

# Development of an Internet System for Composite Design and Thermophysical Property Prediction

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A thermophysical property prediction system for composite materials was developed and is available via Internet access. This system offers users a platform to design new composite materials and to predict properties such as density, specific heat, thermal conductivity, and thermal diffusivity based on the properties of the component materials and the composite structure. The system is composed of a knowledge base, a materials database, and a simulation system. Two simulation methods, an analytical method and a finite element method, are available to calculate the thermal conductivities of the composites. This system has been successfully used to predict the thermal conductivities of SiC whisker-reinforced aluminum alloy matrix composites, thermal-sprayed ZrO<sub>2</sub> thermal barrier coatings, and some other composites. The reliability and effectiveness of this system have proven to be good. [doi:10.2320/matertrans.47.1882]

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**Keywords:** composite material design, property prediction, thermal conductivity, materials database

## 1. Introduction

Thermophysical properties such as specific heat, thermal conductivity, and thermal diffusivity are very important properties for composites used in various structural, non-structural, and functional roles where high levels of heat flux and temperature change occur. Examples of this include nuclear power plants, electronic packaging, and the brake discs of trains and cars. Through careful materials selection and structural design, it is possible to optimize the thermophysical properties of a composite; however, the possible combinations of materials and structures are too numerous to explore through experimental testing. A computer simulation system is necessary to primitively design the constitution and structure of composites in order to decrease the development cost and time. Many computer simulations have been constructed to study the mechanical properties such as strength, toughness, and elasticity of various composites. Few studies, however, have focused on the thermal properties, and software regarding the calculation of composite thermophysical properties is rare.

In our previous work, we developed programs that predict the thermal conductivities of composites using an analytical method<sup>1)</sup> and a finite element method (FEM).<sup>2,3)</sup> The purpose of this work is to develop a publicly accessible platform that integrates the theoretical knowledge, materials data, and simulation tools needed to design a composite with optimized thermophysical properties. This platform will be a helpful materials design tool for material researchers and engineers all over the world.

## 2. System Architecture

The architecture of the system is shown in Fig. 1. The system is composed of four parts: a knowledge base, a materials database, an analytical simulation system, and an FEM simulation system. The knowledge base provides users with the background knowledge required to use this system, such as the basic concepts about composites and the theory of thermophysical property calculations. The analytical and

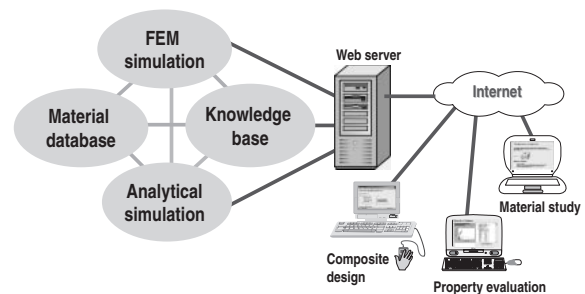


Fig. 1 Architecture of the system. The system is composed of a knowledge base, a materials database, an analytical simulation system, and an FEM simulation system.

FEM simulation systems help users to design a composite and to calculate its properties. The database stores thermophysical property data of known materials. The system was designed to provide world-wide Internet service through a web server. Users can access and operate this service with their web browsers.

## 3. Composite Thermophysical Property Knowledge Base

The basic theory regarding composites and thermophysical properties such as the concepts, equations, and expressions are represented in the knowledge base as conceptual frameworks. The concepts are classified into four groups: composite material, composite structure, property and quantity, and laws and equations. The concepts are described by definitions, symbols, graphs, related concepts, etc. A concept map is used to illustrate the relationships among concepts within the same group. Figure 2 shows the concept map of the composite material group. Figure 3 is the web page describing the concept of Frick expression. Besides the conventional descriptions in the text, graphs, and mathematical expression, a calculator interface is provided to let users perform online calculations with the expression. For concepts such as thermal conductivity and specific heat, the users may also

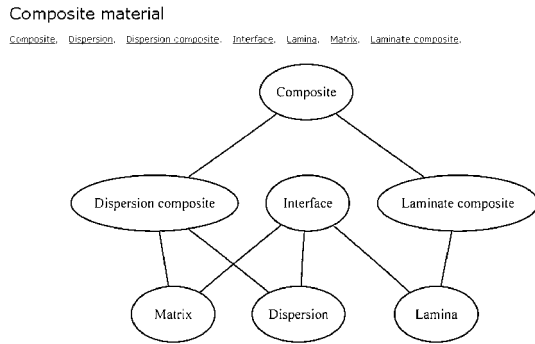


Fig. 2 Concept map showing the relationship among the concepts in the composite material group.

