Composite materials design and property prediction using materials database

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Why composite material?

- **Multi-requirements on material property**

Nuclear power plants	Electronic packaging	Brake disc of cars	Thermal barrier coating
Non-radioactive, high thermal conductivity, thermal shock resistance, strength	high thermal conductivity, low thermal expansion, strength	high thermal conductivity, wear resistance, strength	Low thermal conductivity, low thermal expansion

- **Difficult to be satisfied by single phased material**

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- **Improve material performance by mixing two or three phases**

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- **Infinite combination of materials and structures**

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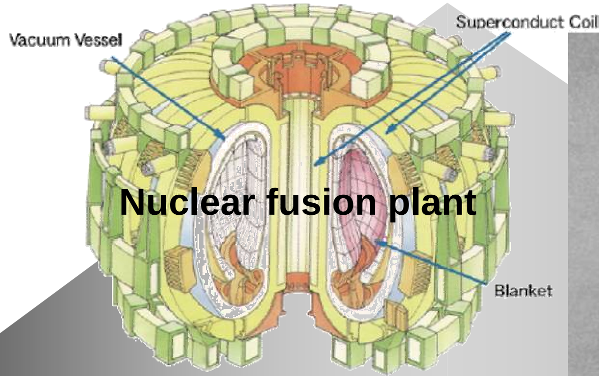
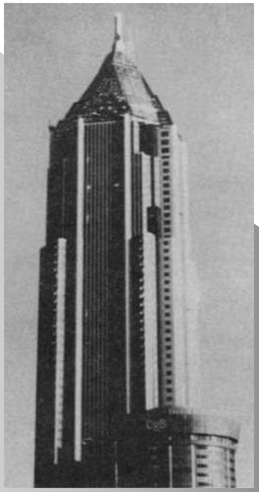
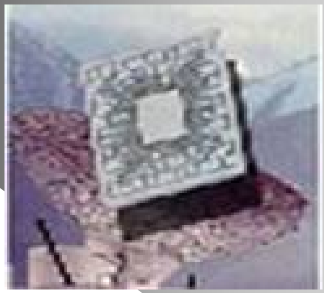
- **Constitutional and structural design and optimization by computer simulation**

Thermophysical property of composite





Composite



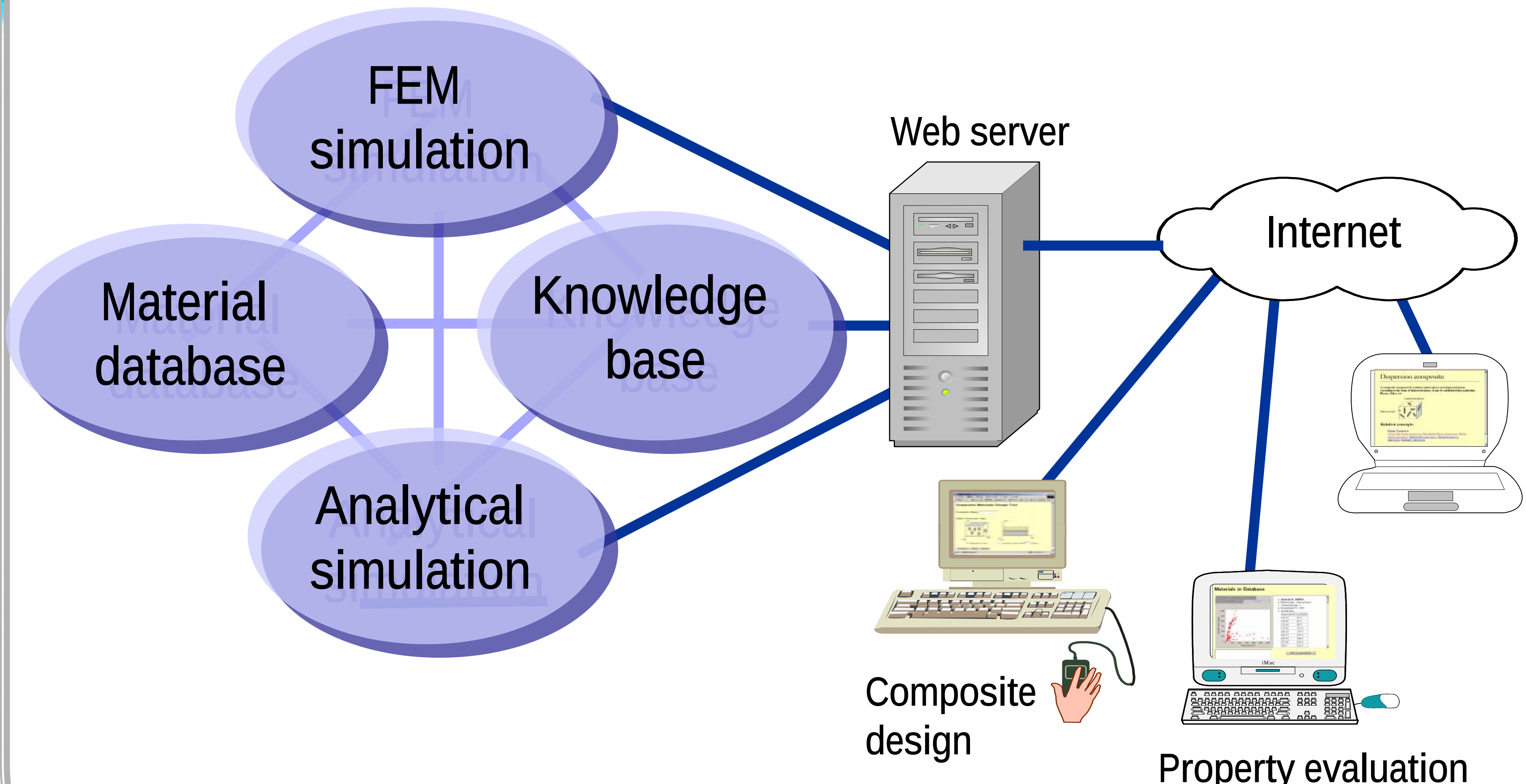
- **Thermal stress**
- **Thermal shock resistance**
- **Energy transfer**

