

## THE ADOPTION OF NOVEL COOLING LIQUIDS FOR ENHANCING HEAT TRANSFER PERFORMANCE OF 3-D INTEGRATED CIRCUITS WITH EMBEDDED MICRO-CHANNEL

by

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*The nanofluids (including MWCNT based nanofluid and SWCNT based nanofluid) and liquid metal Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> are proposed to replace the conventional water as cooling liquid of micro-channel for enhancing heat transfer performance of 3-D integrated circuits (3-D IC) in this paper. An equivalent thermal model of 3-D IC with integrated micro-channel is established to investigate the heat transfer performances for using different cooling liquids. The results show that the steady-state temperature for MWCNT based nanofluid, SWCNT based nanofluid and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquids can be reduced over 25.698%, 28.771%, and 35.735% than the conventional water scheme in a four-layers stacked chip, respectively. Besides, it is found that the steady-state temperature of all die layer in 3-D IC can be further reduced by increasing the micro-channel size and flow velocity of cooling liquid. Therefore, the proposed novel materials (i.e., nanofluids and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub>) as cooling liquids have excellent application prospect in solving thermal problems of 3-D IC.*

*Key words: 3-D IC, micro-channel, heat transfer performance*

### Introduction

The occurrence of 3-D stacking technology has remarkably facilitated the progression of semiconductor integrated circuits, which extend the conventional 2-D IC entering into 3-D space [1]. Compared with 2-D IC, 3-D IC can reduce the total wire length, transmission delay, power dissipation and package size due to its multi-layer stacked structure in the vertical direction. However, the unique structure inevitably leads to the increase of power density of 3-D IC, this can enable the 3-D IC to form the complex thermal problem owing to the excessive temperature rise [2]. Hence, it is extremely vital that the chip designer ought to seek the solution for enhancing the heat transfer performance of 3-D IC.

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In recent years, the micro-channel cooling system has been widely used in high power semiconductor devices due to its excellent heat transfer performance [3-7]. Besides, it is recognized that the integration of micro-channel in 3-D IC is regarded as an effective solution for solving the increasingly serious thermal problem. The micro-channel is embedded in the silicon substrate of each die layer and its interior is filled with cooling liquid. The cooling liquid convey the heat generated by back end of line (BEoL) to the external environment of 3-D IC through heat conduction and convection [8]. Depending on the size of hydraulic diameter,  $D_h$ , the micro-channel can be divided into nanochannel (*i.e.*,  $D_h = 10\text{-}1000$  nm), micro-channel (*i.e.*,  $D_h = 1\text{-}100$   $\mu\text{m}$ ), meso-channel (*i.e.*,  $D_h = 100\text{-}1000$   $\mu\text{m}$ ), and macro-channel (*i.e.*,  $D_h = 1\text{-}6$  mm), respectively [9, 10].

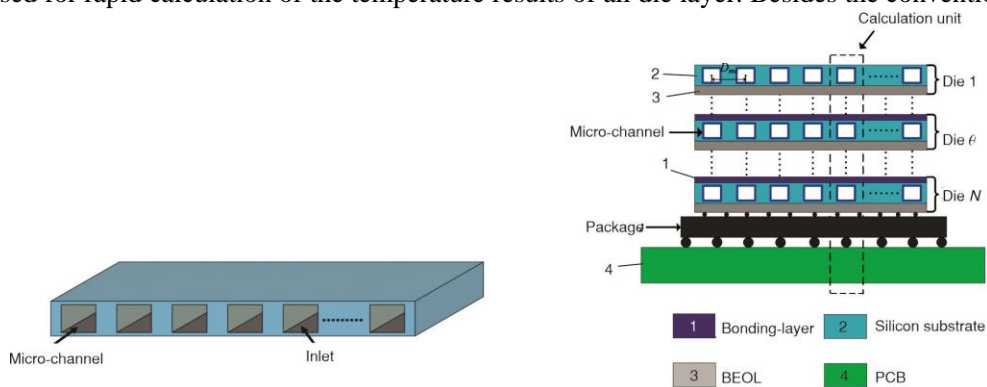
In the available literatures, water is the most common cooling liquid of micro-channel for practical application. However, the heat transfer performance of water as cooling liquid is limited in the light of its small thermal conductivity of  $0.611$  W/mK [11]. Therefore, researchers are urgent to seek the novel materials with better heat transfer performance for replacing the conventional water as cooling liquid to solve the complex thermal problem of 3-D IC due to the excessive temperature rise. Nanofluids have captured the intensive interest from many researchers that are composed of the ultra-fine nanoparticles (such as CNT *etc.*) mixed in fluids (such as oil, water, engine oil, *etc.*) in specific proportions [12-14]. The thermal properties of ultra-fine nanoparticles is far larger than water, which result in the thermal conductivity of nanofluids exceeding water [15, 16]. The CNT are the cylindrical nanostructure of one or more graphene layers, which can be classified into single-wall carbon nanotubes (SWCNT) and multi-wall carbon nanotubes (MWCNT) depending on the number of carbon walls [17]. Based on the statement of [18], the diameters of SWCNT and MWCNT nanoparticles are commonly  $0.8\text{-}2$  nm, and  $5\text{-}20$  nm, respectively. In this work, the SWCNT and MWCNT are adopted as the ultra-fine nanoparticles because their thermal conductivity can reach to  $6600$  W/mK and  $3000$  W/mK, respectively [19]. In view of the small sizes and the large particular surface area of nanoparticles, the SWCNT and MWCNT based nanofluids have a series of excellent performance such as high thermal conductivity, less blockage in the transit of the fluid-flow, longer stabilization and homogeneity [20]. Thus, the MWCNT based nanofluid and SWCNT based nanofluid as cooling liquids are investigated in our work. Besides the nanofluids, the liquid metals are also regarded as a promising potential cooling liquid in the research community in terms of their excellent heat transfer performance. The  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$ , composed of 68% gallium, 20% indium, and 12% tin (calculating by weight), is deemed as the prospective cooling liquid of micro-channel [21]. The thermal conductivity of  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  can exceed  $39$  W/mK, which is far greater than the thermal conductivity of water (*i.e.*,  $0.6$  W/m·K) under the same conditions [22, 23]. Therefore, the heat transfer performance for  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid of micro-channel in 3-D IC is also discussed in this work.

In the practical applications, it is indispensable to investigate the preparation cost of different cooling liquids. The SWCNT and MWCNT nanoparticle powder are the essential materials for the preparation of nanofluids, and their price are usually  $101$  USD and  $64$  USD per gram, respectively [24]. Besides, the price of liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  is usually  $0.38$  USD per gram. Accordingly, the preparation cost for the proposed SWCNT based nanofluid, MWCNT based nanofluid and liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquids are much greater than the conventional water (usually  $0.41$  USD per ton in China) case [25]. Therefore, it is the key factor to reduce the preparation cost of these proposed cooling liquids for the future widespread application.

So far, there are some studies on improving heat transfer performance of micro-channel by replacing the conventional water with other promising cooling liquids that have been

done. Abubakar and Sidik. [26] investigated the heat transfer performance of  $\text{Fe}_3\text{O}_4$ -water as cooling liquid under four volume fractions (0, 0.4, 0.6, and 0.8), respectively. The results illustrated that increasing the volume fractions of nanofluids can improve the heat transfer performance of micro-channel. Kalteh [27] established a numerical model to investigate the heat transfer performance of micro-channel for applying different types of nanofluid as cooling liquid cases in which nine different nanoparticles (*i.e.*,  $\text{Al}_2\text{O}_3$ ,  $\text{CuO}$ ,  $\text{Cu}$ ,  $\text{Fe}$ ,  $\text{Au}$ ,  $\text{Ag}$ ,  $\text{TiO}_2$ ,  $\text{SiO}_2$ , and diamond) are mixed in three different base fluid (*i.e.*, water, ethylene glycol, and engine oil) as nanofluids. The results shown that the diamond based nanofluid as cooling liquid of micro-channel has the highest heat transfer coefficient than other nanofluid. Sarafraz *et al.* [28] studied the heat transfer performance of rectangular micro-channel for using the CNT based nanofluid and water as cooling liquids of micro-channel, respectively, and the experimental results illustrated that the CNT based nanofluid as cooling fluid can effectively reduce the temperature of heat sink as compared with the conventional water case. Amrollahi *et al.* [29] measured the heat transfer coefficients of MWCNT based nanofluid at horizontal tube, the results suggested that the convective heat transfer coefficients of MWCNT based nanofluid can be improved over 33% under the concentration of 0.25 wt.%, as compared with the pure water case. Liu *et al.* [30] proposed the liquid metal GaInSn for replacing the conventional water as cooling liquid, which can enhance heat transfer performance of *T-Y*-type micro-channel evidently. Moreover, in [31-33], it is reported that  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid can efficiently improve the heat transfer performance of micro-channel in heat sink when compared with the pure water case.

