Transactions of the Materials Research Society of Japan 29 [8] 3815-3818 (2004)

An Internet platform of composites design and thermophysical properties evaluation

Yibin Xu, Yoshihisa Tanaka, Masahiro Goto and Koichi Yagi
National Institute for Materials Science
2-2-54 Nakameguro, Meguro-Ku, Tokyo 153-0061, Japan
Fax: 81-03-3713-6577, e-mail: xu.yibin@nims.go.jp

A prototype of composites design and thermophysical properties evaluation system was developed based on Internet technology. The system is featured by ease in constitutional design, fast calculation speed, huge capacity of materials data, and wide accessibility. Component material selection and structural design are done with a Web browser. Specific heat, thermal conductivity and thermal diffusivity of the designed composites can be evaluated online. A materials information server was included to provide materials property data for materials selection and property calculation. The system has been applied to predict the properties of SiC particles reinforced aluminum alloy matrix composite. The predicted values are close to the experimental ones.
Key words: composite design, property calculation, specific heat, thermal conductivity, thermal diffusivity, materials database

1. INTRODUCTION

Composite materials have been widely used today in numerous structure, non-structure and functional application in many engineering sectors. In spite of their great advantages in strength, weariness, thermal properties, etc., the possibility of property management through constitutional design has made composites increasingly attractive in more and more fields. Thermophysical properties such as thermal conductivity, specific heat and thermal diffusivity are important properties in many of the composites' applications [1-2], for example, electronic packaging, heat spreader, fusion applications, etc. Primitive constitutional design is an effective method to develop composites with ideal thermal properties and decrease the development cost and period.

Some commercial software products are available for this purpose, such as FiberSIM and Voxelcon-HG. In these products, finite element method (FEM) is used to analyze the heat conduction inside a composite. The FEM model of the composite is constructed either by a computer-aided design (CAD) user interface or by reading micro-CT (computer tomography scan) images of the material. The difficulties in modeling and long time of computing have become the biggest barrier that obstructs the usage of these products.

Another difficulty in composite design is to select appropriate materials. Usually the selection of materials is made basing on the experiences of the researchers or engineers, thus the options are offset by their personal knowledge.

This work is aimed to construct an easy, fast and widely accessible platform for composite design and properties evaluation.

2. SYSTEM DESIGN AND ARCHITECTURE

The basic concept of this system is to calculate the thermophysical properties of composite using analytical solutions of the effective properties, so that the calculation speed can be significantly improved and some procedures of FEM modeling such as geometry generation and meshing are omitted or greatly simplified. Moreover, templates of basic composite structural models are prepared and built inside the system. Users will not be necessary to design a structure beginning from scratch, but do it by choosing the models and combining them.

A materials information server containing a database management system is included in the system. A large amount of materials property data can be stored and provided as reference information for materials selection and property calculation. The designed composites and its calculated properties can also be stored in the database in order to be reused and shared with other users.

The architecture of this system is shown in Fig.1. The system is developed based on Internet technology and provides the service through a Web server. Users can choose the structural model, view the materials property data inside the database, select the component materials and specify the structural parameters of a composite on a Web browser. The data are sent to the property calculation engines. The calculation engines calculate the density, specific heat, thermal conductivity and thermal diffusivity of the composite, and sent the results back to the Web browser.

3. BASIC COMPOSITE STRUCTURE MODELS

The structures of composite can be generally described by two models: laminate (Fig.2a) and dispersion (Fig.2b). The dispersion composite can be further classified to two types: the effect of dispersion/matrix interface considered or neglected. Whereas, we don't distinguish these two cases for the laminate model because the interface can be considered as an extra layer of this model.

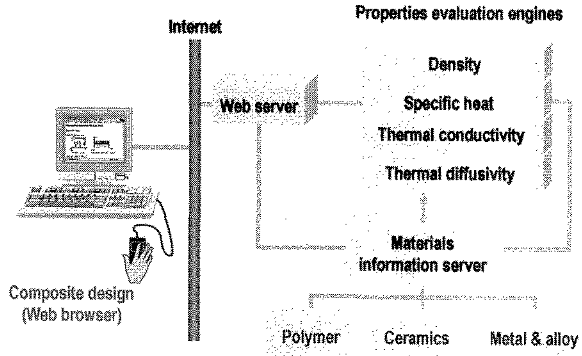

Fig.1 System structure of the composite design and thermal conductivity evaluation platform.