Thermophysical property （thermal conductivity, thermal expansion, heat capacity, etc.）

Objective

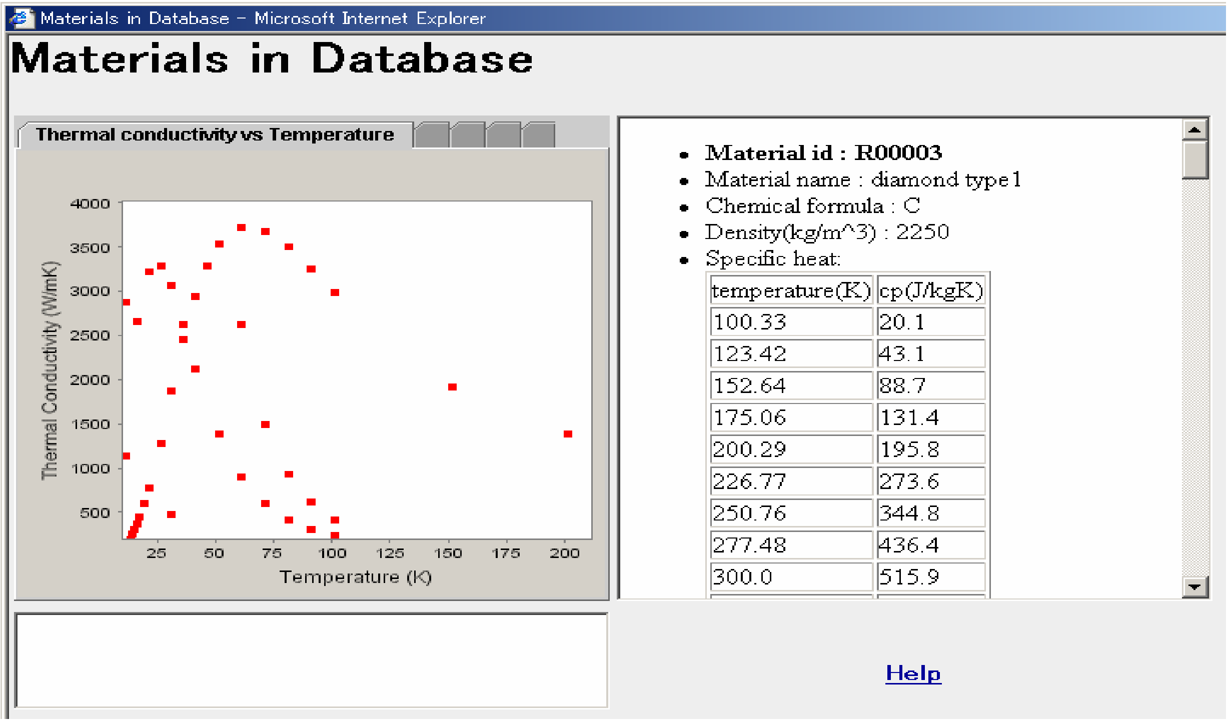
- Develop a platform for design composites with required thermophysical property, basing on the material property data we known.
- Apply the system to material research and evaluate the accuracy of calculation by experiments.

