Effective Thermal Conductivity of Anisotropic Cu–Mo Composites*

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High thermal conductivity and small thermal expansion coefficient are property requirements for heat sink materials, and Cu–Mo composite is an attractive one. Owing to the thermal property of Cu–Mo composite which varies much when the microstructure is changing, the composition and microstructure should be carefully designed to achieve appropriate combination of properties. Consequently it is very important to quantitatively evaluate properties of the composite.

In this research, a method that estimates the thermal conductivity of composites directly from their microstructure assisted with Finite Element Analysis (FEA) and Digital Image Based (DIB) technique was investigated. The effective thermal conductivities of rolled anisotropic Cu–Mo composite plates were evaluated parallel to and perpendicular to the rolling direction. The calculated thermal conductivities perpendicular to the rolling direction were compared with experimental data and found they are in good agreement. Hence, the FEA combined with DIB technique is a very helpful method for estimation of effective thermal conductivity of anisotropic composite materials.

(Received November 7, 2003; Accepted January 23, 2004)

Keywords: microstructural modeling, thermal conductivity, anisotropy, copper-molybdenum composite

1. Introduction

Recent advancement of electrical hardware requires heat sink materials which efficiently release the heat generated in an IC module. Both coefficient of thermal expansion equivalent to that of IC substrates and high thermal conductivity are required for heat sink materials. As for Cu–Mo composites, Cu has high thermal conductivity and Mo has low thermal expansion coefficient. Combining both properties in Cu–Mo composite makes it an attractive heat sink material.¹

Cu–Mo composite has a wide range of composition distribution and diverse microstructure. This leads to a wide variation of thermal properties. When this composite is used for industrial applications, it should be suitably designed to achieve appropriate combination of properties in advance. Consequently it is very important to quantify thermal conductivity and coefficient of thermal expansion in a Cu–Mo composite. Many analytical approaches for the quantitative evaluation of material properties of composites have been reported.²⁻⁴ Most of them, however, involve several restrictions on the morphology of microstructures. This is due to insufficient information about the microstructural geometry or the incapability of dealing with the geometrical complexity of the actual microstructures in numerical modeling. Therefore there are unavoidable potential errors in estimating the material properties by means of the analytical methods.

A method which enables the estimation of material properties of composites directly from the actual microstructure assisted with Digital Image Based (DIB) technique and Finite Element Analysis (FEA) was proposed in our previous work.⁶,⁷ In this method, material properties were estimated directly from the results of FEA. Hence, it offers excellent capability for estimating material properties more exactly than many established methods. In addition, the local distribution of material properties in composite could also be evaluated by this method when the composite is not assumed to be homogeneous in macro scale.

In this research, the same method was applied to estimate the effective thermal conductivity of rolled anisotropic Cu–Mo composite plates parallel to and perpendicular to the rolling direction respectively from their microstructures assisted with FEA. The calculated results obtained perpendicular to the rolling direction were compared with the experimental data by laser flash apparatus. The estimation accuracy of the method assisted with DIB technique and FEA on the thermal conductivity of a composite was then investigated. The thermal conductivities along rolling direction were also successfully estimated using this method.

2. Analysis and Experimental Procedure

2.1 Materials and evaluation

In producing Cu–Mo composite specimens, first, Mo and Cu powders were mixed, compacted and then sintered. These sintered compacts were both rolled and annealed for several times until the desired thickness was reached.

Thermal diffusivity was measured using laser flash technique (Netzsch, LFA-427) at room temperature. Density of the specimens was measured by Archimedes’ method. Specific heat was obtained from the weight percentage of the specific heat of each constituent.⁸ Thermal conductivity was calculated from the thermal diffusivity, specific heat, and density of the specimens. Microstructures were observed by optical microscope.

2.2 Microstructural modeling

The procedure for microstructural modeling conducted in this paper is shown in Fig. 1. Digital Image Based (DIB) geometric modeling technique⁹ was used to reflect the actual morphology of composite microstructure on Finite Element (FE) model. The DIB technique for 2-dimensional models used in this paper can be divided into three parts. First, the image of composite microstructure observed by

*This Paper was Presented at the Autumn Meeting of the Japan Institute of Metals, held in Sapporo, on October 12, 2003
optical micrograph was captured as a digital image by an optical sensor. The second step is the image processing which emphasizes the contrast of colors conducted to the digitalized microstructure in order to separate it into a domain of each component. Finally, the FE model consisting of as many 4-node square finite elements as pixels in digitalized image was made. The digitalized image was converted into FE model by applying material constants of a component to each element from this image. The details of this method are shown in another work.6,7)

2.3 Estimation of thermal conductivity

In this work, the effective thermal conductivity of rolled anisotropic Cu–Mo composite was calculated assisted with DIB modeling described in previous section and FEA. Figure 2 shows the representative optical micrograph of Cu–Mo composites; (a)-I to (c)-I are latitudinal cross-section along z-x plane, and (a)-II to (c)-II are longitudinal cross-section along y-z plane. The effective thermal conductivities parallel to (y-direction) and perpendicular to (z-direction) the rolling direction were estimated respectively from these microstructures. The analysis area was square-shaped at $20 \times 20 \times 10^{-5}$ m$^3$ and divided into 250000 elements by DIB technique. The effective thermal conductivity along the rolling direction was estimated from the y-z cross-section microstructures and that perpendicular to the rolling direction was estimated from the z-x cross-section microstructures respectively.

