COMPLEX COMPOSITE ENGINEERING ARCHITECTURES FOR NUCLEAR AND HIGH-RADIATION ENVIRONMENTS

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Introduction:

Integrated Computational Materials Engineering (ICME) is a novel overarching approach to bridge length and time scales in computational materials science and engineering. This approach integrates all elements of multi-scale modeling (including various empirical and science-based models) with materials informatics to provide users the opportunity to tailor material selections based on stringent application needs. Typically, materials engineering has focused on structural requirements (stress, strain, modulus, fracture toughness etc.) while multi-scale modeling has been science focused (mechanical threshold strength model, grain-size models, solid-solution strengthening models etc.). Materials informatics (mechanical property inventories) on the other hand, is extensively data focused. All of these elements are combined within the framework of ICME to create architecture for the development, selection and design new composite materials for challenging environments.

We propose development of the foundations for applying ICME to composite materials development for nuclear and high-radiation environments (including nuclear-fusion energy reactors, nuclear-fission reactors, and accelerators). We expect to combine all elements of current material models (including thermo-mechanical and finite-element models) into the ICME framework. This will be accomplished through the use of a various mathematical modeling constructs. These constructs will allow the integration of constituent models, which in turn would allow us to use the adaptive strengths of using a combinatorial scheme (fabrication and computational) for creating new composite materials. A sample problem where these concepts are used is provided in this summary.

Background and Significance:

Composite materials have the capability of overcoming the disadvantages of monolithic materials by combining the characteristics of two or more classes of materials. Unfortunately, the development of new composite materials for nuclear (and high-radiation environments) has not kept pace with material developments in other areas like the automotive and aeronautical industries. Some of the factors that have impeded this technology proliferation have been (1) the high level of cost and complexity of testing, (2) lack of material behavior information under these extreme environments, and (3) systems understanding of composite material behaviors. We believe that the combinatorial schemes provided by models like those presented here will mitigate, and perhaps eventually eliminate, the aforementioned drawbacks.

Nuclear energy programs have a tremendous potential for growth in the coming years because of a renewed and energized interest in energy security. Nuclear energy systems have traditionally made rigorous demands on the materials used including dimensional stability (including void swelling, thermal creep, irradiation creep, stress relaxation, and growth), and acceptable strength, ductility, toughness, creep resistance, fatigue-cracking resistance, and corrosion resistance (in the presence of radiation, coolants, and process fluids). Deploying traditional metals and ceramics in these roles has resulted in compromises to performance.

Applications that might be amenable to this kind of treatment are those related to reactor fuel properties as a function of reactor burn-up. If these material behaviors can be described mathematically, they may support mathematic analysis methods as described here. Being able to avoid this or supplement it with reliable calculation results would be a great asset to fast reactor development programs (both in terms of cost and schedule).

Materials, Experiments, and Modeling:

Glidcop® materials were used for the computational test case. The material properties of the two composite materials plus the properties of the constituent materials are provided in the Table 1 below. The table includes fundamental, mechanical, thermodynamic, and electrical properties, as well as a sample nuclear property.

As a very simple test case, we perform an overall estimate of the mixture's suite of properties using the simple linear combinatorial model for all properties:

$$P_i = w_1 p_{1i} + w_2 p_{2i}$$

where,

P_i = the composite material's *ith* property;
p_{ji} = the *jth* constituent's *ith* property; and
w_j = the weight fraction (or volume fraction) of the *jth* constituent.

Because we have the as-measured properties from Glidcop (as shown in Table 1), we can compare the estimated values to the actual values. The results of the comparison, in the form of a percent relative error are provided in Figure 1 below. It is apparent that some properties are amenable to a linear model while others require a different treatment. For example, the large electrical resistivity of alumina overwhelms the calculation for the mixture, and a simple combinatorial model is inappropriate given the nature of electrical resistivity and the areal nature of electrical flow. Therefore, the material model elements for the electrical resistivity would be related to the relative area of the constituents and the electronic interactions.

Table 1. Glidcop Dispersion-Strengthened Copper Material Properties.