System architecture of CompoTherm



Materials database

- Thermophysical property database
  - Density, specific heat and thermal conductivity data extracted from NIMS Materials Database.
  - Data number: 990 (polymers, alloys, ceramics, etc.)



Simulation systems

- Two simulation methods available
  - Analytical method
  - Numerical method (finite element method)
- Fit for different requirements on computational efficiency and accuracy.

Analytical simulation method

- **Analytical solutions used for different composite structures**

<table>
<tr><th colspan="4">Structure model</th><th rowspan="2">Analytical solutions</th></tr>
<tr><th>Structure type</th><th>Dispersion shape</th><th>Dispersion distribution</th><th>Interface</th></tr>
<tr><td rowspan="2">Laminate composite</td><td>--</td><td>--</td><td>No</td><td rowspan="2">Wiener expression (Law of mixture)</td></tr>
<tr><td>--</td><td>--</td><td>Yes</td></tr>
<tr><td rowspan="6">Dispersion composite</td><td>Sphere</td><td rowspan="3">1D, 2D, and 3D</td><td rowspan="3">No</td><td rowspan="3">Equivalent inclusion method</td></tr>
<tr><td>Ellipsoid</td></tr>
<tr><td>Cylinder</td></tr>
<tr><td>Sphere</td><td rowspan="3">1D</td><td rowspan="3">Yes</td><td rowspan="3">Effective medium theory</td></tr>
<tr><td>Ellipsoid</td></tr>
<tr><td>Cylinder</td></tr>
</table>

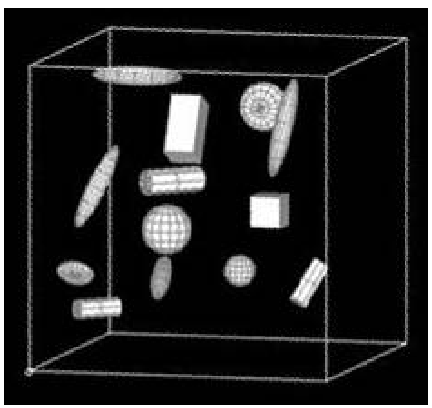
- **Features**
  - **Simple model**
  - **Quick calculation**
  - **Suitable to study the dependence of thermal property on structure**

Demonstration

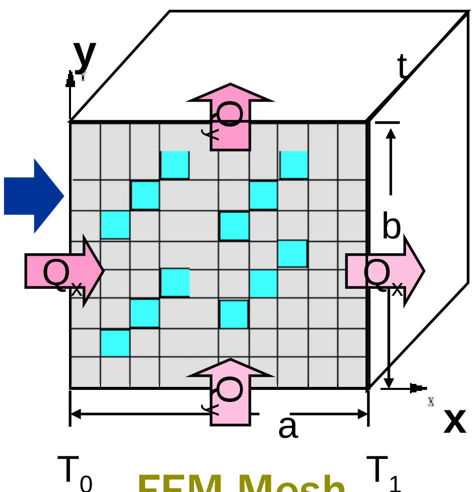
Finite element simulation method

- **Features**
  - **Precise material arrangement**
  - **Composites containing dispersions with different shapes, sizes, materials, etc.**
  - **Material with anisotropy**
  - **Thermal conductivity dependence on temperature**

