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Cold Sprayed Copper-Diamond Composites for Thermal Management of Semiconductor Packages

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Abstract—**Thermal management is key to enabling increasingly powerful chips and heterogeneous integrated 2.5D/3-D systems. Composite materials with high thermal conductivities that can be placed at different levels of proximity to the die provide new solutions for heat dissipation. Here we report the fabrication of thick copper-diamond composite films using cold spray, which is a high-throughput, low-thermal-budget deposition technology. In cold spray, feedstock micro powder is accelerated in a specially designed nozzle by a heated pressurized gas and adheres to the substrate upon high-speed impingement. This process achieves higher deposition rates than other methods used in semiconductor manufacturing (such as electroplating). It also produces films that are denser and much less porous than ones produced by conventional thermal spray techniques. In this work, we first use process and thermal simulations to determine the requirements of the micro diamond powder feedstock, including the diamond core size, metal-clad thickness, core-clad interfacial resistance, and volume fraction to enable the cold spray of copper-diamond composites with thermal conductivities that are higher than copper. Subsequently, we perform a systematic characterization of the diamond powders from several suppliers, including the purity, metal oxygen content, particle morphology, and metal-clad adhesion. This characterization reveals the challenges of meeting all the specs using currently available diamond powders. Finally, we cold spray copper-diamond composite films on a variety of substrates with tunable thicknesses between 100 μm and 2 mm, achieving a thermal conductivity that is approximately 10% higher than cold-sprayed pure copper. Further improvement of the thermal properties relies on continued innovation in powder surface modification and powder storage/shipping methods.**

Keywords—**Cold spray, thermal management copper-diamond composite, 3D heterogeneous integration**

Introduction

The advent of multichip composite devices and in particular, 3-D stacked-die architectures, and necessitates new thermal management solutions to enable heat dissipation from packages with increasing power. Materials with high thermal conductivities are desired that can be either directly deposited on the silicon backside at the wafer level or manufactured into advanced heat spreaders to be attached at the package level.

Recently, composite materials comprised of metal matrices and fillers have been explored as candidates for thermal vias and heat spreaders. Among them, copper-diamond is a favorable combination because both components demonstrate almost the highest thermal conductivities in their respective categories (metal matrix and nonmetal filler), holding promise for composites with thermal conductivities that are higher than copper. However, the existing techniques for manufacturing copper-diamond composites, e.g., electroplating, and different sintering techniques like spark plasma sintering, are neither cost-effective nor scalable when utilized for semiconductor high-volume manufacturing applications [1]. While some achieved favorable thermal conductivities, the fabrication either required unconventional tool configuration as in electroplating (to include diamond) and took a hit on throughput or required a very high thermal budget (>600°C) and needed a separate bonding step to the substrates of interest [2, 3].

Previously, our team reported that cold spray technology provided a new, scalable, and high throughout manufacturing approach to solve some of the thermomechanical challenges of semiconductor packaging [4]. For example, thick metal structures such as blanket copper or aluminum films, when cold sprayed on the die backside at the wafer level, can help with heat spreading and mitigation of package warpage simultaneously (Figs. 1a and 1b).

To study the applicability of cold spray to materials that are more thermally conductive than copper, we evaluate and report in this work the use of this technology to create copper-diamond composites. We first outline the feedstock material specifications, including powder size, morphology, and required chemical modifications to enable the high thermal conductivities that are possible in theory. This is followed by experimental characterizations of various diamond powders, providing important learnings on the material challenges and improvements needed. Finally, we cold spray and characterize the morphologies and thermal conductivities of composite copper-diamond films, discussing the observed deviation from theoretical values.

