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Composite Materials for Thermal Expansivity Matching and High Heat Flux Thermal Management

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Abstract: A description is given of a possible solution of an important practical problem in microelectronics, namely producing a material of thermal expansion coeffiecient to equal that of silicon.

Thermal Management-Control of CTE

Composite materials may solve a number of problems in thermal management where it is necessary to evacuate excess heat from a device and this is done by joining it to a material of the highest possible thermal conductivity. To avoid excessive strain between the conductor and the device, as the temperature fluctuates, it is very desirable to have as close as possible a matching of the coefficients of thermal expansion (CTE) at the interface.

In what follows we shall consider a device based on silicon. Matching the thermal expansion coefficient of silicon is not easy because of its low value. The values of the CTE of a number of relevant materials are shown in Table 1. We also give the thermal conductivity at about room temperature because, other things being equal, we are seeking materials with high thermal conductance. It is seen that that silicon has one of the lowest CTEs, only diamond and fused silica show lower values. Fused silica has a very low thermal conductance.

Table 1. Thermal expansivity and thermal conductance of materials of interest in microelectronics

Material	Diamond	silicon	SiC	GaAs	GaN	AlN	BeO	Fused SiO_2
CTE $[10^{-6}K^{-1}]$	0.8-1.05	2.57	2.8-3.2	5.7	3.5-3.7	2.57 4.2-5.2	5.65	0.5
Thermal conduc. [W/mK]	600-1800	168.var.	1000 var only singl Xtl..	48	100	150	200	1.4

G A Slack and S F Bartram J Appl. Phys **46** (1974) 89-98 and Data in Science and Technology Semiconductors (1991) Springer-Verlag

In the remainder of this paper which we will consider two ways of matching the CTE at the interface and will not deal specifically with how to obtain a large thermal conductivity but it should be borne in mind that in every choice of material the accent is on using only those of high thermal conductivity where possible- so among matrices metallic matrices, notably Au, Ag Cu or Al, are to be preferred.

Matching of thermal expansion coefficients at an interface and not just in a single direction or range of directions may be accomplished by at least three methods by using composite materials.

1) Using a particulate composite provided the distribution of particles is uniform throughout the matrix.
2) The cross section of an aligned fibrous composite shows isotropy in this plane.

3) A balanced and symmetric 0/90 laminate fibrous composite shows isotropy of CTE in its plane- the condition for the value to be negative is considered by McCartney and Kelly [1].

Particulate Composite

The prediction of CTE for a particulate composite is well given by which is the upper bound quoted by Rosen and Hashin [2] and coincides almost exactly with the value found from an exact calculation by Arridge[3].

The expression is:

$$\alpha_c = \alpha_1 V_1 + \alpha_2 V_2 + \frac{4V_1V_2G_1(K_1 - K_2)(\alpha_1 - \alpha_2)}{3K_1K_2 + 4G_1 K} \quad (1)$$

where $\bar{K} = K_1V_1 + K_2V_1$ (2)

Using relation (1) the predicted values of CTE for a composite consisting of diamond particles in silver is compared with experimental results in Fig.1.

The experimental specimens were kindly supplied to me by Dr Ludger Weber at EPFL Lausanne. The agreement with theory is very good but one sees that in order to obtain a value matched to that of silicon a volume fraction of greater the 0.95 is required. Using gold or copper or other matrix of high thermal conductivity does not predict attaining a value of $2.6.10^{-6}$ K^{-1} with any lesser value of V_f. In order to obtain the high values of V_f shown in Fig.1, at the very least particles of no less than three average sizes must be used. For a consideration of the problems see [4].

The alternative to using diamond in one of the noble metals would be to use a material with a negative thermal expansion coefficient in order to match the CTE of silicon- a much lower volume fraction might then be required. However of those, known to me, none shows either sufficient stability or isotropy. A possible exception is M_3XN with X=Cu, Ga or Zn but little is so far known of this material.