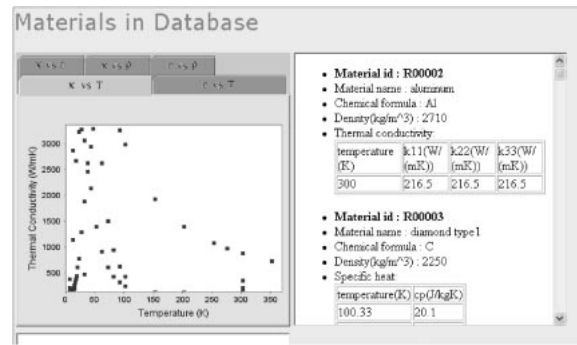


Fig. 4 A graph and numerical values of the thermal conductivity data stored in the materials database.

**Fricke expression**

Expression of effective thermal conductivity of composite with ellipsoid dispersion.

Equation :

$$k_{eff} = k_m \frac{[k_m + S_i(k_d - k_m)](1 - V_d) + k_d V_d}{[k_m + S_i(k_d - k_m)](1 - V_d) + k_m V_d}$$

$$S_i = \frac{a_1 a_2 a_3}{2} \int_0^\infty \frac{ds}{(s + a_1^2) \sqrt{(s + a_1^2)(s + a_2^2)(s + a_3^2)}}$$

$k_{eff}$ : effective thermal conductivity in the direction,  
 $a_1, a_2, a_3$ : semi-axes of ellipsoid  
 $k_m$ : thermal conductivity of matrix  
 $k_d$ : thermal conductivity of dispersion  
 $V_d$ : volume fraction of dispersion

Related concepts  
 Effective thermal conductivity, Dispersion composite, Ellipsoid

(b) Online calculator interface with input fields for: ratio of semi-axes  $a_2$  to  $a_1$  ( $a_2/a_1$ ), ratio of semi-axes  $a_3$  to  $a_1$  ( $a_3/a_1$ ), thermal conductivity of matrix (Wm<sup>-1</sup>K<sup>-1</sup>), thermal conductivity of dispersion (Wm<sup>-1</sup>K<sup>-1</sup>), and volume fraction of dispersion. Includes 'calculate' and 'reset' buttons.

Fig. 3 Web page describing the Fricke expression using text, graphs, mathematical expressions (a), and an online calculator (b).

refer to the database to view the plot graphs and numerical values of these properties.

#### 4. Materials Properties Database

A thermophysical property database is included in the system in order to help the users select appropriate component materials. The database contains data regarding the thermal conductivity, specific heat, density, and thermal diffusivity of metals, ceramics, polymers, etc., extracted from multiple databases<sup>4</sup> of The National Institute for Materials Sciences and relevant literatures. When materials data is required, it is first displayed in the form of graphs such as thermal conductivity versus temperature (Fig. 4), specific

Table 1 Analytical solutions used for different composite structures.

Structure type	Structure model			Analytical solutions
	Dispersion shape	Dispersion distribution	Interface	
Laminate composite	—	—	No	Wiener bounds <sup>5)</sup>
	—	—	Yes	
Dispersion composite	Sphere	1D, 2D and 3D	No	Equivalent inclusion method <sup>6)</sup>
	Ellipsoid		Yes	
	Cylinder		Yes	

heat versus temperature, and so on. The user may select and enlarge an area of the plot, and when the number of the selected materials is less than 20, the description of the materials and the numerical values of the properties are shown.