Materials and Methods

A. LS-DYNA Simulation of Particle Impingement

We conducted an LS-DYNA explicit dynamics simulation of a spherical particle impingement on diamond-embedded copper surface with the Lagrange method. A 3-D model with quarter symmetry is adopted to reduce the computational cost, and the fully coupled thermal-structural analysis is performed. Key parameters used in the simulation are adopted from the literature [5]. Copper follows the Johnson-Cook plasticity relationship and diamond follows linear elasticity. The simulated geometry assumes tied contact between the diamond and the copper clad and omits the nanoscale interlayer in between.

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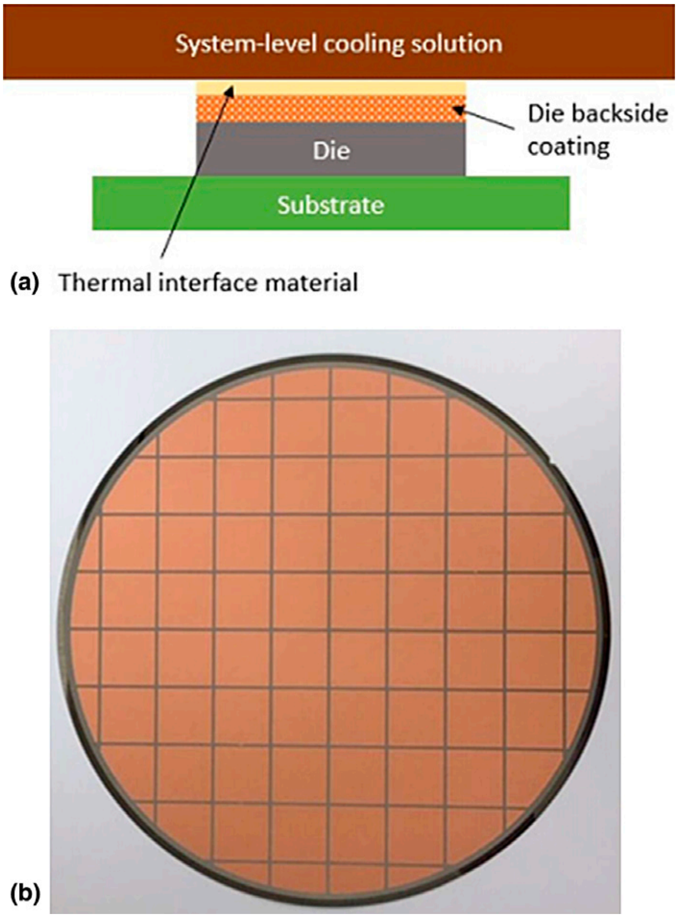

Fig. 1. (a) Schematic illustration of die-backside cold sprayed metal film. (b) Cold-sprayed copper film on a silicon wafer. Images edited from Ref. [1].

The velocity of the particle is estimated using the process parameters, i.e., acceleration pressure and gas temperature, and the dimensional information of the spray nozzle.

B. Microstructure and Chemical Characterization of Copper Cladded Diamond Powders

We observed the cross-section of incoming copper-clad diamond particles and sprayed films using scanning electron microscopy (SEM). We characterized the oxygen content in copper using the standard instrumental gas analysis. The thermal conductivity of the sprayed copper-diamond films was derived from the laser flash diffusivity measurement.

Results and Discussion

A. Cold Spray Unique Benefits in Composite Manufacturing

Cold spray is a solid-state deposition technology. The powder feedstock is fed into a customized converging-diverging nozzle and mixed with a heated pressurized gas, such as nitrogen, helium, or even compressed air. The schematic illustration is shown in Fig. 2. The gas expands and cools down as it flows through the nozzle, while simultaneously accelerating the powder it carries. The substrate temperature during deposition can

