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Characterization of thermal transport properties of $Ag/BaTiO_3$ composites using hot disk: Numerical simulations

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ABSTRACT

In this study, a micromechanics model was considered for simulating transient heat transfer response and predicting various thermal properties, such as thermal conductivity, thermal diffusivity and heat capacity, of composite materials, mimicking the hot disk experimental technique. The micromechanics analyses can give insights with regards to variations in the field variables, i.e. temperature and heat flux, in the hot disk experiment for composite materials. The micromechanics model was generated by randomly placing reinforcement particles within a square matrix medium. The effects of heat source geometry were studied, and the convergence behavior in particle size was investigated. These investigations reveal that, the size of the reinforcement particles should be small relative to the hot disk sensor to extract enough information in characterizing the homogenized material properties of the composite in the hot disk experimental technique. To study the effects of small perturbation in input data on the estimation of the material constants, sensitivity analysis was conducted. Both sensitivity analysis and micromechanics model predictions showed that the prediction accuracy for the effective thermal conductivity is higher than that for effective thermal diffusivity. This conclusion is equivalently applicable to the experimentally measured effective properties obtained by the hot disk technique. The newly presented micromechanics model was used to predict the various effective thermal properties of silver/barium titanate ($Ag/BaTiO_3$) composite. The predictions were then compared to both the experimental and numerical results reported in the literature.

1. Introduction

Piezoelectric ceramics like barium titanate ($BaTiO_3$) and lead zirconate titanate (PZT) have been widely used as actuators and sensors. These materials undergo cyclic electro-mechanical loading during service, which leads to heat generation. Thermal management is an important aspect in a wide range of applications for the integrity and reliability of devices. Thermal conductivity, thermal diffusivity and heat capacity are basic thermal transport properties of materials, and understanding these thermal properties of materials is crucial for the design and performance of many devices under harsh thermal environment, such as thermal management of electronic packages in semiconductor industry. In order to improve the overall performance of devices, composites are often considered. For example, metal or polymer phases were blended into $BaTiO_3$ and PZT to improve its fracture toughness and ductility. Consequently, in addition to the mechanical properties of each individual phase the macroscopic effective thermal properties also need to be characterized. The aim of this work is to understand the effects of different microstructural morphologies of composites on their effective thermal properties determined from hot disk technique.

In general, two types of experimental techniques exist to measure the thermal conductivity of materials, i.e. steady state and transient techniques. The steady state technique includes the radial heat flow method and the guarded hotplate method [1], while the transient method includes the hot wire, laser flash [1], 3ω method [2,3], the differential photoacoustic method [4], the thermal-wave technique [5], etc. The advantage of the transient technique is that it provides rapid measurements of thermal conductivity. Hot disk technique, as a transient plane source technique, has gain popularity due to its rapidness and accuracy. Furthermore, this technique can provide both thermal conductivity and thermal diffusivity of the specimen at the same time. During the measurement, certain amount of heat was generated on the hot disk sensor, made of double spiral of nickel wire embedded in Kapton polyimide film, by supplying a constant current. At the same time, it also records the temperature changes of the specimen. The sensor was sandwiched between two plates of materials

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of which thermal properties are measured. The recorded temperature change ΔT, determined from the electrical resistance change of the nickel sensor, is related to the thermal properties of surrounding samples by $\Delta T(t) = F(\tau)/K$, where $\tau = \sqrt{\alpha t/r^2}, K$ and κ are the thermal conductivity and thermal diffusivity of the specimen, and r is the radius of the nickel sensor [6]. The selection of experimental time window in different conditions was studied in the hot dick configuration by conducting sensitivity analysis [7]. The hot disk method, which involves prescribing spatial heat source through the spiral wire, reading the temperature changes from the spiral wire, and averaging the temperature changes in obtaining the basic thermal properties of materials, is shown reliable in determining the thermal properties of homogeneous materials. This is because the field variables in homogeneous materials are spatially continuous, which corresponds to the analytical solutions used in determining the spatial and temporal variations in temperature and flux in the hot disk experiment. This study examines the procedures in the hot disk technique in determining the thermal properties in heterogeneous materials, where the thermal field variables are not necessarily continuous.

Various micromechanics models have been developed to predict the effective thermal conductivity of composite materials. Most of those models were based on idealized assumptions, such as spherical or ellipsoidal inclusions, linear thermo-elastic behaviors of constituent materials, perfect bonding at the interfaces, etc. Based on these simplifications analytical solutions were obtained for the effective thermal conductivities [8–12]. In some cases the effect of thermal barrier at phase boundaries on the effective thermal conductivity was important and cannot be neglected [13,14]. Unit cell micromechanics models were also considered in [15,16] to numerically predict the effective thermal conductivity of composite. This method is based on simplified microstructural geometry and can easily be adjusted to take nonlinear material properties into consideration. In another type of micromechanics model, the detailed microstructures of the composite were modeled directly. The microstructures can either be randomly generated by computer algorithms [17–20], or obtained from scanning electronic microscopy (SEM) images [21–27]. Finite element methods based on steady state heat transfer are then employed to solve a boundary value problem, from which the effective properties can be calculated. In these models, nonlinear behavior of constituents and complex reinforcement shapes can be easily incorporated. They can also simulate the detailed local field fluctuations, such as heat flux concentration and flowing paths.