Based on these aforementioned discussions, the conventional water is replaced with the nanofluids and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$ , which can obviously improve the heat transfer performance of micro-channel. However, at present few researches have investigated the nanofluids and liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquids of micro-channel for enhancing the heat transfer performance of 3-D IC on the basis of the available literatures. In addition, till date most researches concerning 3-D IC with integrated micro-channel are carried out by the COMSOL or ANSYS simulation, while the studies for proposing the numerical computation thermal model to quickly calculate temperature of 3-D IC with integrated micro-channel are still rare. Meanwhile, it is widely known that the numerical computation model can evidently reduce the running time of CPU and memory consumption as compared with the COMSOL or ANSYS simulation. Therefore, a numerical computation thermal model of 3-D IC with integrated micro-channel is proposed for rapid calculation of the temperature results of all die layer. Besides the conventional



**Figure 1. The geometric structure diagrams; (a) 3-D view of micro-channel and (b) section view of *N*-layers stacked chip with embedded micro-channel**

water, other potential cooling liquids including of nanofluids and liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  for using in 3-D IC are also investigated in this paper. In order to verify the correctness of our proposed computational thermal model, thus its results are compared with the COMSOL simulation. The main contributions of this work are evaluated as:

- The novel cooling liquids concerning SWCNT based nanofluid, MWCNT nanofluid and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  are proposed to replace the conventional water as cooling liquid of micro-channel for improving heat transfer performance of 3-D IC.
- A computation thermal model is established in this work to improve operating efficiency of solving steady-state temperature of 3D-IC with embedded micro-channel.
- The heat transfer performance of 3-D IC can be improved by increasing the micro-channel size and flow velocity of cooling liquid.

## Computational model

### Modeling method

The geometric structure diagram concerning micro-channel and 3-D IC with embedded micro-channel are exhibited in fig. 1, where the  $N$ -layers stacked chip includes package, BEOL, silicon substrate, bonding-layer and micro-channel. At present, the epoxy material is the most commonly used material as bonding-layer of 3-D IC owing to its low curing shrinkage and high thermostability. The 3-D IC is constructed on the printed circuit board (PCB). Especially, the BEOL is an essential part of 3-D IC that contains transistor devices and metal wire. The heat is generated by BEOL that must be convey to the external ambient of chip in time. Additionally, it is assumed that the micro-channel is uniformly embedded in the center of silicon substrate with the same distance  $D_{mc}$  and each micro-channel has same geometric dimensions.

In this work, only a square structure unit of 3-D IC as shown in fig. 2 is discussed since the overall structure is configured as the symmetrical structure. Herein,  $L$  is the side length of calculation unit, and the cross-section area of calculation unit is  $L \times L$ ,  $w$  and  $h$  are the width and height of the micro-channel, and  $Q_\theta$  ( $\theta = 1, 2, \dots, N$ ) represents heat generated by  $\theta^{\text{th}}$  die layer. Moreover, the boundary conditions and assumptions for the proposed computation model are listed as:

- The ambient temperature and inlet temperature of micro-channel are fixed in the calculation process.
- The flow is considered as the steady and fully developed in each channel.
- All materials in 3-D IC possess the homogeneous spatial structure, where their thermophysical parameters are isotropic.
- The total amount of heat generated by heat source is fixed, which is evenly distributed on the surface of BEOL.

The methodology for the proposed computation model is also listed as:

- Step 1: Derive the equivalent thermal resistance of PCB, package, BEOL, silicon substrate, bonding-layer and micro-channel, respectively. Especially, the equivalent thermal

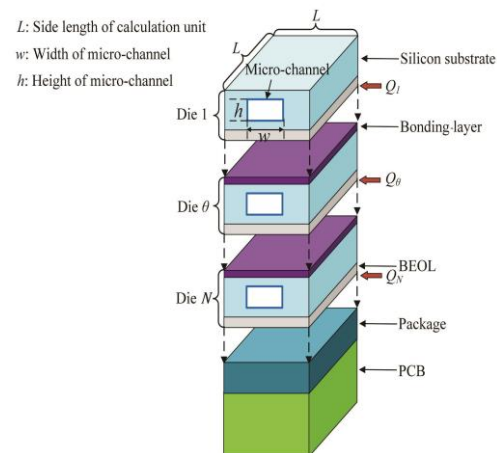


Figure 2. The structure diagram of calculation unit



of PCB and thermal resistance of package for the calculation unit respectively. For the  $\theta^{\text{th}}$  die layer ( $\theta = 1, 2, \dots, N$ ),  $R_{\text{BEOL},\theta}$  and  $R_{\text{bond},\theta}$  represent the thermal resistance of  $\theta^{\text{th}}$  BEOL and bonding-layer of calculation unit, respectively.  $R_{\text{con},\theta T}$ ,  $R_{\text{con},\theta B}$ ,  $R_{\text{con},\theta L}$ , and  $R_{\text{con},\theta R}$  are the conduction thermal resistance of silicon substrate of calculation unit under top direction, bottom direction, left direction and right direction respectively. The  $R_{\text{conv}}$  is the convection thermal resistance between solid and fluid, which is determined by physical parameters of micro-channel and cooling liquid. The  $R_{\text{cl}}$  and  $T_{\text{BEOL},\theta}$  denote the thermal resistance of cooling liquid and the temperature of BEOL in  $\theta^{\text{th}}$  die layer, respectively. The  $T_{\text{mc},\theta T}$ ,  $T_{\text{mc},\theta B}$  are the temperature of top wall and bottom wall of micro-channel, respectively. The  $T_{\text{out},\theta}$  and  $T_{\text{avg},\theta}$  represent outlet temperature of micro-channel and average temperature of cooling liquid for  $\theta^{\text{th}}$  die layer, respectively.

For the calculation unit, the thermal resistance in vertical direction can be written [34]:

$$R = \frac{t}{kA} \quad (1)$$

where  $t$  and  $k$  are the thickness and thermal conductivity of materials, respectively, and  $A$  – the cross-sectional area in the heat flow direction. According to eq. (1) and [2],  $R_{\text{PCB}}$ ,  $R_{\text{pk}}$ ,  $R_{\text{BEOL},\theta}$ ,  $R_{\text{con},\theta T}$ ,  $R_{\text{con},\theta B}$ ,  $R_{\text{con},\theta L}$ ,  $R_{\text{con},\theta R}$ , and  $R_{\text{bond},\theta}$  ( $\theta = 1, 2, \dots, N$ ) can be derived as:

$$R_{\text{PCB}} = \frac{t_{\text{PCB}}}{k_{\text{PCB}}L^2} \quad (2)$$

$$R_{\text{pk}} = \frac{t_{\text{pk}}}{k_{\text{pk}}L^2} \quad (3)$$

$$R_{\text{BEOL},\theta} = \frac{t_{\text{BEOL},\theta}}{k_{\text{BEOL},\theta}L^2} \quad (4)$$

$$R_{\text{con},\theta B} = R_{\text{con},\theta T} = \frac{t_{\text{si},\theta} - h}{2k_{\text{si}}L^2} \quad (5)$$

$$R_{\text{con},\theta L} = R_{\text{con},\theta R} = \frac{2h}{k_{\text{si}}(L - w)L} \quad (6)$$

$$R_{\text{bond},\theta} = \frac{t_{\text{bond},\theta}}{k_{\text{bond}}L^2} \quad (7)$$

Based on [35],  $R_{\text{conv}}$  and  $R_{\text{cl}}$  can be deduced as:

$$R_{\text{conv}} = \frac{1}{h_{\text{cl}}A_m} \quad (8)$$

$$R_{\text{cl}} = \frac{1}{\rho_{\text{cl}}V_{\text{cl}}c_{\text{cl}}} \quad (9)$$

where  $\rho_{\text{cl}}$  and  $c_{\text{cl}}$  are the density and specific heat capacity of cooling liquid, respectively,  $h_{\text{cl}}$ ,  $A_m$ , and  $V_{\text{cl}}$  represent the convective heat transfer coefficient, heat transfer area and volume flow-rate, which can be expressed as eq. (10) to eq. (12), respectively [36]:

$$h_{cl} = \frac{Nu k_{cl}}{D_h} \quad (10)$$

$$A_m = wL + 2hL \quad (11)$$

$$V_{cl} = Uwh \quad (12)$$

where  $k_{cl}$  and  $U$  denote the thermal conductivity and flow velocity of cooling liquid, respectively. According to the [37], the Nusselt number and hydraulic diameter,  $D_h$ , are expressed as eqs. (13) and (14), respectively. Accordingly, the eq. (13) can be used to derive the convective heat transfer coefficient in the light of eq. (10):

$$Nu = 0.1165 \left( \frac{D_h}{D_{mc}} \right)^{0.81} \left( \frac{h}{w} \right)^{-0.79} Re^{0.62} Pr^{1/3} \quad (13)$$