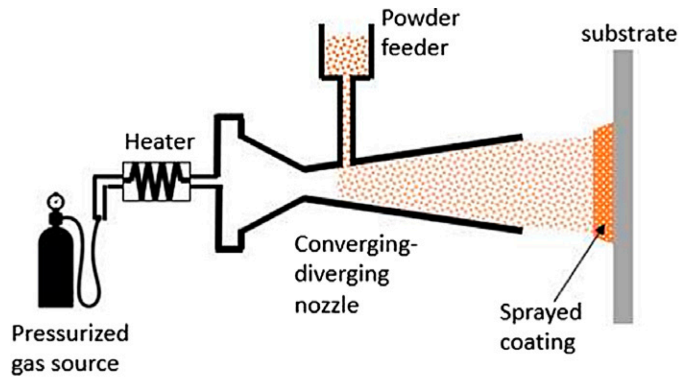

Fig. 2. Schematic illustration of the cold spray equipment.

be kept below 100-200°C, making cold spray compatible with low thermal budget substrates. Additionally, the sprayed film's properties can be tuned with greater flexibility than other high-temperature deposition techniques since the deposition temperature during cold spray remains much lower than the material's melting or phase transition temperatures. Finally, cold spray has a deposition rate (μm/min) that is several orders of magnitude faster than other approaches typically used in semiconductor manufacturing (e.g., electroplating or chemical vapor deposition). All these advantages make cold spray well suited for the fast deposition of high thermal conductivity copper-diamond composites provided that powders with low impurity, low oxidation levels, and high crystallinity are used as precursors.

B. Feedstock Material Design and Challenges

We first use effective medium theory to study the dependency of the composite's thermal conductivity on the diamond particles' diameter, thermal boundary resistance R_b, and volume fraction in the copper matrix. The theory approximates the filler particles to be nonpercolated spheres and k_c, k_p, k_m in eq. (1) refers to thermal conductivities of the composite, diamond filler and copper matrix, and d is the filler particle diameter.

$$\frac{k_c}{k_m} = \frac{[k_p(1+2\alpha)+2k_m]+2\phi[k_p(1-\alpha)-k_m]}{[k_p(1-2\alpha)+2k_m]-\phi[k_p(1-\alpha)-k_m]} \quad (1)$$

$$\alpha = \frac{2R_b k_m}{d} \quad (2)$$

Since R_b is nonzero, the diameter of the diamond particles needs to exceed a threshold value for the composite's thermal conductivity to exceed that of copper, as shown in Fig. 3a and b. Below this threshold diameter, the thermal boundary resistance dominates due to phonon scattering at the copper-diamond interface and causes the composite's thermal conductivity to drop below that of copper. Consequently, smaller diamond powders impose stricter requirements on how low the value of R_b needs to be. As R_b increases, the thermal benefit from the inclusion of the diamond filler in the matrix gradually diminishes.

One unique challenge during the cold spray of hard and brittle powders such as unclad diamonds is their fracture and/or rebounding from the film upon impingement. For the case of copper-diamond composites, this reduces both the volume fraction as well as the effective diameter of diamond particles in