In this study, a micromechanics model based on transient heat transfer analysis was developed to study the effective thermal conductivity, thermal diffusivity and heat capacity of composite materials, which mimics the hot disk experimental technique. The micromechanics analyses can also give in depth understanding on limitation in conducting hot disk experiment for composite materials. The procedure in extracting the thermal properties in hot disk experimental technique is based on heat conduction in homogeneous media. Consequently, the temperature and heat flux distribution are supposed to be continuous and smooth. For composite materials, however, fluctuations exist due to the contrast in thermal properties between the matrix and reinforcement. The influences of the material heterogeneity on the temperature and heat flux profiles were studied by the presented micromechanics models. The detailed microstructure of the model was built based on randomly generating reinforcement particles in a square matrix medium. The effects of heat source geometry and particle size were studied. Sensitivity analysis were carried out to study the effects of small perturbations on the input data. Various effective thermal properties of Ag/$BaTiO_3$ composite were predicted and compared to experimental and numerical results previously reported in [28].

2. Conduction of heat in the hot disk test

The conduction of heat in an isotropic and homogeneous infinite media in the hot disk test is described by the following parabolic partial differential equation [29]:

$$\begin{aligned} &K\nabla^2 T + Q = \rho c \tfrac{\partial T}{\partial t} \\ &T(\vec{x}, 0) = T_0(\vec{x}) \end{aligned} \tag{1}$$

where K is the thermal conductivity, ρ is materials density, c is the specific heat at constant pressure, and Q is the volumetric heat source with the unit $\mathrm{Js^{-1}\ m^{-3}}$. The above governing equations is used in the hot disk test.

If the problem under consideration is two dimensional and axisymmetric the above partial differential equation can be simplified by using the cylindrical coordinate with spatial variation only in the radial direction [30]:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{Q}{K} = \frac{1}{\kappa}\frac{\partial T}{\partial t} \tag{2}$$

where $\kappa = K/\rho c$ is the thermal diffusivity. The Green's function corresponding to Eq. (2) is given as the following [30]:

$$G(r, t; r', t') = \frac{1}{4\pi\kappa(t - t')}\exp\left[-\frac{r^2 + r'^2}{4\kappa(t - t')}\right] I_0\left(\frac{rr'}{2\kappa(t - t')}\right) \tag{3}$$

where $I_0(\bullet)$ is the Bessel function of first kind with zero order,

$$I_0(x) = \frac{1}{2\pi}\int_0^{2\pi} e^{x\cos\theta} d\theta = \frac{1}{\pi}\int_0^{\pi} e^{x\cos\theta} d\theta \tag{4}$$

Note that $(Q_0/\rho c)G(r, t; r', t')$ represents the solution to an impulse point heat source of magnitude Q_0 at location r' and time t'. Q_0 in $\mathrm{Jm^{-1}}$ represents the heat released per unit length at the point source.

When the heat source is arbitrarily distributed in the material the solution can be expressed as the following by using the above green function:

$$\begin{aligned} T(r,t) &= T_0 + \tfrac{\kappa}{K}\int_0^t \int_0^\infty Q(r',t')G(r,t;r',t')(2\pi r')dr'dt' \\ &= T_0 + \tfrac{\kappa}{K}\int_0^t \int_0^\infty \tfrac{Q(r',t')}{4\pi\alpha(t-t')}\exp\left[-\tfrac{r^2+r'^2}{4\kappa(t-t')}\right] I_0\left(\tfrac{rr'}{2\kappa(t-t')}\right)(2\pi r')dr'dt' \end{aligned} \tag{5}$$

where T_0 is the initial temperature, and the unit of Q is $\mathrm{Js^{-1}\ m^{-3}}$.

2.1. Concentric ring heat source

When the material is continuously heated by a set of n concentric ring heat sources, $Q(r', t')$ can be expressed as the following [31]:

$$Q = Q_0\sum_{i=1}^{n}\delta\left(r' - \frac{ia}{n}\right)H(t) \tag{6}$$

It is assumed that n concentric ring heat sources are equally spaced, and that the largest radius of the rings has a value a. As a result, the location of the i-th ring is at ia/n, and the total length of the rings is $(n+1)\pi a$. $H(\bullet)$ is the Heaviside step function. The unit of Q_0 is $\mathrm{Js^{-1}\ m^{-2}}$. Substituting Eq. (6) for the heat source term $Q(r', t')$ in the general solution (5), we arrive at the solution to an infinite plane continuously heated by a series of equally spaced concentric rings:

$$\begin{aligned} T(r,t) = T_0 + \frac{Q_0\kappa}{K}\sum_{i=1}^{n}\int_0^t &\frac{1}{4\pi\kappa(t-t')} \\ &\times \exp\left[-\frac{r^2 + a_i^2}{4\kappa(t-t')}\right] I_0\left(\frac{ra_i}{2\kappa(t-t')}\right)(2\pi a_i)dt' \end{aligned} \tag{7}$$