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Path dependent models to predict property changes in graphite irradiated at changing irradiation temperatures

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INTRODUCTION

Property changes occur in materials subjected to irradiation. The bulk of experimental data and associated empirical models are for isothermal irradiation. The form that these isothermal models take is usually closed form expressions in terms of fluence and irradiation temperature.

Irradiation temperature changes do however occur due to operational requirements. Isothermal models are no longer applicable, since experimental observations after an irradiation temperature change demonstrate that properties do not change instantaneously from one isothermal curve to the other. The properties are path-dependent, but the isothermal models are usually point functions.

SCALED FLUENCE METHOD

An option is the scaled fluence method proposed by Price and Haag [1], which was adopted in the KTA code [2]. The technique requires access to the isothermal property curves, which are transposed horizontally after an irradiation temperature change. Gaps in the resulting property curves are removed by an exponentially decaying function. The method is illustrated in **Figure 1**.

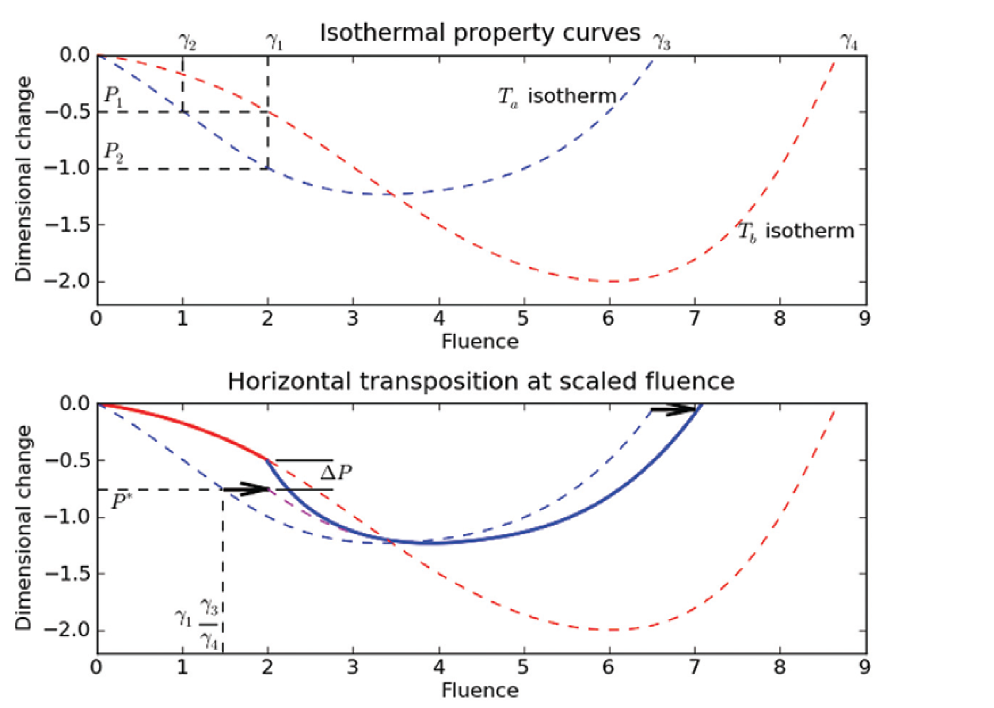

Figure 1: Illustration of scaled fluence method

STATE VARIABLE EVOLUTION MODEL

In this work, path dependency is accounted for by using a state variable evolution model. A property P is evolved by integrating an evolution equation of the form $\frac{dP}{d\gamma} = f(P,T)$. Here γ is the fluence, f is the evolution equation and T is the irradiation temperature. Such an internal state variable model is similar to the metal plasticity model developed by Follansbee and Kocks [3].

WIGNER SHRINKAGE STRAIN

As first example, consider Wigner shrinkage strain, L. Isothermal curves are depicted in **Figure 2(a)**. These curves can be modelled by assuming 3 independent mechanisms i.e. $L = L_1 + L_2 + L_3$, where L_1, L_2 and L_3 evolve as a function of temperature. Evolution equations of the form

$$\frac{dL_1}{d\gamma} = \theta_1 \,(1 - \frac{L_1}{L_{1s}}),\ \frac{dL_2}{d\gamma} = \theta_2 \,(1 - \frac{L_2}{L_{2s}}),\ \frac{dL_3}{d\gamma} = \theta_3 \,(1 + \frac{L_3}{L_{3s}})$$

are assumed, with θ_1, θ_2, θ_3, L_{1s}, L_{2s} and L_{3s} temperature dependent material parameters. **Figure 2** demonstrates the results when applied to Dragon grade 95 graphite. The model parameters are estimated by integrating the evolution equation and minimising the resulting least squares error iteratively. The increased accuracy as compared to the scaled fluence method, after an increase in irradiation temperature from 900 °C to 1200 °C in **Figure 2(b)**, is especially noteworthy.