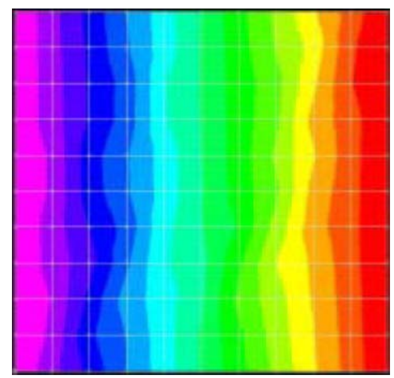
Demonstration



Geometry



FEM Mesh



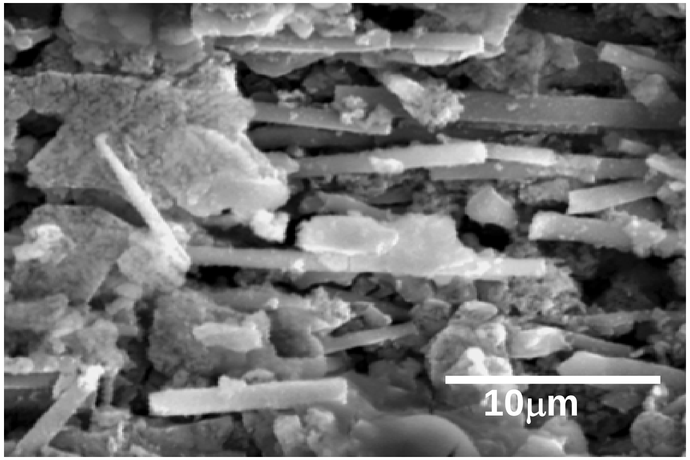
Heat transfer simulation

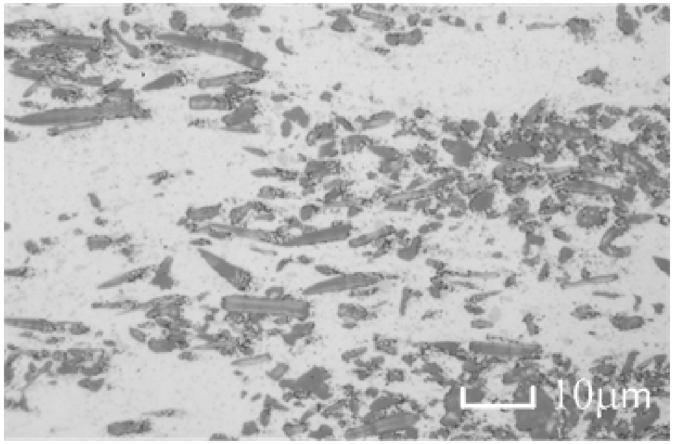
$$\begin{bmatrix} \kappa_{xx} & \kappa_{xy} & \kappa_{xz} \\ \kappa_{yx} & \kappa_{yy} & \kappa_{yz} \\ \kappa_{zx} & \kappa_{zy} & \kappa_{zz} \end{bmatrix}$$

Thermal conductivity

Example of Application (1)