$$D_h = \frac{2wh}{w+h} \quad (14)$$

where  $Re$  and  $Pr$  represent the Reynolds number and Prandtl number. Based on [38], the corresponding expressions for them can be written as eqs. (15) and (16), respectively. Here,  $\mu_{cl}$  is dynamic viscosity of cooling liquid:

$$Re = \frac{\rho_{cl} D_h U}{\mu_{cl}} \quad (15)$$

$$Pr = \frac{\mu_{cl} c_{cl}}{k_{cl}} \quad (16)$$

The relationship between temperature, thermal resistance, and heat flow can be derived by using the Kirchhoff's Current Law [39]. For the  $\theta = N$  die layer, we can derive:

$$\frac{T_{BEOL,N} - T_{amb}}{R_{pk} + R_{PCB}} + \frac{T_{BEOL,N} - T_{mc,NB}}{R_{BEOL,N} + R_{con,NB}} = Q_N L^2 \quad (17)$$

$$\frac{T_{mc,NB} - T_{mc,NT}}{R_{con,NL}} + \frac{T_{mc,NB} - T_{avg,N}}{R_{conv} + R_{cl}} + \frac{T_{mc,NB} - T_{mc,NT}}{R_{con,NR}} = \frac{T_{BEOL,N} - T_{mc,NB}}{R_{BEOL,N} + R_{con,NB}} \quad (18)$$

$$\frac{T_{mc,NT} - T_{BEOL,(N-1)}}{R_{con,NT} + R_{bond,N}} = \frac{T_{mc,NB} - T_{mc,NT}}{R_{con,NL}} + \frac{T_{mc,NB} - T_{mc,NT}}{R_{con,NR}} \quad (19)$$

For the middle die layer ( $\theta = N - 1, N - 2, \dots, 3, 2$ ), we can deduce:

$$\frac{T_{BEOL,\theta} - T_{mc,\theta B}}{R_{BEOL,\theta} + R_{con,\theta B}} = Q_N L^2 + \frac{T_{mc,(\theta+1)T} - T_{BEOL,\theta}}{R_{con,(\theta+1)T} + R_{bond,(\theta+1)}} \quad (20)$$

$$\frac{T_{mc,\theta B} - T_{mc,\theta T}}{R_{con,\theta L}} + \frac{T_{mc,\theta B} - T_{avg,\theta}}{R_{conv} + R_{cl}} + \frac{T_{mc,\theta B} - T_{mc,\theta T}}{R_{con,\theta R}} = \frac{T_{BEOL,\theta} - T_{mc,\theta B}}{R_{BEOL,\theta} + R_{con,\theta B}} \quad (21)$$

$$\frac{T_{mc,\theta T} - T_{BEOL,(\theta-1)}}{R_{con,\theta T} + R_{bond,\theta}} = \frac{T_{mc,\theta B} - T_{mc,\theta T}}{R_{con,\theta L}} + \frac{T_{mc,\theta B} - T_{mc,\theta T}}{R_{con,\theta R}} \quad (22)$$

For the  $\theta = 1$  die layer, we can solve:

$$\frac{T_{\text{BEOL},1} - T_{\text{mc},1B}}{R_{\text{BEOL},1} + R_{\text{con},1B}} = Q_1 L^2 + \frac{T_{\text{mc},2T} - T_{\text{BEOL},1}}{R_{\text{con},2T} + R_{\text{bond},2}} \quad (23)$$

$$\frac{T_{\text{mc},1B} - T_{\text{mc},1T}}{R_{\text{con},1L}} + \frac{T_{\text{mc},1B} - T_{\text{avg},1}}{R_{\text{conv}} + R_{\text{cl}}} + \frac{T_{\text{mc},1B} - T_{\text{mc},1T}}{R_{\text{con},1R}} = \frac{T_{\text{BEOL},1} - T_{\text{mc},1B}}{R_{\text{BEOL},1} + R_{\text{con},1B}} \quad (24)$$

$$\frac{T_{\text{mc},1T} - T_{\text{amb}}}{R_{\text{con},1T}} = \frac{T_{\text{mc},1B} - T_{\text{mc},1T}}{R_{\text{con},1L}} + \frac{T_{\text{mc},1B} - T_{\text{mc},1T}}{R_{\text{con},1R}} \quad (25)$$

The relationship between the temperature of bottom wall of micro-channel  $T_{\text{mc},\theta B}$ , inlet temperature of micro-channel  $T_{\text{in},\theta}$  and outlet temperature of micro-channel  $T_{\text{out},\theta}$  can be given by eq. (26) [40]. In addition, the average temperature of cooling liquid  $T_{\text{avg},\theta}$  can be defined by eq. (27):

$$\ln \frac{T_{\text{mc},\theta B} - T_{\text{out},\theta}}{T_{\text{mc},\theta B} - T_{\text{in},\theta}} = - \frac{1}{R_{\text{conv}} R_{\text{cl}}} \quad (26)$$

$$T_{\text{avg},\theta} = \frac{T_{\text{in},\theta} + T_{\text{out},\theta}}{2} \quad (27)$$

### **The relationship between pump power and flow velocity of cooling liquid**

As the pump power is kept unchanged, the relationship between flow velocity of cooling liquid and geometric dimensions of micro-channel is mutual restraint. Both flow velocity of cooling liquid and geometric dimensions of micro-channel all can affect heat transfer performance of 3-D IC. Hence, it is prominent to investigate the impacts of different micro-channel size on the heat transfer performance of 3-D IC. Based on [41], the relationship between flow velocity of cooling liquid and pump power can be given by:

$$U = D_h \sqrt{\frac{P_p}{2w h_{\text{nf}} \text{Re} \mu_{\text{cl}} S}} \quad (28)$$

$$n = N \frac{S}{L} \quad (29)$$

$$f \text{Re} = 4.70 + 19.64 \frac{w^2 + h^2}{w + h} \quad (30)$$

where  $P_p$ ,  $n$ ,  $S$ , and  $f$  are the pump power, number of channels, side length of chip and friction factor, respectively.

### **Thermophysical properties of nanofluids as cooling liquid**

According to [42, 43], the thermophysical parameters for MWCNT based nanofluid and SWCNT based nanofluid as cooling liquids of micro-channel can be obtained by the eqs. (31)-(34). Here the water is adopted as the carrier of nanofluids:

$$\rho_{\text{nf}} = \phi \rho_{\text{np}} + (1 + \phi) \rho_{\text{wt}} \quad (31)$$

$$c_{nf} = \phi c_{np} + (1 + \phi) c_{wt} \quad (32)$$

$$k_{nf} = \frac{1 - \phi + \left(\frac{4\phi}{\pi}\right) \sqrt{\frac{k_{np}}{k_{wt}}} \operatorname{arctg}\left(\frac{\pi}{4} \sqrt{\frac{k_{np}}{k_{wt}}}\right)}{1 - \phi + \left(\frac{4\phi}{\pi}\right) \sqrt{\frac{k_{wt}}{k_{np}}} \operatorname{arctg}\left(\frac{\pi}{4} \sqrt{\frac{k_{wt}}{k_{np}}}\right)} k_{wt} \quad (33)$$

$$\mu_{nf} = \frac{\mu_{wt}}{(1 - \phi)^{2.5}} \quad (34)$$

where  $\phi$ ,  $\rho_{np}$ ,  $c_{np}$ , and  $k_{np}$  are volume fraction, density, specific heat capacity and thermal conductivity of nanoparticles, respectively,  $\rho_{wt}$ ,  $c_{wt}$ ,  $k_{wt}$ , and  $\mu_{wt}$  represent density, specific heat capacity, thermal conductivity and dynamic viscosity of water, respectively, and  $\rho_{nf}$ ,  $c_{nf}$ ,  $k_{nf}$ , and  $\mu_{nf}$  denote density, specific heat capacity, thermal conductivity and dynamic viscosity of nanofluids, respectively.