Property	AL-60	AL-15	Cu	Al_2O_3
Melting Point (degC)	1083	1083	1083	2054
Density @ 20C (g/cc)	8.81	8.9	8.96	3.96
Electrical Resistivity @ 20C (uOhm-cm)	2.21	1.86	1.7	2.50E+12
Thermal Conductivity @ 20C (W/m-K)	322	365	398	46
CTE 20-150C (um/m-C)	16.6	16.6	16.4	5.5
Modulus of Elasticity (tension) (GPa)	130	130	110	370
Tensile Strength, flat as cons. (MPa)	517	413	344	300
Yield Strength, flat as cons. (MPa)	413	331	333	
Hardness, flat as cons. (HRB)	81	62	37	
Thermal capture cross sections (barnes)	0.315	0.32	0.322	0.011

If the set of materials-properties equations could be expressed in a linear fashion and we could construct a matrix equation for a combined material as

$$\vec{P} = \underline{M}\vec{p},$$

where the vector $\vec{P}$ is the set of integral materials properties, the vector $\vec{p}$ is the set of individual component materials properties, and the translation matrix contains the general model of how the individual component properties combine to obtain the integral composite material properties. One key point is that the vector $\vec{P}$ contains *i* elements where i is the number of properties being considered. However, the vector $\vec{p}$ contains $n \times i$ elements, where *n* is the number of constituent materials. Clearly, therefore, the model matrix will be non-square and therefore non-invertible, and one goal of such a computational model would be to effectively invert the matrix to facilitate aggregation of various materials to obtain a pre-specified suite of material properties. However, we can construct other numerical methods such as iteration to perform this activity. The correlation matrix *M* can include "scale factors," "interface interaction," "defect interactions," and other engineering factors (including thermo-mechanical factors).

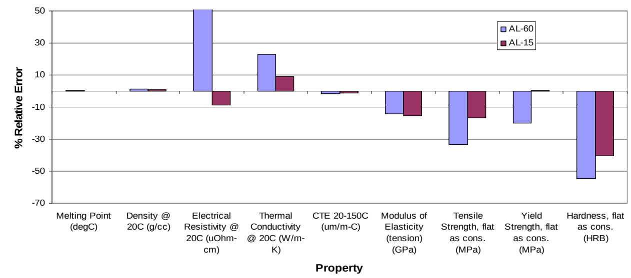

Figure 1. Relative error in linear material property analysis.

As an example we consider a simple analysis of the tensile strength in Glidcop® copper-alumina composites. A linear model yields a very poor representation of the integral material properties. We add two terms to the linear model to account for residual stress at the alumina particle interfaces and to account for the residual stress in the surrounding copper matrix. This yields the following form:

$$\begin{bmatrix} \sigma_{AL-60} \\ \sigma_{AL-15} \end{bmatrix} = \begin{bmatrix} 1 - v_{\mathrm{Al2O3}}^{AL-60} & v_{\mathrm{Al2O3}}^{AL-60} & v_{\mathrm{Al2O3}}^{AL-60} & v_{\mathrm{aff}}^{AL-60} \\ 1 - v_{\mathrm{Al2O3}}^{AL-15} & v_{\mathrm{Al2O3}}^{AL-15} & v_{\mathrm{Al2O3}}^{AL-15} & v_{\mathrm{aff}}^{AL-15} \end{bmatrix} \begin{bmatrix} \sigma_{UTS}(\mathrm{Cu}) \\ \sigma_{UTS}(\mathrm{Al_2O_3}) \\ \sigma_{\mathrm{Residual}} \\ \sigma_{Y}(\mathrm{Cu}) \end{bmatrix}$$

Inserting data from matweb.com yields estimated tensile strengths of

$$\begin{bmatrix} \sigma_{60} \\ \sigma_{15} \end{bmatrix} = \begin{bmatrix} 503 \\ 384 \end{bmatrix},$$

which compares quite well (3% and 6% relative error for the AL-60 and AL-15, respectively) to the data in Table 1, thereby providing at least one example of the capability of mathematical models. Performing an inverse analysis, i.e., determination of a material combination based on required properties is a key capability of this method.

References:

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