- **Prediction of thermal conductivity of SiCw/Al composite**

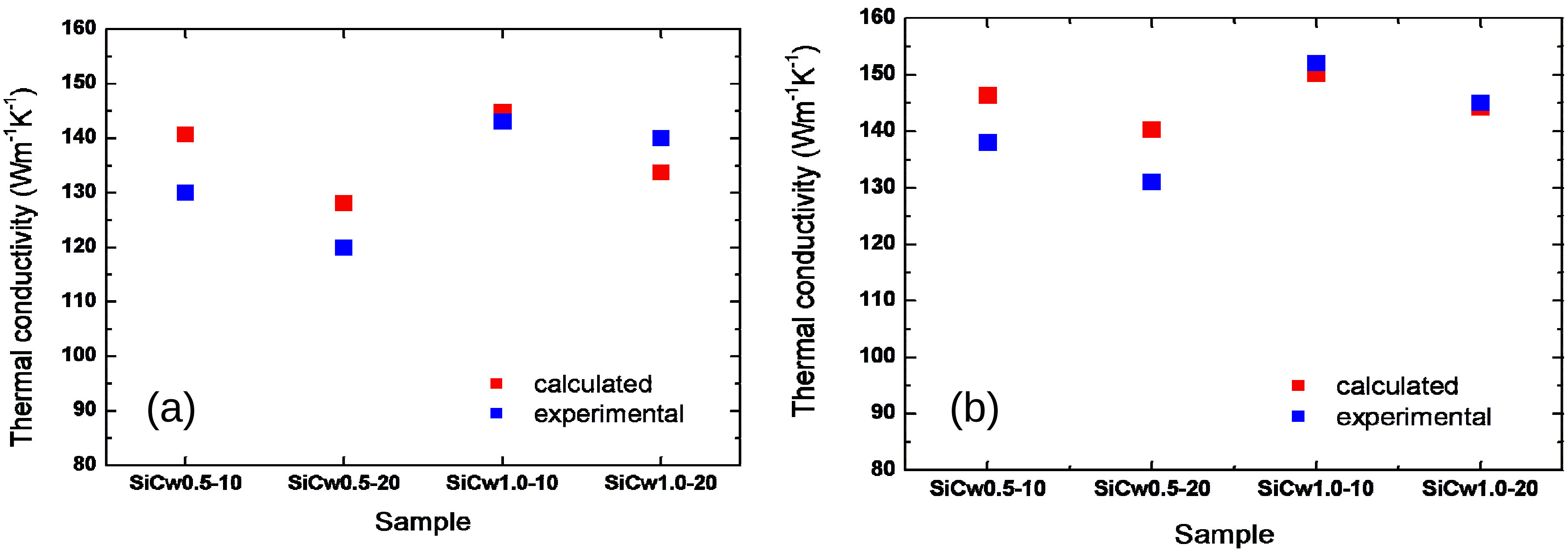




- **Samples**

Specimen	SiCw0.5-10%	SiCw0.5-20%	SiCw1.0-10%	SiCw1.0-20%
Matrix	Al alloy A2024			
SiC whisker diameter (μm)	0.5	0.5	1.0	1.0
SiC volume fraction	10%	20%	10%	20%

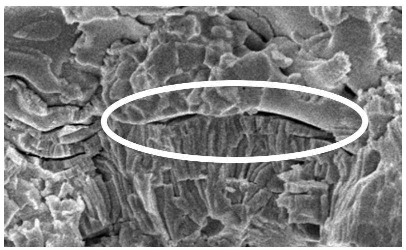
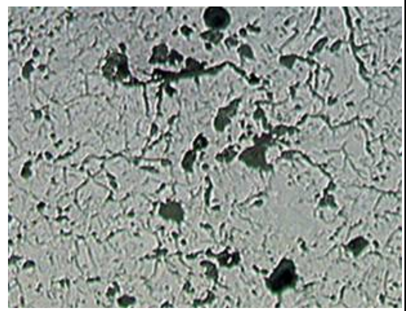
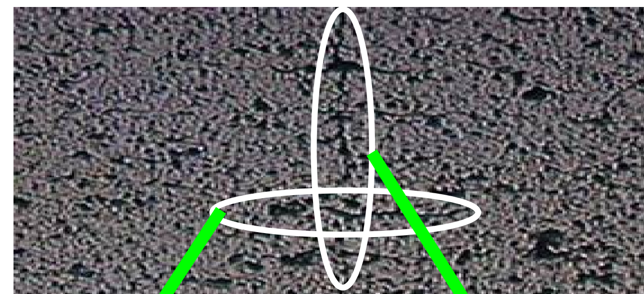
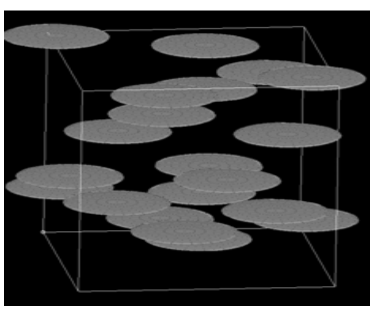
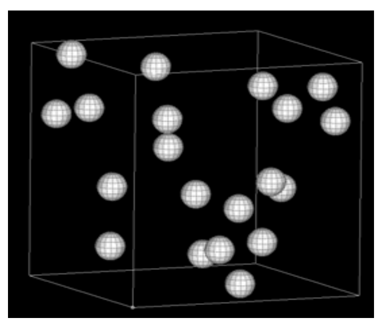
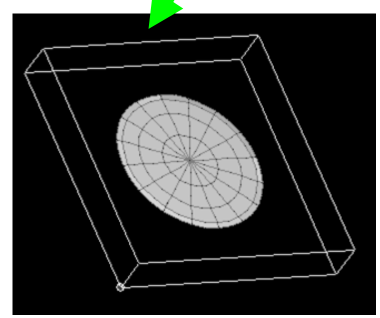
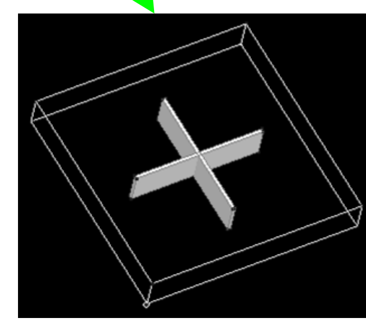
Example of Application (1)