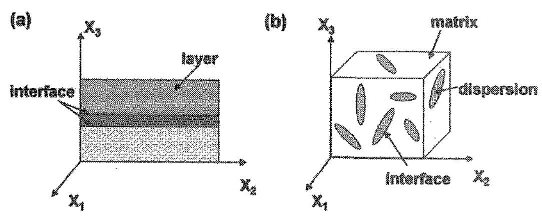

Fig.2 Basic composite structure models built inside the system, (a) laminate model (b) dispersion model.

The shape of a dispersion is approximately represented by a rotation ellipsoid with semi-axes a and c, with c as rotation axis. When the length of a and c are equal, it represents a sphere; and when the length of c tends to infinite, it represents a cylinder. According to the orientation of dispersion, the dispersion composite can be classified as 1 dimensional (1D) orientation, when the c axes of all dispersions are aligned unidirectionally; 2 dimensional (2D) orientation, when the c axes are located in a plane, and 3 dimensional (3D) orientation for the other cases.

The above models are built inside this system as basic models to construct a composite. With combination of them, construction of more complicated structure is possible.

4. COMPOSITE CONSTITUTIONAL DESCRIPTION

The Extensible Markup Language (XML) is used as the data format to describe the constitution and properties of composites. A XML schema has been specified, in which, each material is treated as one object, general information such as name and chemical formula, properties of density, specific heat, thermal conductivity and thermal diffusivity are recorded as elements. Thermal conductivities and thermal diffusivity are recorded by the three diagonal elements of their diagonal matrix for each temperature point (Fig.3a).

The structure of material is classified into homogenous material, laminate composite and dispersion composite. The constitutional parameters of laminate and dispersion composite are described by hierarchically structured elements as shown in Fig.3b. The component material itself can be a composite as well. With this data structure, composites with composed models can be described.

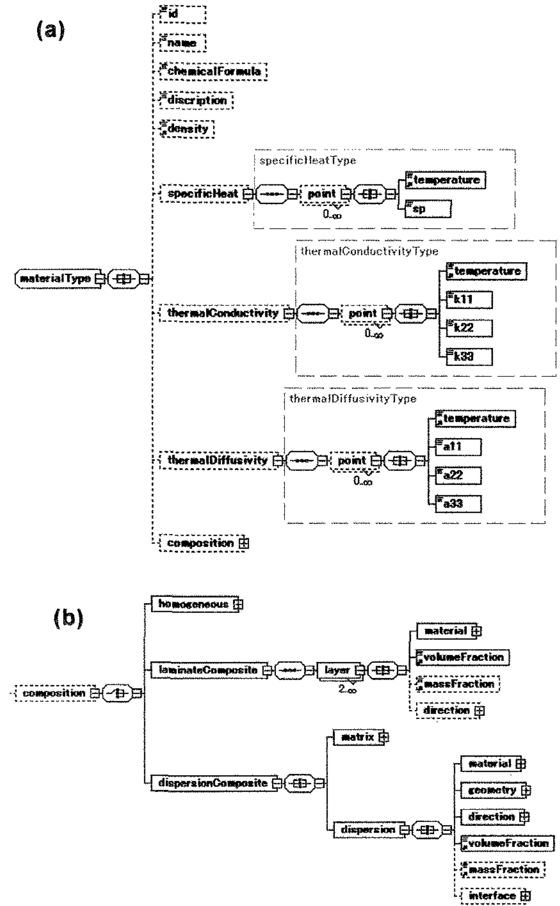

Fig.3 XML schema describing the constitution, structure and properties of composites.