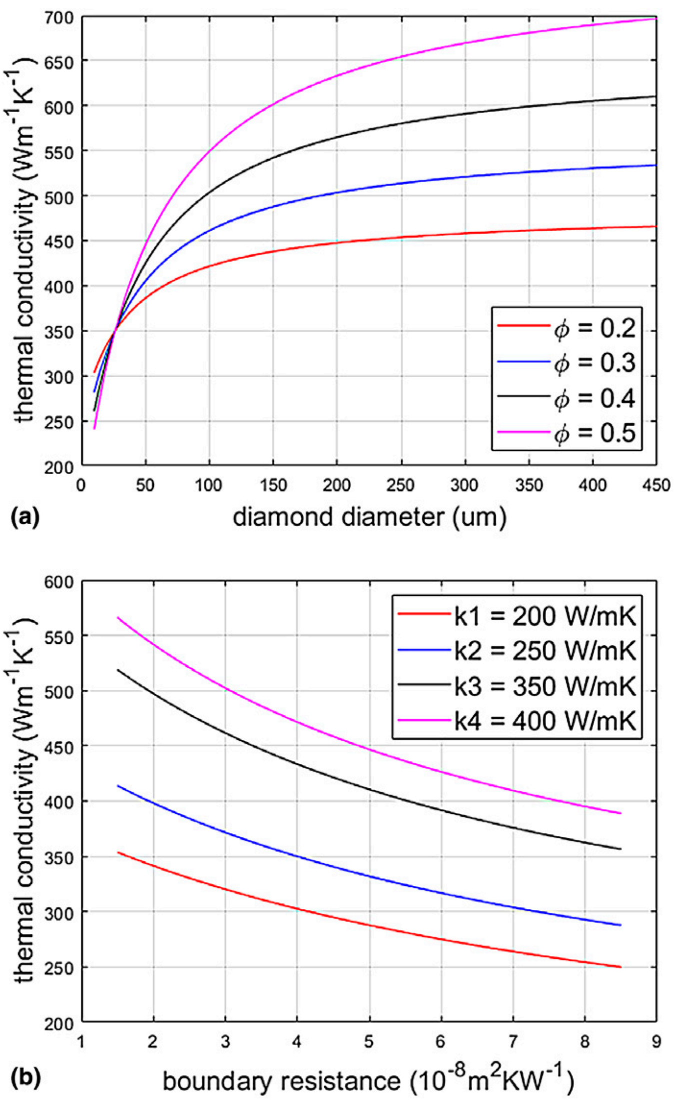

Fig. 3. (a) Modeling results for the thermal conductivity of a copper-diamond composite as a function of diamond volume fraction (ϕ) and diamond particle diameter. (b) Modeling results for the thermal conductivity of a copper-diamond composite as a function of Cu-diamond boundary resistance and Cu matrix thermal conductivity.

the sprayed film, degrading the effective thermal conductivity. To address this issue, copper cladding is proposed to protect the diamond core. To determine the minimum required clad thickness, LS-DYNA explicit dynamics simulation is used to evaluate the stress levels experienced by diamond particles of different core diameters and clad thicknesses. The von Mises stress evolution of a 74 μm diameter diamond core with 0, 2, 5, and 10 μm copper clad is shown in Fig. 4. With thicker cladding, the stress in the diamond core drops significantly, to as low as 15-30% of the uncladded case. However, thicker cladding also increases the interfacial resistance between the diamond cores and the Cu matrix, especially if the cladding has any significant oxidation. The benefits and disadvantages of using thick cladding must both be considered during the optimization of the film's effective conductivity.