**Matrix equation of heat transfer in 3-D IC**

The equations from eqs. (17)-(25) contain  $3N$  variables, which can be solved by the matrix equation as:

$$FT = M \quad (35)$$

where  $F$  is a  $3N \times 3N$  multi-dimension sparse matrix that can be defined as:

$$F = \begin{bmatrix} \beta_1 & \beta_2 & 0 & 0 & 0 & 0 & 0 & \overbrace{0 \dots 0}^{3N-7} \\ \beta_3 & \beta_4 & \beta_5 & 0 & 0 & 0 & 0 & \overbrace{0 \dots 0}^{3N-7} \\ 0 & \beta_6 & \beta_7 & \beta_8 & 0 & 0 & 0 & \overbrace{0 \dots 0}^{3N-7} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \overbrace{0 \dots 0}^{3(N-\theta)-1} & \beta_9 & \beta_{10} & \beta_{11} & 0 & 0 & 0 & \overbrace{0 \dots 0}^{3\theta-5} \\ \overbrace{0 \dots 0}^{3(N-\theta)-1} & 0 & \beta_{12} & \beta_{13} & \beta_{14} & 0 & 0 & \overbrace{0 \dots 0}^{3\theta-5} \\ \overbrace{0 \dots 0}^{3(N-\theta)-1} & 0 & 0 & \beta_{15} & \beta_{16} & \beta_{17} & 0 & \overbrace{0 \dots 0}^{3\theta-5} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \overbrace{0 \dots 0}^{3N-7} & 0 & 0 & 0 & \beta_{18} & \beta_{19} & \beta_{20} & 0 \\ \overbrace{0 \dots 0}^{3N-7} & 0 & 0 & 0 & 0 & \beta_{21} & \beta_{22} & \beta_{23} \\ \overbrace{0 \dots 0}^{3N-7} & 0 & 0 & 0 & 0 & 0 & \beta_{24} & \beta_{25} \end{bmatrix} \quad (36)$$

where  $\theta$  is in the range of 2 to  $(N - 1)$ , and  $\beta_i$  ( $i = 1, 2, 3, \dots, 25$ ) can be solved as:

$$\beta_1 = \frac{1}{R_{pk} + R_{PCB}} + \frac{1}{R_{BEOI,N} + R_{con,NB}} \quad (37-1)$$

$$\beta_2 = \beta_3 = -\frac{1}{R_{BEOI,N} + R_{con,NB}} \quad (37-2)$$

$$\beta_4 = \frac{1}{R_{con,NL}} + \frac{1}{R_{conv} + R_{cl}} + \frac{1}{R_{con,NR}} + \frac{1}{R_{BEOI,N} + R_{con,NB}} \quad (37-3)$$

$$\beta_5 = \beta_6 = -\frac{1}{R_{con,NL}} - \frac{1}{R_{con,NR}} \quad (37-4)$$

$$\beta_7 = \frac{1}{R_{con,NT} + R_{bond,N}} + \frac{1}{R_{con,NL}} + \frac{1}{R_{con,NR}} \quad (37-5)$$

$$\beta_8 = -\frac{1}{R_{con,NT} + R_{bond,N}} \quad (37-6)$$

$$\beta_9 = -\frac{1}{R_{con,(\theta+1)T} + R_{bond,(\theta+1)}} \quad (37-7)$$

$$\beta_{10} = \frac{1}{R_{BEOI,\theta} + R_{con,\theta B}} + \frac{1}{R_{con,(\theta+1)T} + R_{bond,(\theta+1)}} \quad (37-8)$$

$$\beta_{11} = \beta_{12} = -\frac{1}{R_{BEOI,\theta} + R_{con,\theta B}} \quad (37-9)$$

$$\beta_{13} = \frac{1}{R_{con,\theta L}} + \frac{1}{R_{conv} + R_{cl}} + \frac{1}{R_{con,\theta R}} + \frac{1}{R_{BEOI,\theta} + R_{con,\theta B}} \quad (37-10)$$

$$\beta_{14} = \beta_{15} = -\frac{1}{R_{con,\theta L}} - \frac{1}{R_{con,\theta R}} \quad (37-11)$$

$$\beta_{16} = \frac{1}{R_{con,\theta T} + R_{bond,\theta}} + \frac{1}{R_{con,\theta L}} + \frac{1}{R_{con,\theta R}} \quad (37-12)$$

$$\beta_{17} = -\frac{1}{R_{con,\theta T} + R_{bond,\theta}} \quad (37-13)$$

$$\beta_{18} = -\frac{1}{R_{con,2T} + R_{bond,2}} \quad (37-14)$$

$$\beta_{19} = \frac{1}{R_{BEOI,1} + R_{con,1B}} + \frac{1}{R_{con,2T} + R_{bond,2}} \quad (37-15)$$

$$\beta_{20} = \beta_{21} = -\frac{1}{R_{BEOI,1} + R_{con,1B}} \quad (37-16)$$

$$\beta_{22} = \frac{1}{R_{\text{con},1L}} + \frac{1}{R_{\text{conv}} + R_{\text{cl}}} + \frac{1}{R_{\text{con},1R}} + \frac{1}{R_{\text{BEOL},1} + R_{\text{con},1B}} \quad (37-17)$$

$$\beta_{23} = \beta_{24} = -\frac{1}{R_{\text{con},1L}} - \frac{1}{R_{\text{con},1R}} \quad (37-18)$$

$$\beta_{25} = \frac{1}{R_{\text{con},1T}} + \frac{1}{R_{\text{con},1L}} + \frac{1}{R_{\text{con},1R}} \quad (37-19)$$

The  $3N \times 1$  matrix  $T$  represents the specific temperature of the stacked layer that can be expressed as:

$$T = [T_{\text{BEOL},N}, T_{\text{mc},NB}, T_{\text{mc},NT} \cdots T_{\text{BEOL},\theta}, T_{\text{mc},\theta B}, T_{\text{mc},\theta T} \cdots T_{\text{BEOL},1}, T_{\text{mc},1B}, T_{\text{mc},1T}]^T \quad (38)$$

The  $M$  is also a  $3N \times 1$  matrix, which is depended on the initial physical parameters of 3-D IC, and its expression can be solved by:

$$M = \left[ Q_N L^2 + \frac{T_{\text{amb}}}{R_{\text{pk}} + R_{\text{PCB}}} \frac{T_{\text{avg},N}}{R_{\text{conv}} + R_{\text{cl}}} 0 \cdots Q_\theta L^2 \frac{T_{\text{avg},\theta}}{R_{\text{conv}} + R_{\text{cl}}} 0 \cdots Q_1 L^2 \frac{T_{\text{avg},1}}{R_{\text{conv}} + R_{\text{cl}}} \frac{T_{\text{amb}}}{R_{\text{con},1T}} \right]^T \quad (39)$$

## Results and discussions

The heat transfer performance of 3-D IC with embedded micro-channel for applying different cooling liquids (*i.e.*, water, nanofluids and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$ ) are studied in this section. The thermophysical property parameters of water, nanoparticles (*i.e.*, SWCNT and MWCNT) and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  under ambient temperature are shown in tab. 1 [42, 44, 45].

**Table 1. The thermophysical property parameters of water, nanoparticles, and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$**

Materials	Density, [kgm <sup>-3</sup> ]	Specific heat capacity [Jkg <sup>-1</sup> K <sup>-1</sup> ]	Thermal conductivity [Wm <sup>-1</sup> K <sup>-1</sup> ]	Dynamic viscosity [Pa·s]
Water	996	4178	0.611	$8.59 \times 10^{-4}$
MWCNT	1600	796	3000	–
SWCNT	2600	425	6600	–
$\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$	6363.2	346.4	25.378	$2.22 \times 10^{-3}$

In this work, the 3-D IC is configured as a four-layers stacked chip, and the impacts of different micro-channel size on heat transfer performance of 3-D IC are analyzed by utilizing our proposed computational thermal model. All relevant physical and geometric parameters are shown in tab. 2. Additionally, it is assumed that each die layer has same physical configuration, in the meantime each BEOL layer generates the same amount of heat. All the computation results of our proposed model are carried out by MATLAB R2020b. In order to ensure the correctness of our proposed model, where the computation results are validated against the COMSOL simulation and previous study (*i.e.*, [46]), respectively. Here, the [46] has also proposed a numerical computation model to obtain steady-state temperature of 3-D IC with integrated micro-channel. Our computer configuration for CPU and memory are the Intel i7-12650H and 32 GB, respectively.

**Table 2. All relevant physical and geometric parameters of calculation unit**

Parameters	Values
Chip size ( $S \times S$ )	2000 $\mu\text{m} \times 2000 \mu\text{m}$
Unit size ( $L \times L$ )	80 $\mu\text{m} \times 80 \mu\text{m}$
Thickness and thermal conductivity of PCB ( $t_{\text{PCB}}$ and $k_{\text{PCB}}$ )	500 $\mu\text{m}$ , 0.8 W/mK
Thickness and thermal conductivity of package ( $t_{\text{pk}}$ and $k_{\text{pk}}$ )	200 $\mu\text{m}$ , 4.1 W/mK
Thickness and thermal conductivity of BEOL ( $t_{\text{BEOL}}$ and $k_{\text{BEOL}}$ )	10 $\mu\text{m}$ , 1.4 W/mK
Thickness and thermal conductivity of silicon substrate ( $t_{\text{si}}$ and $k_{\text{si}}$ )	60 $\mu\text{m}$ , 130 W/mK
Thickness and thermal conductivity of bonding-layer ( $t_{\text{bond}}$ and $k_{\text{bond}}$ )	5 $\mu\text{m}$ , 0.3 W/mK
Width and height of micro-channel ( $w$ and $h$ )	60 $\mu\text{m}$ , 50 $\mu\text{m}$
Center distance of micro-channel ( $D_{\text{mc}}$ )	80 $\mu\text{m}$
Heat generated by each die layer ( $Q$ )	$1.25 \times 10^6 \text{ W/m}^2$
Ambient temperature and inlet temperature of micro-channel ( $T_{\text{amb}}$ and $T_{\text{in},\theta}$ )	28 $^{\circ}\text{C}$

### Heat transfer performance of novel cooling liquids

In this work, the specific temperature of each stacked die layer is calculated by utilizing our proposed computational thermal model, which take the different type of cooling liquids (*i.e.*, water, nanofluids, and liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$ ) into account. Here, the micro-channel size is kept unchanged and the flow velocity of cooling liquid is set as 1 m/s. In addition, the volume fraction of SWCNT and MWCNT as nanoparticles in nanofluid are all adopted as 0.03 [47].