### 5. Composite Thermophysical Property Prediction

#### 5.1 Analytical simulation system

To design a composite with optimum properties, we first need to know the dependence of the properties on the constitution and structure of the composite. Analytical simulations provide easy modeling and fast calculations, and are therefore most suitable for this purpose. The details of the analytical simulation system have been reported previously.<sup>1)</sup> Here, we simply summarize the larger points. The analytical solutions used to calculate the thermal conductivity of composites with different structures are shown in Table 1. According to the structure of the designed composite, the system automatically selects the appropriate solution to calculate. The density and the specific heat of the composite are calculated using the law of mixtures, and the thermal diffusivity is calculated using the expression  $\alpha = \frac{\kappa}{\rho c_p}$ , where  $\alpha$  is the thermal diffusivity,  $\kappa$  is the thermal conductivity,  $\rho$  is the density, and  $c_p$  is the specific heat of the composite.

Figure 5(a) shows the web user interface for designing a dispersion composite. When clicking the button “refer to materials database”, the window in Fig. 4 will open, and the data in the materials database will be plotted and displayed. If

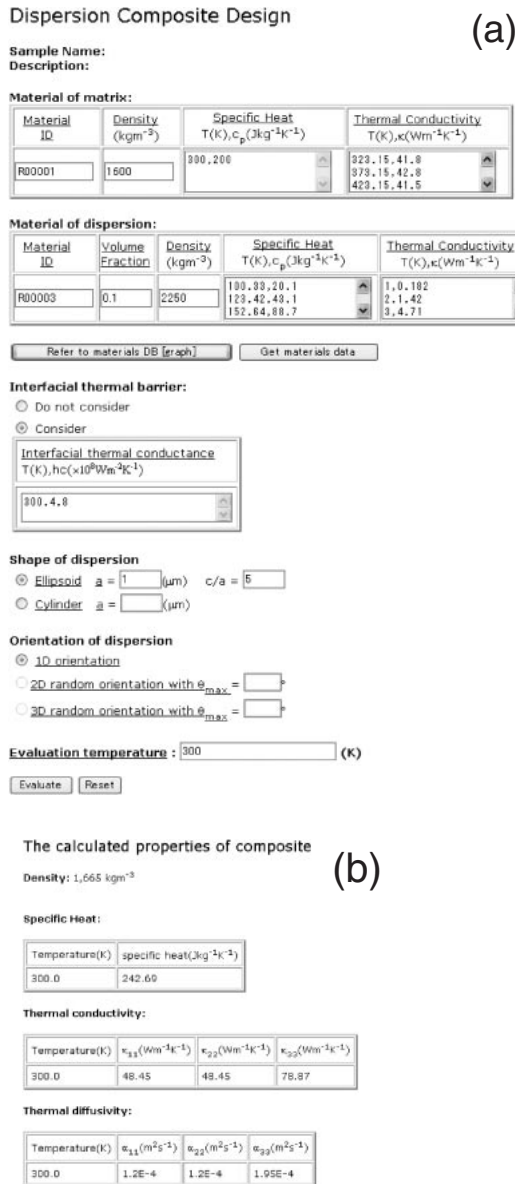


Fig. 5 Web user interface to design a dispersion composite (a), and the calculation results for the density, specific heat, thermal conductivity, and thermal diffusivity (b).

the user wants to use a material in the database as a matrix or dispersion, inputting the materials identification number into the “Material ID” space and clicking the button “Get materials data” is all that is required. The density, specific heat, and thermal conductivity will then be imported to the form. After inputting the structural parameters and evaluating temperatures and clicking the button “Evaluate”, the user will obtain the calculated density, specific heat, thermal conductivity, and thermal diffusivity of the composite, as shown in Fig. 5(b). The time to calculate the above properties is usually within 1 second, which makes calculating a large number of combinations of different materials and structural parameters in order to find the dependence of the properties on these parameters possible.

