhelm, S. Knippscheer, S. Levchuk, G. Mitic, Proceedings of IPACK2007-ASME InterPACK, Vancouver, BC, pp. 389-397, (2007)
3. S. Knippscheer, “Advanced Metal Diamond Composites – Love and Heat Relationship”, Electronics Cooling, vol.14(4), (November 2008)
4. Kyocera, “Single Crystal Sapphire”, datasheet, Aug. 2015
5. D. P. H. Hasselman, L. F. Johnson, J. Compos. Mater. 21(6), pp.508-515, (1987)
6. M. Seiss, T. Mrotzek, U. Jäntsch, M. Klimenkov, J. Reiser, W. Knabl, „The interface in molybdenum-copper-composites used for thermal management applications “, manuscript submitted to 33rd Semiconductor Thermal Measurement and Management Symposium, (2017)
7. J. Hartmann, O. Nilsson, J. Fricke, High Temp – High Press, Vol. 25, pp. 403-410, (1993)
8. M. Seiss, T. Mrotzek, N. Dreer, W. Knabl, Mater. Sci. Forum, Vols. 825-826, pp.297-304, (2015)
9. C. Kittel, Introduction to Solid State Physics, Second Edition, John Wiley & Sons (1956)