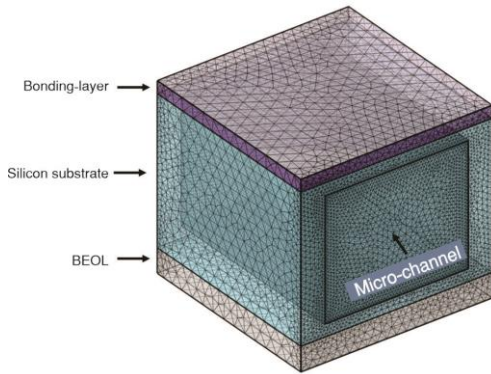
### Results of heat transfer performance for using different cooling liquids

The calculation temperature results of each BEOL die layer for water, nanofluids and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquids are listed in tab. 3. As shown in tab. 3, it is obvious that the nanofluids and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquids have lower temperature than the conventional water scheme for any stacked die layer. Meanwhile it is inferred from tab. 3 that the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid has the lowest temperature when compared with the other cooling liquids (*i.e.*, water and nanofluids) for all stacked die layer. Using the  $\theta = 3$  die layer as an example, the temperature reduction for MWCNT based nanofluid, SWCNT based nanofluid and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid schemes are exceeding 25.698%, 28.771%, and 35.735%, respectively, as compared with the conventional water scheme. Therefore, the nanofluids and liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  for substituting the traditional water as cooling liquids of micro-channel have excellent application prospect in enhancing the heat transfer performance of 3-D IC.

**Table 3. The temperature results of each BEOL layer for using different cooling liquids**

Type of cooling liquid	Temperature of BEOL layer, $T_{\text{BEOL},\theta}$ ( $^{\circ}\text{C}$ )			
	$\theta = 1$	$\theta = 2$	$\theta = 3$	$\theta = 4$
Water	40.914	53.470	58.830	63.921
MWCNT based nanofluid	37.585	42.258	43.712	47.261
SWCNT based nanofluid	37.127	40.828	41.904	45.269
$\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$	35.948	37.445	37.807	40.719

The simulation models for adopting the water, nanofluids and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquids of micro-channel are established to verify the accuracy of our proposed computational thermal model by utilizing COMOSL simulation in this work, respectively. The mesh type of our COMOSL simulation model is adopted as the tetrahedral division, where the general size of mesh elements is configured as *extremely fine*, and the corresponding single die layer of



**Figure 4. The single die layer of calculation unit with embedded micro-channel for adopting the tetrahedral mesh with the extremely fine division**

calculation unit is shown in fig. 4. Herein, the smallest element size is predefined in COMSOL simulation, which can guarantee the grid convergence. The COMSOL software utilized an iterative scheme to solve the governing partial differential equations, and the prescribed converging tolerance is 0.0001. The equations are solved iteratively behind till the individual values reach stability, or converge.

In the simulation process of solving steady-state temperature, the governing equations of mass, momentum, and energy can be listed as [48]:

- The continuity equation for the fluid:

$$\nabla(\rho_{cl}U) = 0$$

- The momentum equation for the fluid:

$$(U\nabla)\rho_{cl}U = -\nabla p + \mu_{cl}\nabla^2U$$

- The energy equation for the fluid:

$$\rho_{cl}c_{cl}U\nabla T = k_{cl}\nabla^2T$$

- The energy equation for the solid:

$$k_s\nabla^2T = 0$$

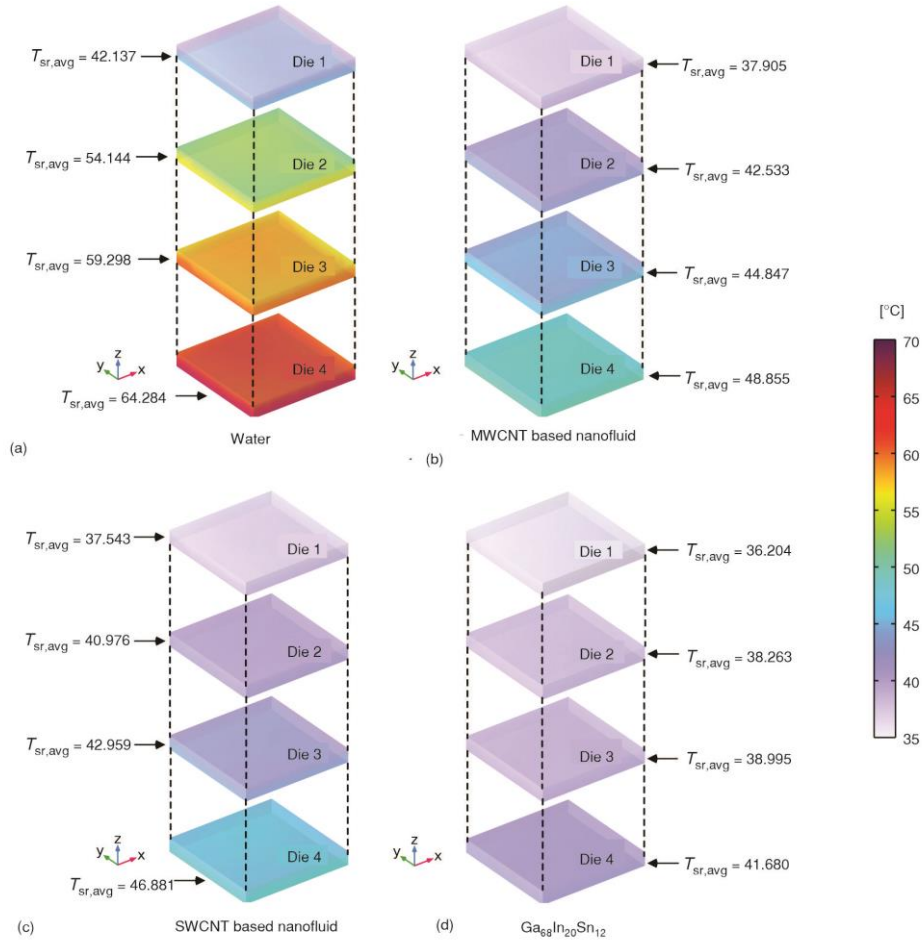
where  $p$  and  $k_s$  represent the pressure and thermal conductivity of solid, respectively.

The boundary condition and assumptions for COMSOL simulation model are listed as [49]:

- The heat transfer in solid and fluid module are coupled by using the non-isothermal flow feature.
- The micro-channel inlet boundary conditions are configured as uniform temperature  $T_{in}$  with a uniform flow velocity  $U$ .
- The flow is assumed to be steady and fully developed in each channel.
- The ambient temperature of physical field is adopted as  $T_{amb}$ .
- The top surface of  $\theta = 1$  die layer and bottom surface of PCB of 3-D IC are configured as natural convection, and other surfaces are set as adiabatic state.

The corresponding temperature results of COMSOL simulation of all BEOL die layer for using different cooling liquids are exhibited in fig. 5. Herein, the simulation temperature of each BEOL die layer are obtained by the average steady-state temperature  $T_{sr,avg}$ . The  $T_{sr,avg}$  is defined as  $T_{sr,avg} = T_{sr,sum}/P_{sum}$ , where  $T_{sr,sum}$  represents the total temperature of all extracted points, and  $P_{sum}$  denotes the number of all extracted points. In addition, the points separated by  $5 \mu m$  in the  $x$ -,  $y$ -. and  $z$ -directions on the BEOL die layer are selected as the extracted points, and the corresponding total extracted points are 867 in this work. Based on the analysis of results, it can be found that the conclusions obtained from fig. 5 have close agreement with the tab. 3.