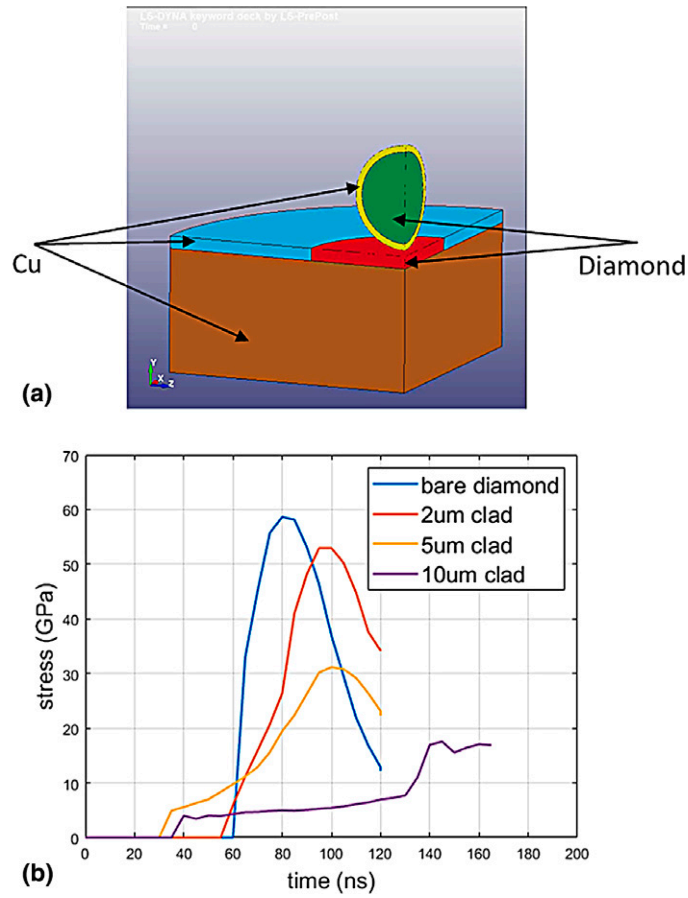

Fig. 4. (a) Simulated geometry and (b) stresses in diamond using LS-DYNA.

C. *Diamond Micro Powder Evaluation*

We investigated several commercially available Cu-clad diamond powders (Table I). The cladding oxygen concentrations range between 750 and 6,000 ppm. Those relatively high oxidation levels significantly reduce the thermal conductivity compared with pure copper. Reducing oxidation during powder manufacturing and shipping, while necessary for enabling the cold spray of high thermal conductivity composites, was a common challenge for all the diamond suppliers we collaborated with.

Cross-sectional SEM images of the Cu-clad diamond particles are shown in Fig. 5. The claddings show good overall coverage of the diamond cores, but nanoscale gaps are present, as indicated by the arrows. Cladding peel-off from the core due to impingement on the substrate during cold spray could result in diamond fracture/rebounding and low volume fraction in the composite films. Consequently, it is important to maintain good adhesion between the cladding and core at all interfaces.

Table I
Summary of the Oxygen Content and Cladding Thickness of Three Cu-Clad Diamond Powders Obtained from Different Suppliers

Powder type	Oxygen content	Nominal cladding thickness
A (Supplier 1)	6,000 ppm	9 μm, uniform
B (Supplier 2)	1,000 ppm	2 μm, nonuniform
C (Supplier 3)	750 ppm	9 μm, uniform