5. THEORETICAL FOUNDATION OF THERMOPHYSICAL PROPERTY CALCULATION

5.1 Thermal conductivity

The theory of thermal conductivity of composites is well established [3-8]. For most of the common composite structures, analytical solutions of effective thermal conductivity are available. The analytical solutions used in this system and their corresponding structure models are listed in Table 1.

A package of calculation modules including these analytical solutions has been developed [9]. According to the constitutional description file of a composite, the appropriate solution is automatically selected to calculate its thermal conductivity.

Table 1 Analytical solutions of effective thermal conductivity of composites

Composites structure model				Analytical solution & reference
	Shape of dispersion	Orientation of dispersion	Inter-face	
Lamina-te	-	-	No	Wiener [3]
	-	-	Thin	Hasselman[4]
	-	-	Thick	Wiener [3]
Disper-sion	Sphere	-	No	Maxwell [5]
	Cylinder	1D	No	Rayleigh [6]
	Ellipsoid	1D, 2D, 3D	No	Hatta et.al [7]

Sphere	-	Thin	Hasselman[4]
Cylinder	1D	Thin	Hasselman[4]
Cylinder	1D	Thick	Markworth[8]

5.2 Density, specific heat and thermal diffusivity

The density ρ of the composite is calculated using the following expression:

$$\rho = \sum_{i=1}^{n} V_f^i \rho_i \cdot$$

Where, V_f^i and ρ_i are the volume fraction and density of the ith component, respectively.

Kopp-Neuman's Law is used to calculate the specific heat of composite, which can be written as

$$c_p = \frac{\sum_{i=1}^{n} V_f^i \rho_i c_p^i}{\sum_{i=1}^{n} V_f^i \rho_i} \cdot$$

Where c_p is the specific heat of composite and c_p^i the specific heat of the *i*th component.

The thermal diffusivity is calculated using the relationship of

$$D = \frac{\kappa}{\rho c_p} \cdot$$

Where D and κ are the thermal diffusivity and thermal conductivity of the composite, respectively.

6. SYSTEM DEVELOPMENT

This system is developed based on Java technology. The interface of composite design is generated by JavaServer Pages (JSP). Data transfer between the Web browser and the calculation engine is carried out by Java servlets. Apache HTTP server is used as the Web server, and Jakarta Tomcat as the Java servlet and JSP engine.

Excelon eXtensible Information Server (XIS) is used to manage the materials database. Data of materials are recorded as XML files, each for one material, according to the XML schema described in section 4. The material id is a unique number to distinguish the material, and is also used as the name of the XML file. Materials are classified as real materials whose data are obtained experimentally and virtual materials whose data are calculated by this system. The data of real materials and virtual materials are preserved in two data stores separately. The virtual materials data store permits authorized users to upload data to it.

7. APPLICATION TO SiC/AA6061 COMPOSITE

As an example of applications, this system has been used to predict the thermophysical properties of SiC particles reinforced aluminum alloy (AA6061) composite. The scanning electronic microscope photograph of the composite is shown in Fig.5. The average radius of the particles is about 0.5μm, and the volume fraction of SiC is 10%.

The structure model of the composite can be described as spherical SiC particles randomly distributed inside the matrix, and we wish to take into account of the effect of particle/matrix interface.

In the constitutional design window shown in Fig.6, we input the general information of the material, checked the structure model of "Dispersion type with interfacial effect", and then clicked the button "Continue".

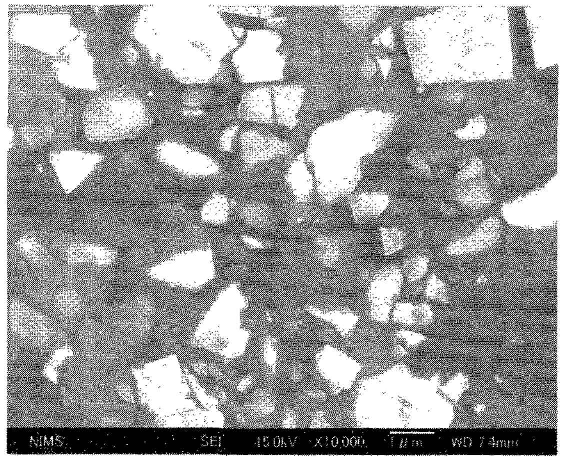

Fig.5 Microstructures of 10vol% particulate SiC reinforced aluminum alloy matrix composites.