Moreover, the comparison results for our proposed computational model and COMSOL simulation are shown in fig. 6. In the meantime, the corresponding relative error results of



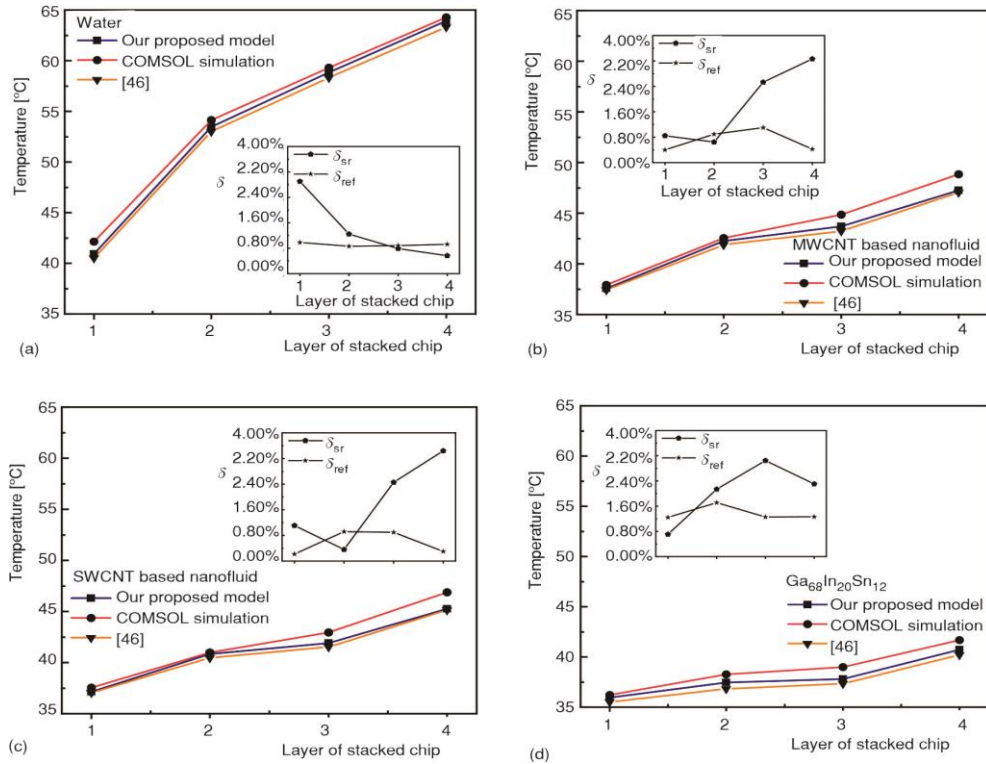
**Figure 5. The simulation temperature results of all BEOL die layer for using different cooling liquids; (a) water as cooling liquid, (b) MWCNT based nanofluid as cooling liquid, (c) SWCNT based nanofluid as cooling liquid, and (d)  $Ga_{68}In_{20}Sn_{12}$  as cooling liquid**

all stacked die layer for them are depicted in fig. 6. Where the relative error is defined as  $\delta = |T_{cr} - T_{sr,avg}|/T_{sr,avg}$ . Herein  $T_{cr}$  represents the temperature of our proposed computational model. Besides, in order to further ensure the accuracy of our proposed numerical computation model, their numerical results are validated with the numerical model of [46]. Meanwhile, the corresponding relative error results of all stacked die layer involved in them are also described in fig. 6, and the relative error is expressed as  $\delta_{ref} = |T_{cr} - T_{ref}|/T_{ref}$ . Wherein  $T_{ref}$  denotes that the temperature results are obtained by the numerical model of [46].

From the displayed fig. 6, it is evidently seen that the results of our proposed computation thermal model are fairly consistent with the COMOSL simulation results and the computation results of [46] in all cooling liquids, and the maximum relative error for them is less than 4%.

The differences of memory consumption and running time of CPU between our proposed numerical computation model, COMOSL simulation model and the numerical model of

[46] are investigated in this section. The corresponding results of all cooling liquids for them are listed in tab. 4, respectively.



**Figure 6.** The comparison results for our proposed computational thermal model, COMSOL simulation and the numerical model of [46]; (a) water as cooling liquid, (b) MWCNT based nanofluid as cooling liquid, (c) SWCNT based nanofluid as cooling liquid, and (d)  $Ga_{68}In_{20}Sn_{12}$  as cooling liquid

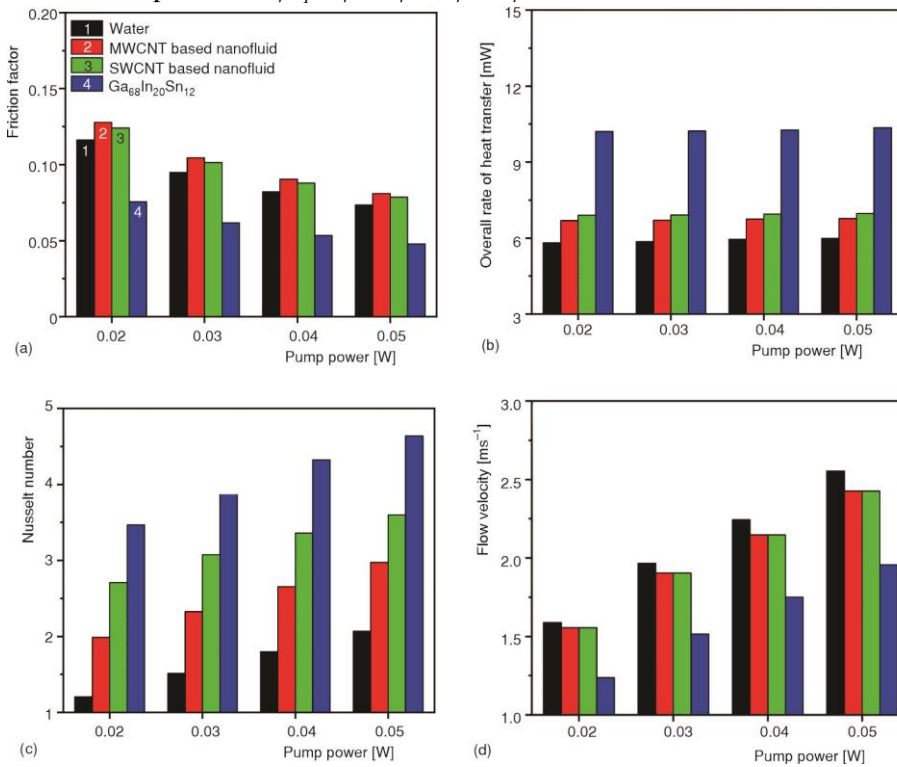
**Table 4.** The memory consumption and running time of CPU for solving temperature results of different types of cooling liquids

Working fluid type	Memory consumption and running time of CPU		
	Our proposed model	COMSOL simulation	[46]
Water	5.1 GB and 181 s	13.1 GB and 1479 s	7.8 GB and 547 s
MWCNT based nanofluid	5.2 GB and 196 s	13.3 GB and 1580 s	7.9 GB and 559 s
SWCNT based nanofluid	5.3 GB and 209 s	13.4 GB and 1588 s	8.0 GB and 584 s
$Ga_{68}In_{20}Sn_{12}$	5.3 GB and 203 s	13.2 GB and 1509 s	7.9 GB and 563 s

As described in tab. 4, it is remarkable that our proposed computation model can effectively reduce the memory consumption and running time of CPU as compared with the COMSOL simulation and the numerical model of [46]. Taking the  $Ga_{68}In_{20}Sn_{12}$  as cooling liquid as an instance, the memory consumption of our proposed model can be reduced over 59.848% and 32.911% than the COMSOL simulation and [46], respectively, and the corresponding running time of CPU for them can be reduced over 86.547% and 63.943%, respectively. Consequently, our proposed computation thermal model can prominently reduce memory consumption and significantly improve CPU operating efficiency when compared with COMSOL simulation and the similar study (*i.e.*, [46]).

### Discussions of thermophysical parameters for using different cooling liquid

In order to analyze the heat transfer performance for using different cooling liquid cases, the key thermophysical parameters concerning friction factor, rate of heat transfer, Nusselt number and flow velocity are investigated in this work when the range of pump power is from 0.02 to 0.05 W [50, 51]. The corresponding results are depicted in fig. 7, respectively. Here, according to Newton's law of cooling, the rate of heat transfer for  $\theta^{\text{th}}$  die layer can be defined as  $\psi_{\theta} = A_m h_{cl}(T_{mc,\theta B} - T_{avg,\theta})$  [52]. The overall rate of heat transfer  $\psi_{ov}$  for all die layer of 3-D IC can be expressed as  $\psi_{eq} = \psi_1 + \psi_2 + \psi_3 + \psi_4$ .



**Figure 7. The key thermophysical parameters with different pump power for using different cooling liquids; (a) friction factor, (b) overall rate of heat transfer, (c) Nusselt number and (d) flow velocity**

As shown in fig. 7(a), it can be seen that the friction factor of  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid is smaller than other cooling liquids. The reason behind this is that the kinematic viscosity ( $= \mu_{cl}/\rho_{cl}$ ) of  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  is much smaller than other cooling liquids, thus the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid has a lower friction factor based on the eqs. (15) and (30).

As depicted in fig. 7(b), the overall rate of heat transfer for MWCNT based nanofluid, SWCNT based nanofluid and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid cases are larger than water as cooling liquid case. In the meantime, it can be observed from fig. 7(b) that the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid case has the largest overall rate of heat transfer as compared with other cooling liquid cases. This can be explained that the overall rate of heat transfer decreases with the increase of convection thermal resistance  $R_{\text{conv}}$  based on the aforementioned discussion and eq. (8).