Thermal conductivity of SiCw/Al perpendicular (a) and parallel (b) to the whisker.

Example of Application (2)

- **ZrO_2 thermal barrier coating**

	Inter-splat crack (<1μm)	**Pore (1-10 μm)**	**Branch crack (>10 μm)**	**Segment crack (>10 μm)**
images				
FEM models				

Example of Application (2)

- Samples

Coating condition

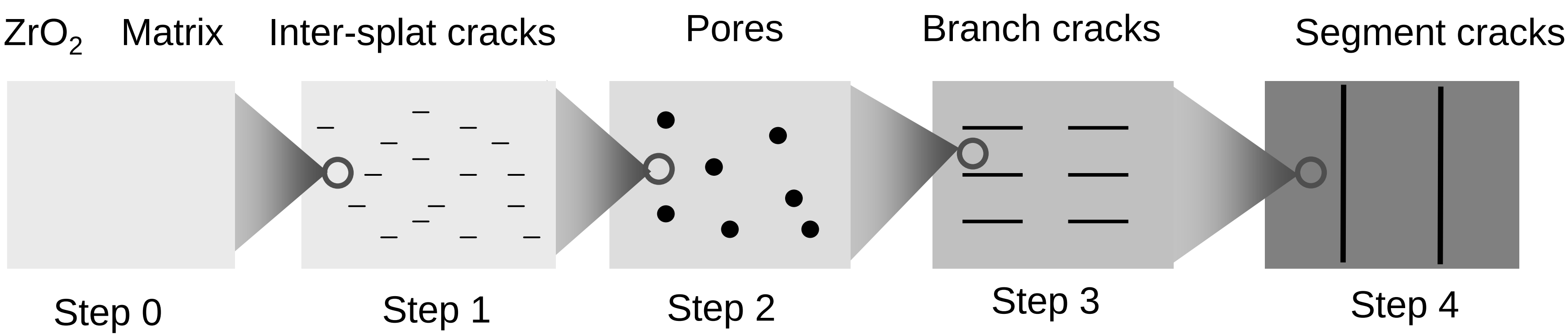
	Plasma power (KW)	Spray distance (mm)	Substrate temp. (℃)
C1	25.6	100	500
C2	34.2	80	650
C3	37.8	60	800

Volume fraction of pores

	Segment cracks	Branch cracks	Pores	Inter-splat cracks
C1	1.85%	0.68 %	4.67 %	5.36%
C2	2.25%	0.36%	4.07%	4.20%
C3	3.78%	0.29 %	1.83 %	1.89%

Example of Application (2)

- **Multi-scaled simulation**



Comparison of the calculated and measured transverse thermal conductivity κ_T (W/mK)

	Step0 (matrix)	Step1 (inter-splat crack)	Step2 (pore)	Step3 (branch crack)	Step4 (segment crack)	Exp.	Dev.
C1	2.30	1.10	1.03	0.95	0.93	0.98	4.1%
C2	2.30	1.27	1.20	1.16	1.14	1.12	1.8%
C3	2.30	1.78	1.73	1.71	1.63	1.68	3.0%

Conclusion

- An Internet platform for designing composites with required thermophysical property with connection to materials database has been developed.
- The accuracy and reliability of the system has been proved by experiments.