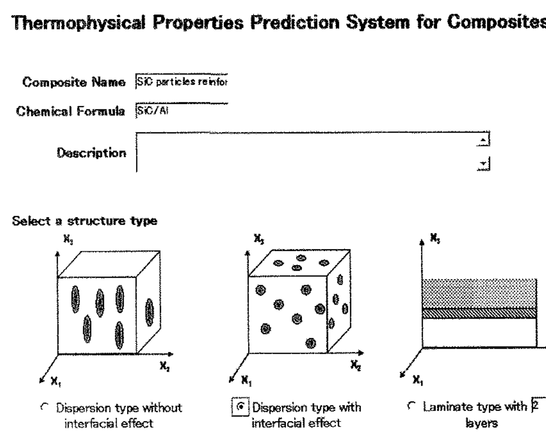

Fig.6 Window for inputting the general information and selecting the structure model of the composite.

In the next window, we selected the model of "Spherical particle" (Fig.7), and input the data of component materials (Fig.8). By clicking the button "Refer to materials DB", we viewed the data in the database and found that the properties of AA6061 alloy and SiC particle are preserved in it (Fig.9), so just copied the materials' identification numbers into the form of Fig.8 and input the size and volume fraction of the dispersions.

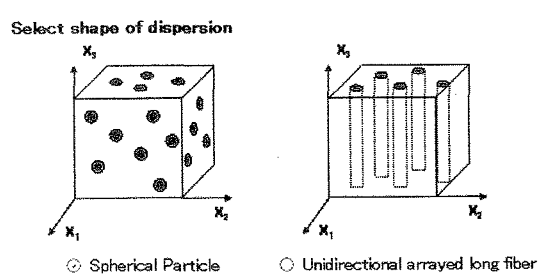

Fig.7 Window for selecting the shape of dispersion.

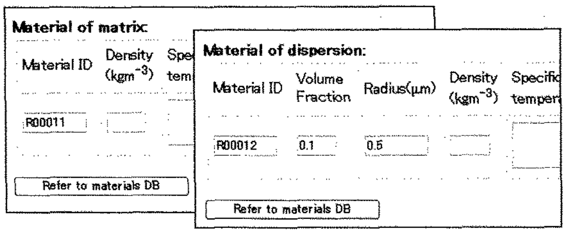

Fig.8 Window for inputting data of matrix and dispersion.

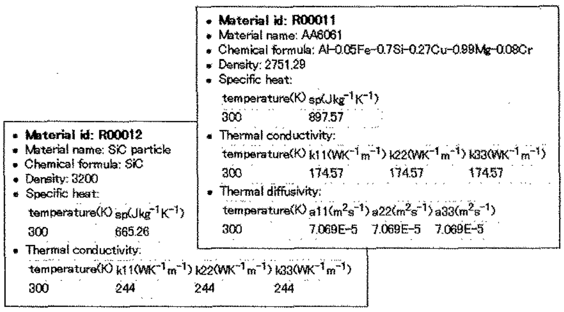

Fig.9 Display the data inside the database.

The interfacial thermal conductance of SiC/Al alloy around room temperature is reported to be in the order of 10^8 $Wm^{-2}K$ [10]. Input the temperature and interfacial thermal conductance in the form of Fig.10, specified the temperature at which the properties would be calculated and clicked the button "Evaluate", then we got the calculation result as shown in Fig.11.

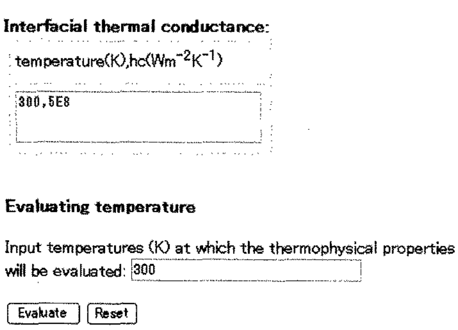

Fig.10 Windows for inputting interfacial thermal conductance and evaluating temperature.