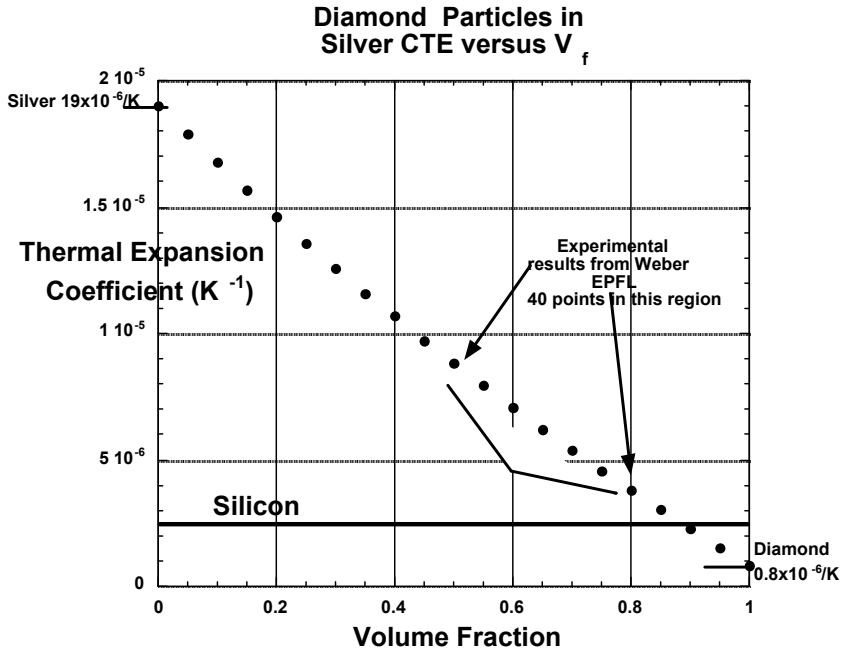

Fig.1. Measured and Predicted CTE of diamond particles in silver.

Aligned Composite

Provided the composite shows transverse isotropy it will show planar isotropy of the CTE in the transverse plane. The analytic formulae for estimating this from the properties of the two components of the composite are very robust and have been published by McCartney [3]. The relevant formula is also repeated in [1]. One set of fibres which might enable matching of the CTE of silicon when introduced into one of the matrices of very high thermal conductance are the diamond fibres developed by May and his colleagues at Bristol [6]. Dr May very kindly provided me with some of these. We have determined the thermal conductivity of these fibres ourselves and find for those containing more than 90% CVD diamond a value greater than 500 w/mK.

These fibres consist of CVD diamond deposited upon a core of tungsten wire. Using the known properties of tungsten and those of diamond given in Field's compilation [7] we have determined the properties of the compound fibre and the estimated values are shown in table 2 using an obvious notation. It is to be noted that the predicted axial and transverse properties of these fibres are very similar because the elastic and thermal properties of tungsten are isotropic and those of diamond nearly so. This is in contrast to most high performance fibres, in particular in contrast with carbon fibres. These compound diamond fibres show similar values of the axial and the transverse CTE, whereas carbon fibres have much larger transverse CTEs than in the axial direction.

Table 2. Predicted properties of tungsten/diamond fibres

E ax	E tr	PR ax	PR tr	Bulk mod tr	Shear mod ax	Shear Mod tr	CTE ax	CTE tr
843 GPa	832 GPa	0.1	0.1	485 GPa	375 GPa	371 GPa	$1x10^{-6}$	$1x10^{-6}$

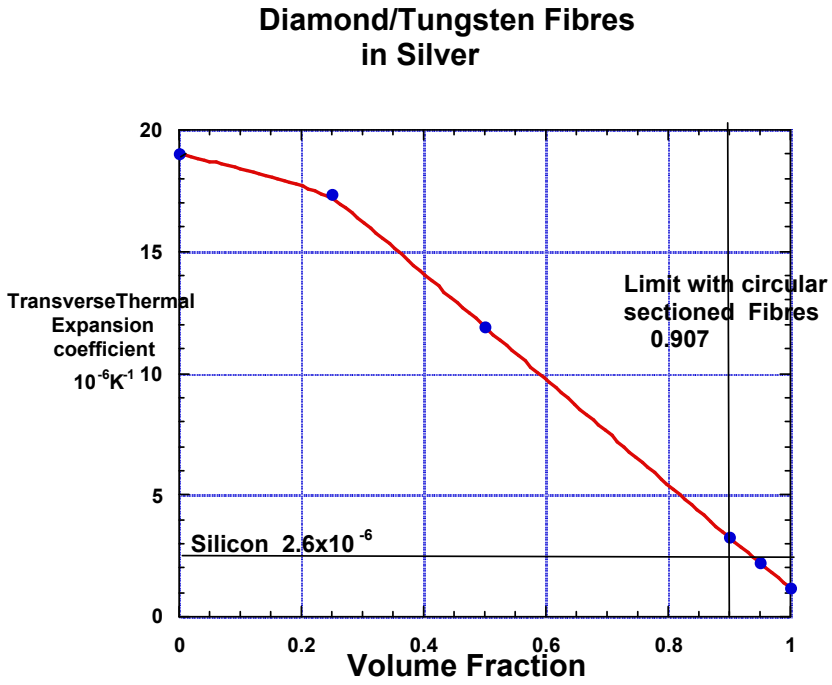

Fig.2. Predicted transverse CTE of diamond fibres in silver as function of V_f.

The predicted transverse CTE of an aligned composite consisting of these fibres in silver is shown in Fig.2. Because these fibres are expected to show a transverse CTE smaller than that of silicon it is possible to predict exact matching though only at extreme values of the volume fraction is it possible to match silicon's CTE exactly. However, no other fibre known to me, shows a transverse CTE within the necessary range.

Conclusions

When matching coefficients of thermal expansion at an interface, accurate match may be obtained by using laminated composites (not dealt with here) but this method is not easily coupled with very high thermal conductance. For best thermal conductance the use of an aligned composite containing fibres of high conductance and of a prescribed lateral thermal expansion coefficient is best.

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