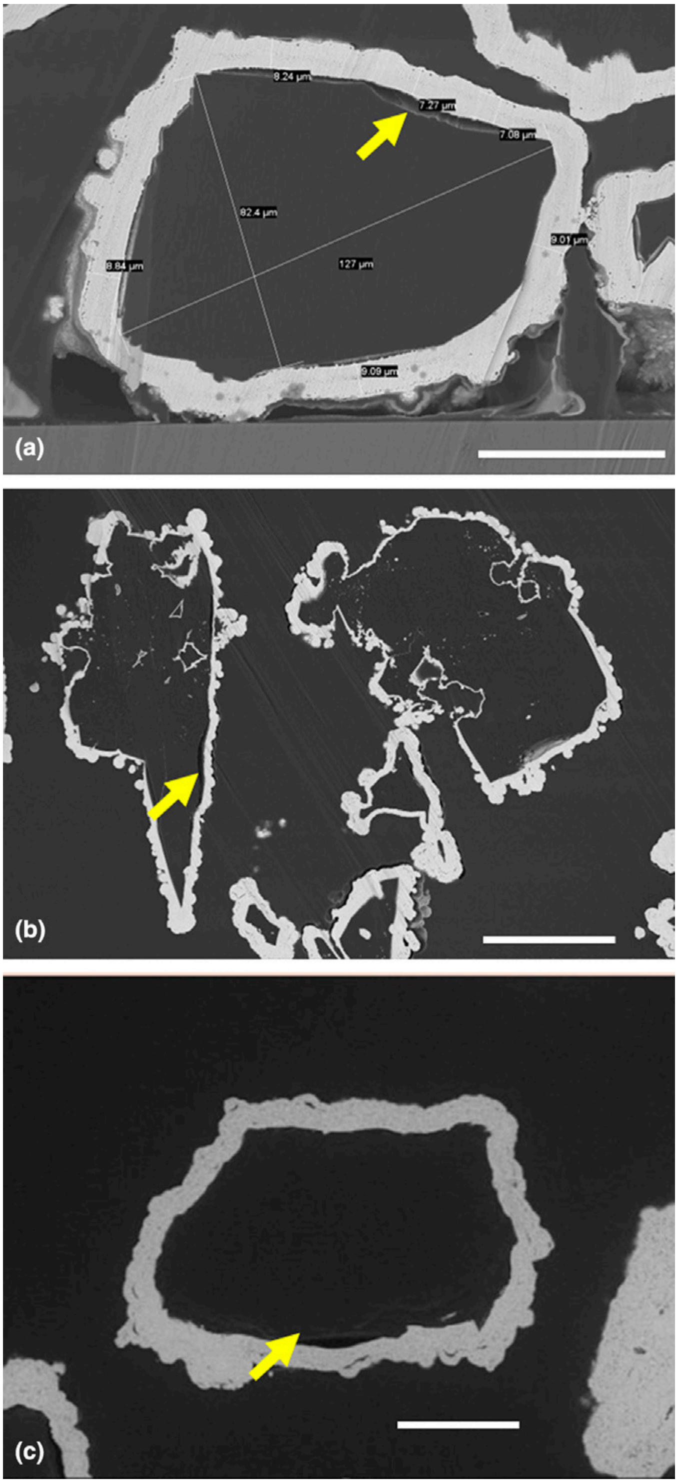

Fig. 5. SEM cross-sectional images of powders (a–c), showing different diamond core shapes and Cu cladding thicknesses. The scale bar in each image is 50 μm. Yellow arrows point at gaps between the diamond core and copper clad.

D. Composite Deposition and Thermal Conductivity

Composite copper-diamond films were deposited on different substrates, including metal and sacrificial panel substrates. Fig. 6a shows a cross-sectional view of a composite film with cladded diamond B. Using image analysis, the diamond volume fraction in the matrix is estimated to be around 8.3%. A and C showed comparable lower volume fractions in the range of 3-7%. Higher volume fractions may be achievable by optimizing the spray process parameters and feedstock type. The zoom-in view of the diamond core in the composite film is shown in Fig. 6b. While cold spray rendered good physical contact between the diamond and the copper matrix due to high-momentum impingement, diamond fracture, and size reduction were observed. Image analysis showed that the average diamond core size dropped from 70 μm to 32.8 μm. The improvement of clad-to-core adhesion in the incoming particles should help with maintaining the structural integrity of the diamond.