Based on the eqs. (13)-(16), the Nusselt number for all cooling liquids can be solved, which are exhibited in fig. 7(c). The fig. 7(c) shows that the Nusselt number of MWCNT based nanofluid, SWCNT based nanofluid and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquids are larger than the conventional water case, meanwhile the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid has the largest Nusselt number in comparison with other cooling liquid cases. Besides, it can be seen from fig.7(c) that the Nusselt number for all cooling liquids increases as the pump power increases. This is due to the fact that the flow velocity of cooling liquid increases with the increase of the pump power, thereby resulting in the increase of Reynolds number, then lead to the Nusselt number increase according to eqs. (13) and (15).

The results of fig. 7(d) show that the flow velocity of water as cooling liquid is greater than other cooling liquids under the same pump power condition. The reason for this phenomenon is that the equivalent dynamic viscosity of water is smaller than other cooling liquids, and the flow velocity decreases as dynamic viscosity increases based on the eq. (28).

#### *Discussions of heat transfer performance for using different cooling liquid*

Based on the results of this section, it is concluded that the steady-state temperature of all die layer for using the MWCNT based nanofluid, SWCNT based nanofluid and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquids are lower than the conventional water case. Meanwhile the steady-state temperature of all die layer for the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid is lower than other cooling liquids. The reason behind this is that the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  has the largest thermal conductivity as compared with other cooling liquids, in the meantime the water has the smallest thermal conductivity in comparison with other cooling liquids. Therefore, the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  and water as cooling liquids have the smallest and largest convection thermal resistance when compared with other cooling liquids based on eqs. (8) and (10). Consequently, the 3-D IC with integrated micro-channel for the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  as cooling liquid has the lowest steady-state temperature as compared with the cases of MWCNT based nanofluid, SWCNT based nanofluid and water as cooling liquids. Certainly, the nanofluids and liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  can be regarded as an effective solution for substituting the traditional water as cooling liquid of micro-channel to enhance heat transfer performance of 3-D IC in the future application.

In addition, it can be inferred that our proposed computation thermal model can obviously reduce memory consumption and running time of CPU when compared with COMSOL simulation. This can be explained that the COMSOL simulation software is implemented by a steady-state solver to calculate the temperature results, which is required to execute the steps for discrete grid and iterative calculations. There is no doubt that these steps need to spend more CPU execution time and memory consumption. However, the numerical computation model has no the steps of discrete grid and iterative calculation in the process of solving steady-state temperature.

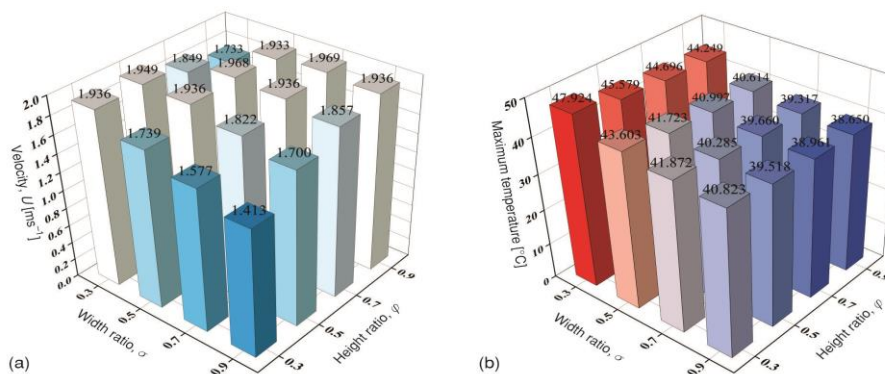
#### ***Effects of micro-channel size on heat transfer performance of 3-D ICs***

The flow velocity of cooling liquid and the contact area between the micro-channel and cooling liquid are determined by micro-channel size according to eqs. (11), (12), and (28), which can affect the value of convection thermal resistance and thermal resistance of cooling liquid. Hence, it is crucial to investigate the effects of micro-channel size on heat transfer performance of micro-channel. Therefore, the effects of micro-channel size on steady-state temperature of 3-D IC are investigated in this section. Here, the pump power is fixed and its value is set as 0.05 W. And the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  is adopted as the cooling liquid of micro-channel in this

section owing to its excellent heat transfer performance. Besides, the  $\sigma$  ( $\sigma = w/L$ ) and  $\varphi$  ( $\varphi = h/t_{si}$ ) are defined as the width ratio of micro-channel and height ratio of micro-channel, respectively. In addition, it is reported from [53, 54] that the ranges of width ratio  $\sigma$  of micro-channel and height ratio  $\varphi$  of micro-channel are all adopted as from 0.3 to 0.9.

#### Results for effects of micro-channel size on heat transfer performance of 3-D ICs

The calculation results concerning flow velocity of cooling liquid and the maximum temperature are exhibited in fig. 8. As depicted fig. 8(a), it is found that the maximum and minimum flow velocity of cooling liquid are 1.969 m/s (*i.e.*, when  $\sigma = 0.7$  and  $\varphi = 0.9$ ) and 1.413 m/s (*i.e.*, when  $\sigma = 0.9$  and  $\varphi = 0.3$ ) under different micro-channel size, respectively. Consequently, the effects of geometry size of micro-channel on the flow velocity of cooling liquid ought to be taken into consideration when the pump power is fixed. In order to further investigate the impacts of micro-channel size on the temperature of 3-D IC, the corresponding calculation results regarding the maximum temperature of four-layers stacked chip versus the micro-channel size are presented in fig. 8(b). Here, the pump power is still kept unchanged. As shown in fig. 8(b), it is suggested that the maximum temperature of all die layer occurs its lowest value of 38.650 °C when the micro-channel size reach to its maximum value (*i.e.*, the maximum micro-channel size with  $\sigma = 0.9$  and  $\varphi = 0.9$ ). Meanwhile, it can be inferred that the maximum temperature of all die layer for the maximum micro-channel size case (*i.e.*,  $\sigma = 0.9$  and  $\varphi = 0.9$ ) can be reduced over 19.351% than the minimum micro-channel size case (*i.e.*,  $\sigma = 0.3$  and  $\varphi = 0.3$ ). Apparently, expanding the micro-channel size can significantly improve the heat transfer performance of 3-D IC as the pump power is fixed.

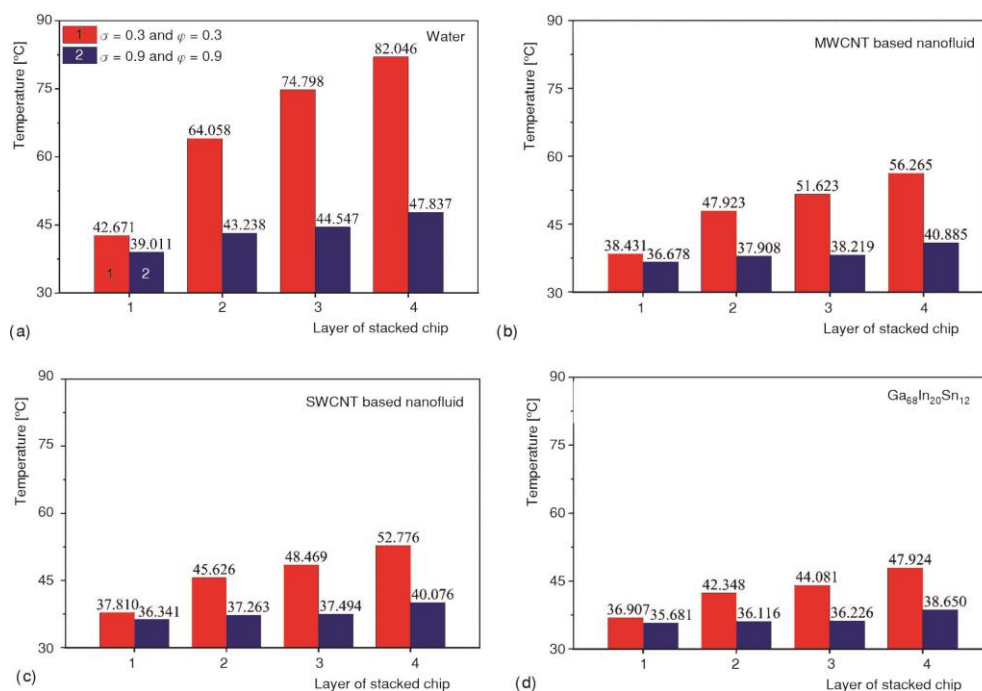


**Figure 8.** The calculation results concerning; (a) flow velocity of cooling liquid vs. micro-channel size and (b) the maximum temperature of 3-D IC vs. micro-channel size

The heat transfer performance of different type of cooling liquids under the maximum micro-channel size (*i.e.*,  $\sigma = 0.9$  and  $\varphi = 0.9$ ) and the minimum micro-channel size (*i.e.*,  $\sigma = 0.3$  and  $\varphi = 0.3$ ) are investigated, and the corresponding temperature results are displayed in fig. 9.