5.2 FEM simulation system

Although the analytical method has a lot of advantages,

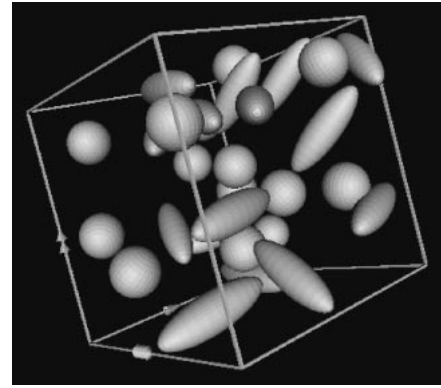


Fig. 6 Structural model of a composite containing randomly distributed spheres and ellipsoids, two different types of dispersions, generated by the FEM simulation system.

solutions are not available for some complicated structures, for example, a composite containing dispersions with different shapes, sizes, or materials; and also if the component materials have anisotropy in their thermal conductivity, etc. In these cases, the FEM method should be used. In our system, the FEM simulation is also available to calculate the thermal conductivity of composites.

Using commercial FEM software to design a dispersion composite is an enormously time consuming task because for each dispersion, the material, geometry, coordinates, and vectors of direction must be specified manually. We have developed a new method to simplify the generation of geometric models of composites containing randomly distributed dispersions.<sup>2,3)</sup> With this method, for the same type of dispersions, users just need to once specify their material, geometry, number, volume fraction, and orientation type the same way as in the case of the analytical simulation. The computer will then automatically create the coordinates and vectors of direction for each dispersion. Figure 6 shows a geometric model containing spherical and ellipsoid dispersions generated using this method. After the geometrical model is built, an FEM mesh is automatically created using the voxel-based method according to user-specified refinement. Depending on the mesh refinement, the computing time varies from several minutes to hours. An e-mail will be sent to the user when the process is finished, and the user can go to the web address to view the calculated result.

6. Application Examples

This system has been used to evaluate the thermal conductivity of some factual composites,<sup>8-10)</sup> the results of which are summarized and plotted in Fig. 7. The largest deviation between the calculated and experimental values was less than 10%, which is considered to be in good agreement. We have also used the system to estimate the dispersion/matrix interfacial thermal conductance of SiC particle-reinforced aluminum alloy matrix composites<sup>11)</sup> from the measured thermal conductivity of the composites. The SiC/Al interfacial thermal conductance was estimated to be between 1.1 and 4.1 × 10<sup>8</sup> Wm<sup>-2</sup> K<sup>-1</sup>, which is consistent with the value of 1.2 × 10<sup>8</sup> Wm<sup>-2</sup> K<sup>-1</sup>, calculated using phonon diffuse mismatch model and Debye theory.<sup>12)</sup>

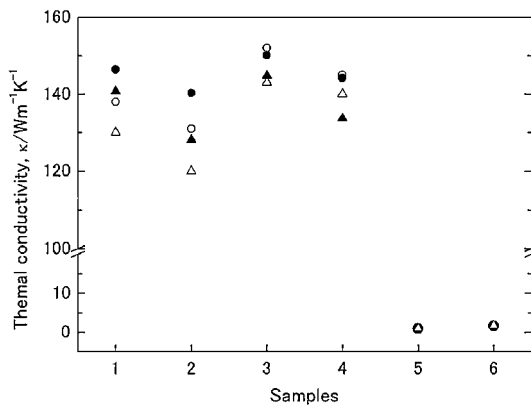


Fig. 7 Comparison of the calculated thermal conductivity using this system and the experimental data. Samples 1 to 4 are SiC whisker-reinforced Al alloy matrix composites. Samples 1 and 2 have a whisker diameter of  $0.5\mu\text{m}$  and volume fractions of 10 and 20%, respectively. Samples 3 and 4 have a whisker diameter of  $1\mu\text{m}$  and volume fractions of 10 and 20%, respectively. ● is the calculated thermal conductivity in the direction perpendicular to the whiskers, and ▲ is that parallel to the whiskers. ○ and △ are the experimental data respectively. Sample 5 and 6 are thermal-sprayed ZrO<sub>2</sub> thermal barrier coatings made under different coating conditions. ● is the calculated and △ is the measured thermal conductivity perpendicular to the coating.

## 7. Conclusion

A composite design and thermophysical property prediction system was developed, which integrates the functions of materials design and simulation. This system is available with Internet access at <http://composite.nims.go.jp/>. This system is expected to be a useful tool for researchers and

engineers to primitively design the constitution and structure of composites in order to obtain required thermophysical properties.

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