The calculated density, thermal diffusivity and thermal conductivity were 2796.16 kgm^{-3}, 6.94×10^{-5} m^2s^{-1} and 168.97 $Wm^{-1}K^{-1}$, respectively. The experimentally measured values of this material were 2804.63 kgm^{-3}, 7.16×10^{-5} m^2s^{-1} and 174.81 $Wm^{-1}K^{-1}$ [11]. The prediction values are close to the experimental ones.

In the windows of Fig.11, by clicking the button "Upload to materials DB", the calculation result might be uploaded to the materials database after user authentication.

5. CONCLUSION

In this paper, we reported a web-based system of composites design and thermophysical properties prediction. With this system, the users can design the constitution and structure of a composite, and evaluated its density, specific heat, thermal conductivity and thermal diffusivity. A materials information server is equipped to provide materials data needed in composite design and property calculation. This system is expected to be a useful tool to help the users primitively design a composite with ideal thermophysical properties.

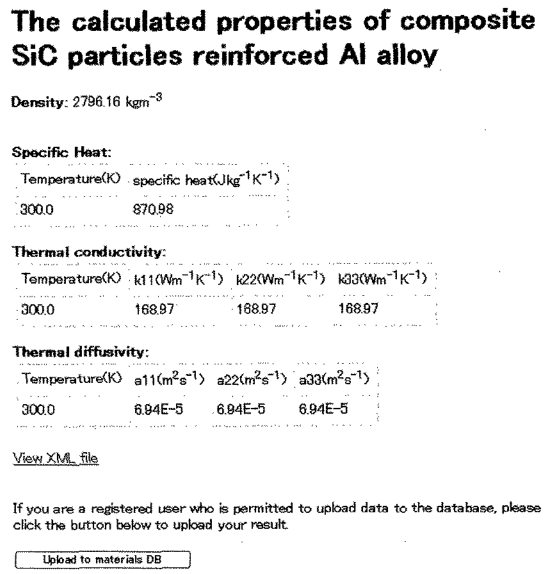

Fig.11 Window of calculation result.

ACKNOWLEDGEMENTS

A part of this study was financially supported by the Budget for Nuclear Research of the Ministry of Education, Culture, Sports, Science and Technology, based on the screening and counseling by the Atomic Energy Commission.

REFERENCES

[1] D. P. H. Hasselman, K. Y. Donaldson, J. American Ceramic Society 75 (11) (1992) 3137-3140.
[2] W. Kowbek, C. A. Bruce, K. L. Tsou, K. Patel, J. C. Withers, G. E. Youngblood, J. Nuclear Materials 283 (287) (2000) 570-573.
[3] O. Wiener, Abh. Math. Phys. Kl. Kgl. Sächs. Ges. Wiss. 32 (1912) 509-604.
[4] D. P. H. Hasselmen, L. F. Johnson, J. Composite Materials 21 (1987) 508-515.
[5] J. C. Maxwell, "A Treatise on Electricity and Magnetism", Vol. 1, 3rd ed. Oxford University Press, London, 1892, pp.435-449.
[6] L. Rayleigh, Phil. Mag. 34 (1892) 481-502.
[7] H. Hatta and M. Taya, J. Applied Physics 58(7) (1985) 2478-2486.
[8] A. J. Markworth, J. materials Science Letters 12 (1993) 1487-1489.
[9] Y. Xu, J. Kinugawa and K. Yagi, Materials Transactions 44(4) (2003) 629-632.
[10] D. P. H. Hasselman, K. Y. Donaldson and A. L. Geiger, J. Am. Ceram. Soc. 75 (11) (1992) 3137-3140.
[11] Y. Xu, Y. Tanaka, M. Goto, Y. Zhou, K. Yagia, J. Applied Physics 95(2) (2004) 722-726.

(Received October 13, 2003; Accepted April 24, 2004)