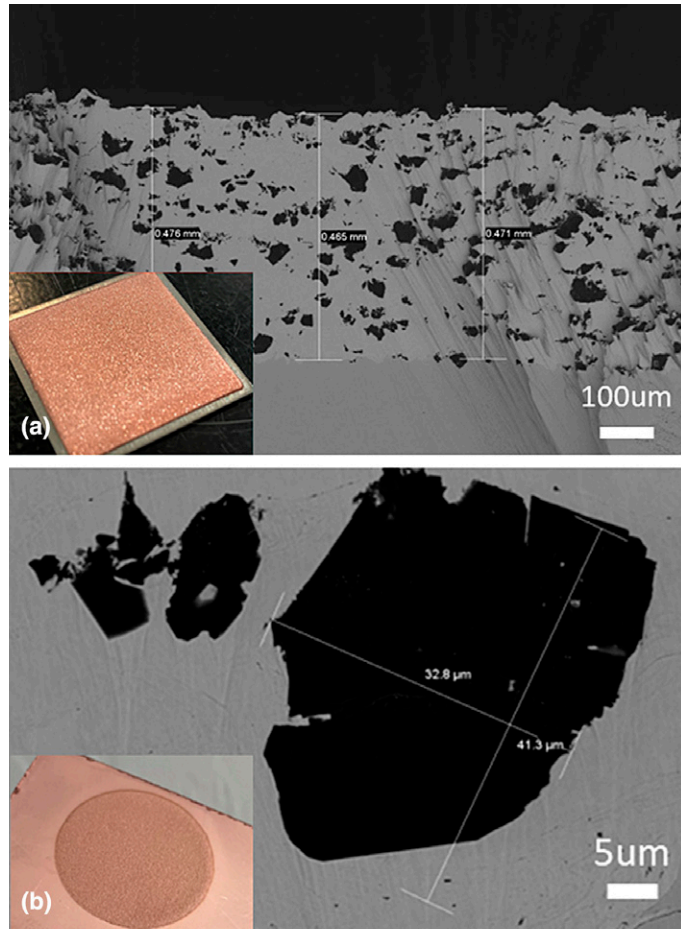

Fig. 6. (a) Film morphology of composite made from powder B. Inlet: image of the composite films deposited on stainless steel. (b) Zoom-in image of diamond particles in the film. Inlet: image of the composite films on sacrificial panel substrate.

The thermal conductivities of the composites using the three diamond powders, and of a cold-sprayed film of pure copper, were measured after sacrificial substrate removal and are shown in Fig. 7. Cold-sprayed pure copper demonstrated close-to-bulk thermal conductivity, which indicates low oxidation and porosity, consistent with our previous report [4]. While composite B has the highest diamond volume fraction among the three composites, its thermal conductivity is well below that of pure copper. This is attributed to one or more of

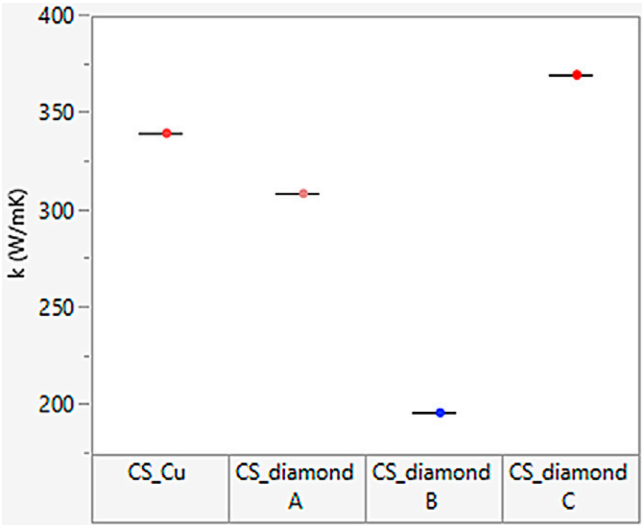

Fig. 7. Thermal conductivity of cold sprayed pure copper, composite using particle A, particle B, and particle C.

several factors, including: (1) the degradation of the copper matrix due to peeling off and mixing of highly oxidized Cu-cladding during powder B impingement, (2) diamond core size reduction during powder B impingement (see "section B. Feedstock Material Design and Challenges" above), and (3) high thermal boundary resistance between the diamond particles and Cu matrix due to the powder B interlayer thickness. The best-performing film is composite C, demonstrating about a 10% improvement in thermal conductivity relative to cold-sprayed copper alone. It is worth noting that powder C had the lowest oxygen content and interlayer thickness among the three powders. With better clad-to-diamond adhesion, a higher diamond volume fraction may be achieved in the film, leading to potentially higher thermal conductivity.

Conclusion

In this paper, we reported copper-diamond composites manufactured using cold spray technology for the thermal management of electronics. On the process side, cold spray offers a pathway for low porosity, and low oxidation deposition. We used modeling and experiments to identify the key material requirements for enabling high thermal conductivity composites. As the first and primary gating item, few existing materials today on the market meet all those requirements, leaving significant room for improvement. We believe material innovation efforts that are jointly driven by conventional diamond suppliers and semiconductor experts (e.g., in powder plating, vacuum deposition, and defect metrology) will provide the solutions needed.

Acknowledgments

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