Boundary conditions were applied to the FE model made by DIB technique as shown in Fig. 3; an arbitrary uniform difference of temperature, $\Delta T$, a distance $d$, which is the distance between surfaces in the estimated direction and periodic condition on the rest of the surfaces. In this paper, the $\Delta T$ set was 10K. The average heat flux, $Q$, was obtained subsequently using FEA and the effective thermal conductivity, $\kappa_{\text{eff}}$, of the model was determined by the following equation,

$$
\kappa_{\text{eff}} = \frac{Q}{\Delta T/d}
$$
The effective thermal conductivities of Cu–Mo composites normal to the rolling direction were calculated by Equivalent Inclusion (EI) method, and were compared with those measured by laser flash technique. The thermal conductivity of Cu and Mo used in this estimation was 381.5 W/mK and 150.9 W/mK respectively, those were measured by laser flash technique.

2.4 Equivalent inclusion method

The effective thermal conductivities of Cu–Mo composites perpendicular to the rolling direction were calculated by Equivalent Inclusion (EI) method, and also calculated by the EI method. In the EI method, the shape of inclusion was assumed to be an oblate spheroid elongated to the rolling direction; i.e. the spheroidal rotation axis corresponded to the rolling direction, and the aspect ratio was determined from their microstructure as shown in Table 1.

3. Results and Discussion

The effective thermal conductivities of Cu–Mo composites perpendicular to the rolling direction were estimated from their microstructure assisted with FEA, then measured by laser flash technique, and also calculated by the EI method. These results are plotted in Fig. 4.

On the other hand, the calculated value by EI method is higher than the experimental data for rolling ratio more than 0.9 though they correspond well with each other in low rolling ratio. This disagreement is caused by the omission that the EI method is defined to be just a symmetrical oblate spheroid to the rolling direction and only disclose the change of microstructure elongated to the rolling direction. The

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\kappa_{\text{eff}} = \frac{Q\Delta T}{d}.
\]  

The Cu–Mo system only has a 0.061 at% of molybdenum eutectic solid solution under the melting temperature of copper. Hence it was assumed that there is no thermal barrier at the interfaces in this Cu–Mo composite. The thermal conductivity of Cu and Mo used in this estimation was 381.5 W/mK and 150.9 W/mK respectively, those were measured by laser flash technique.

These results are plotted in Fig. 4. The thermal conductivities of Cu–Mo composites calculated by the method of present study are in agreement with the experimental data better than those were obtained from two-dimensional analysis which represented unidirectional fiber reinforced composite. Three-dimensional analysis should be conducted in coming research, and the result will be presented in immediate future.

Both thermal conductivity and thermal expansion coefficient are important for heat sink materials, though only the thermal conductivity of Cu–Mo composites was evaluated in this work. Thermal expansion coefficient can be estimated by just providing the suitable boundary conditions for the same model, and it is now under study.

4. Conclusion

The thermal conductivities of Cu–Mo composites calculated by the method assisted with DIB technique and FEA were evaluated by comparing the experimental results. As for the calculated results perpendicular to the rolling direction, the values are in agreement with the experimental data better.

Table 1 Average aspect ratio (z/y) of Mo phase for Cu–Mo composites.

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<td>(a)</td>
<td>0.333</td>
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<td>(b)</td>
<td>0.269</td>
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<td>(c)</td>
<td>0.174</td>
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Fig. 5 The effective thermal conductivities pararell to and normal to the rolling direction estimated from their microstructure assisted with FEA.

Fig. 4 The effective thermal conductivities of Cu–Mo composites normal to the rolling direction estimated from their microstructure assisted with FEA, and calculated by equivalent inclusion method compared with measured results by laser flash technique.

\[
\kappa_{\text{eff}} = \frac{Q\Delta T}{d}.
\]
than those calculated by the EI method. Additionally, thermal conductivities calculated along the rolling direction were sufficiently obtained in present work. Consequently we consider the method using FEA and DIB technique is very helpful for designing Cu–Mo heat sinks. Hopefully it can be put into practical use for other material systems.

REFERENCES