As described in fig. 9, it is implied that the temperature of each die layer can be obviously reduced by expanding the micro-channel size when the pump power is fixed. Using the  $\theta = 4$  die layer as an example, the temperature for water, MWCNT based nanofluid, SWCNT based nanofluid and  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  under the maximum micro-channel size case are reduced by 41.695%, 27.335%, 24.064%, and 19.351% than the minimum micro-channel size case, respectively. Besides, it can be concluded from fig. 9 that the heat transfer performance of nanofluids

and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquids is still better than the conventional water as cooling liquid scheme. Taking the  $\theta = 3$  die layer as an example, the reduction percentages of temperature for MWCNT based nanofluid, SWCNT based nanofluid and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquids under the maximum micro-channel size scheme are exceeding 14.533%, 16.224%, and 19.205%, respectively, as compared with the conventional water scheme. Apparently, the nanofluids and liquid metal Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> can be applied as the promising cooling liquids of micro-channel for enhancing heat transfer performance of 3-D IC.



**Figure 9. The specific temperature of each die layer of 3-D IC for applying different type of cooling liquids under the maximum micro-channel size and the minimum micro-channel size; (a) water as cooling liquid, (b) MWCNT based nanofluid as cooling liquid, (c) SWCNT based nanofluid as cooling liquid, and (d) Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquid**

*Discussions for effects of micro-channel size on heat transfer performance of 3-D IC*

According to the results of this section, it can be deduced that the heat transfer performance of 3-D IC can be effectively enhanced by expanding the micro-channel size. This is due to the fact that the convective thermal resistance and thermal resistance of cooling liquid decrease with the increase of micro-channel size, thereby reducing the steady-state temperature. Besides, it is demonstrated that the nanofluids and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquids under the maximum micro-channel size scheme still have better heat transfer performance in comparison with the conventional water as cooling liquid. This can be explained that the nanofluids and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquids possess a lower convection thermal resistance as compared with the traditional water case on the basis of the aforementioned discussions. Therefore, expanding the micro-channel size can be seemed as a prospective method for enhancing heat transfer performance of 3-D IC.

### **Effects flow velocity of cooling liquid on heat transfer performance of 3-D IC**

The effects of flow velocity of cooling liquid on heat transfer performance of 3-D IC are investigated for this section. In order to obtain the different flow velocity of cooling liquid, the pump power is no longer kept unchanged. Here, the geometric dimensions of micro-channel are set as the maximum micro-channel size with  $\sigma = 0.9$  and  $\varphi = 0.9$ , and the  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$  is selected as the cooling liquid of micro-channel.

#### *Results for effects flow velocity of cooling liquid on heat transfer performance of 3-D IC*

The temperature results versus flow velocity of cooling liquid are shown in tab. 5. As illustrated in tab. 5, it is indicated that the temperature of all die layer decreases with the increase of flow velocity of cooling liquid. For instance, the temperature reduction for the die layer  $\theta = 2$  can exceed 2.5 °C when the flow velocity of cooling liquid increases from 0.5 m/s to 2 m/s. Besides, it is also found that the pump power also increases as the flow velocity of cooling liquid increases. As an instance, the pump power is increased over 17 times as the flow velocity of cooling liquid increases from 0.5 m/s to 2 m/s.

**Table 5. The temperature results of 3-D IC under different flow velocity of cooling liquid**

Flow velocity of cooling liquid	Pump power	Temperature of BEOL layer, $T_{\text{BEOL},\theta}$ [°C]			
		$\theta = 1$	$\theta = 2$	$\theta = 3$	$\theta = 4$
0.5 m/s	0.003 W	37.050	38.662	39.080	41.841
1 m/s	0.013 W	36.217	37.035	37.239	39.791
1.5 m/s	0.030 W	35.863	36.416	36.555	39.022
2 m/s	0.053 W	35.660	36.081	36.188	38.607

#### *Discussions for effects flow velocity of cooling liquid on heat transfer performance of 3-D IC*

According to the results of tab. 5, it can be implied that the heat transfer performance of 3-D IC can be further improved by increasing the flow velocity of cooling liquids. The reason behind this is that the volume flow-rate increases as the flow velocity of cooling liquid increases, then lead to the decrease of thermal resistance of cooling liquid combining of eqs. (9) and (12). Meanwhile, the power consumption of the pump will increase as the flow velocity of cooling liquid increases based on eq. (28). Therefore, the constraint relationship between the pump power and the flow velocity of cooling liquid ought to be considered in the thermal design of 3-D IC.

### **Conclusions**

This paper proposed the novel cooling liquids (*i.e.*, MWCNT based nanofluids, SWCNT based nanofluid and liquid metal  $\text{Ga}_{68}\text{In}_{20}\text{Sn}_{12}$ ) for replacing the conventional water to enhance heat transfer performance of 3-D IC with integrated micro-channel. In order to quickly obtain the steady-state temperature of 3-D IC for using different types of cooling liquids, the corresponding numerical thermal model is established. Moreover, the effects of micro-channel size and flow velocity of cooling liquid on heat transfer performance of 3-D IC are investigated by using our proposed computation model in this work. The main findings of this work are listed as follows.

- The reduction of steady-state temperature for MWCNT based nanofluid, SWCNT based nanofluid and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquid cases are exceeding 25.698%, 28.771%, and 35.735%, respectively, as compared with the conventional water case.
- Expanding the micro-channel size can be regarded as an effective method to improve heat transfer performance of 3-D IC. The steady-state temperature for water, MWCNT based nanofluid, SWCNT based nanofluid and Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquid cases can be reduced by 41.695%, 27.335%, 24.064% and 19.351% when the width ratio and height ratio of micro-channel increase from 0.3 to 0.9.
- The steady-state temperature of 3-D IC decreases with the increase of flow velocity of cooling liquid. Meanwhile the pump power will increase as the flow velocity of cooling liquid increases.
- The results of our proposed computation thermal model have close agreement with the results of COMSOL simulation, and the maximum relative error involved in them is not exceeding 4%. In the meantime, the memory consumption and running time of CPU for our proposed computation thermal model can be reduced over 59.848% and 86.547% than COMSOL simulation, respectively.

In the light of the presented results in this paper, it can be expected that the proposed new technology for utilizing the nanofluids and liquid metal Ga<sub>68</sub>In<sub>20</sub>Sn<sub>12</sub> as cooling liquids can be as an emerging technology to improve the heat transfer performance of 3-D IC.

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### Nomenclature

$A$	– cross-sectional area, [m <sup>2</sup> ]	$Q$	– heat generated, [Wm <sup>-2</sup> ]
$A_m$	– heat transfer area, [m <sup>2</sup> ]	$R$	– thermal resistance, [KW <sup>-1</sup> ]
$c$	– specific heat capacity, [Jkg <sup>-1</sup> K <sup>-1</sup> ]	Re	– Reynolds number, [–]
$D_h$	– hydraulic diameter, [m]	$S$	– side length of chip, [m]
$D_{mc}$	– distance of each micro-channel, [m]	$T$	– temperature, [°C]
$f$	– friction factor, [–]	$t$	– thickness, [m]
$h$	– height of micro-channel, [m]	$U$	– flow velocity, [ms <sup>-1</sup> ]
$h_{cl}$	– heat transfer coefficient, [Wm <sup>-2</sup> K <sup>-1</sup> ]	$V_{cl}$	– volume flow-rate, [m <sup>3</sup> s <sup>-1</sup> ]
$k$	– thermal conductivity, [Wm <sup>-1</sup> K <sup>-1</sup> ]	$w$	– width of micro-channel, [m]
$L$	– side length of calculation unit, [m]		
$n$	– number of channels, [–]	<i>Greek symbols</i>	
Nu	– Nusselt number, [–]	$\beta$	– matrix elements
$P_p$	– pump power, [W]	$\delta$	– relative error
Pr	– Prandtl number, [–]	$\mu$	– dynamic viscosity, [Pa·s]

$\rho$  – density, [kgm<sup>-3</sup>]  
 $\phi$  – volume concentration  
 $\psi$  – heat transfer rate, [mW]

#### Subscripts

amb – ambient  
 avg – average  
 bond – bonding-layer of 3D-ICs  
 cl – cooling liquid  
 con – conduction  
 conv – convection  
 cr – calculation results  
 in – inlet  
 mc – micro-channel  
 nf – nanofluid

np – nanoparticles  
 out – outlet  
 ov – overall  
 pk – package of 3D-IC  
 ref – reference  
 sr – simulation results  
 si – silicone  
 wt – water

#### Acronyms

BEoL – back end of line  
 IC – integrated circuits  
 MWCNT – multi-wall carbon nanotubes  
 PCB – printed circuit board  
 SWCNT – single-wall carbon nanotubes

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