YOUNG'S MODULUS

Percentage change in Young's modulus Y is modelled as

$$\frac{dY}{d\gamma} = \theta_1 \,(1 - \frac{Y}{Y} + \frac{C}{Y}) \ \text{with}\ \frac{dC}{d\gamma} = a_1 C^{a_2}$$

where θ_1, Y_s, a_1 and a_2 are temperature dependent material parameters. Application to data from Price and Haag [1] is demonstrated in **Figure 3**.

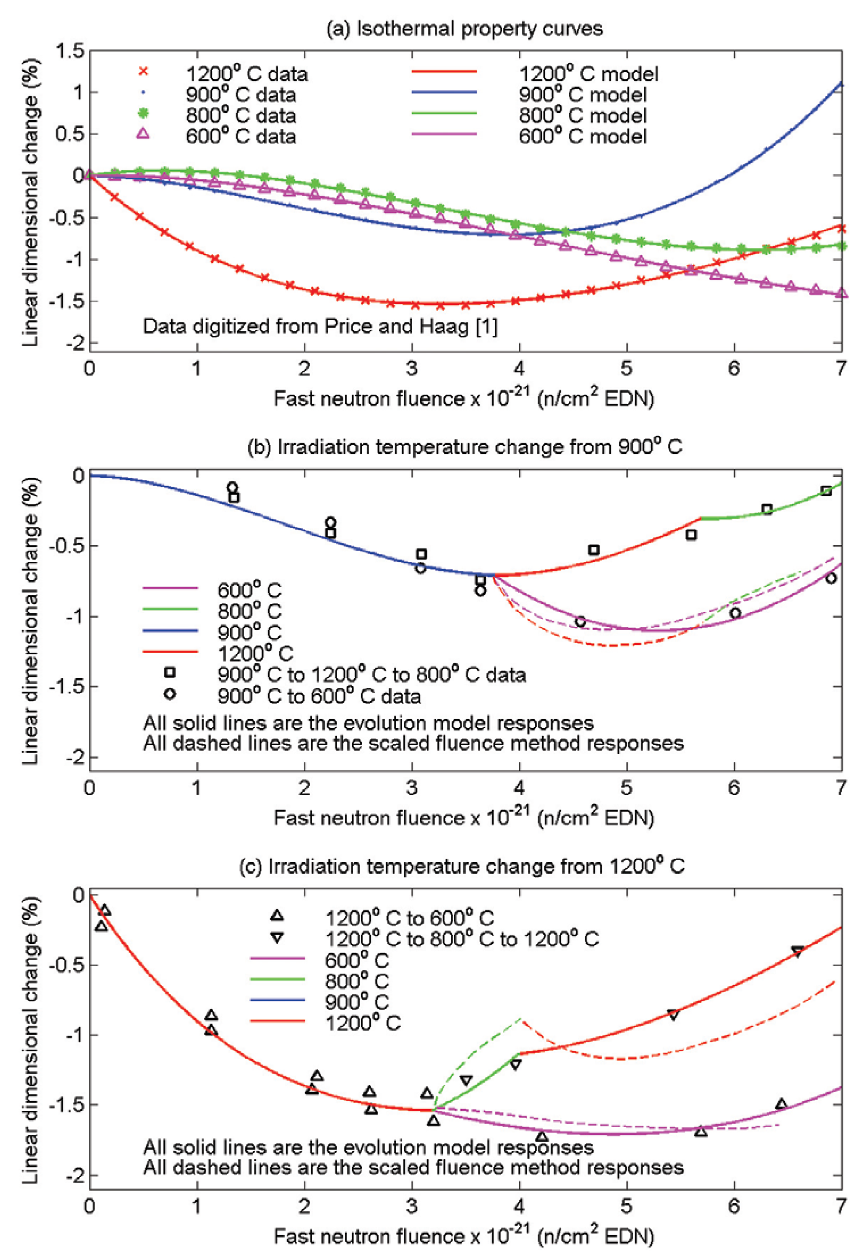

Figure 2: Wigner shrinkage strain

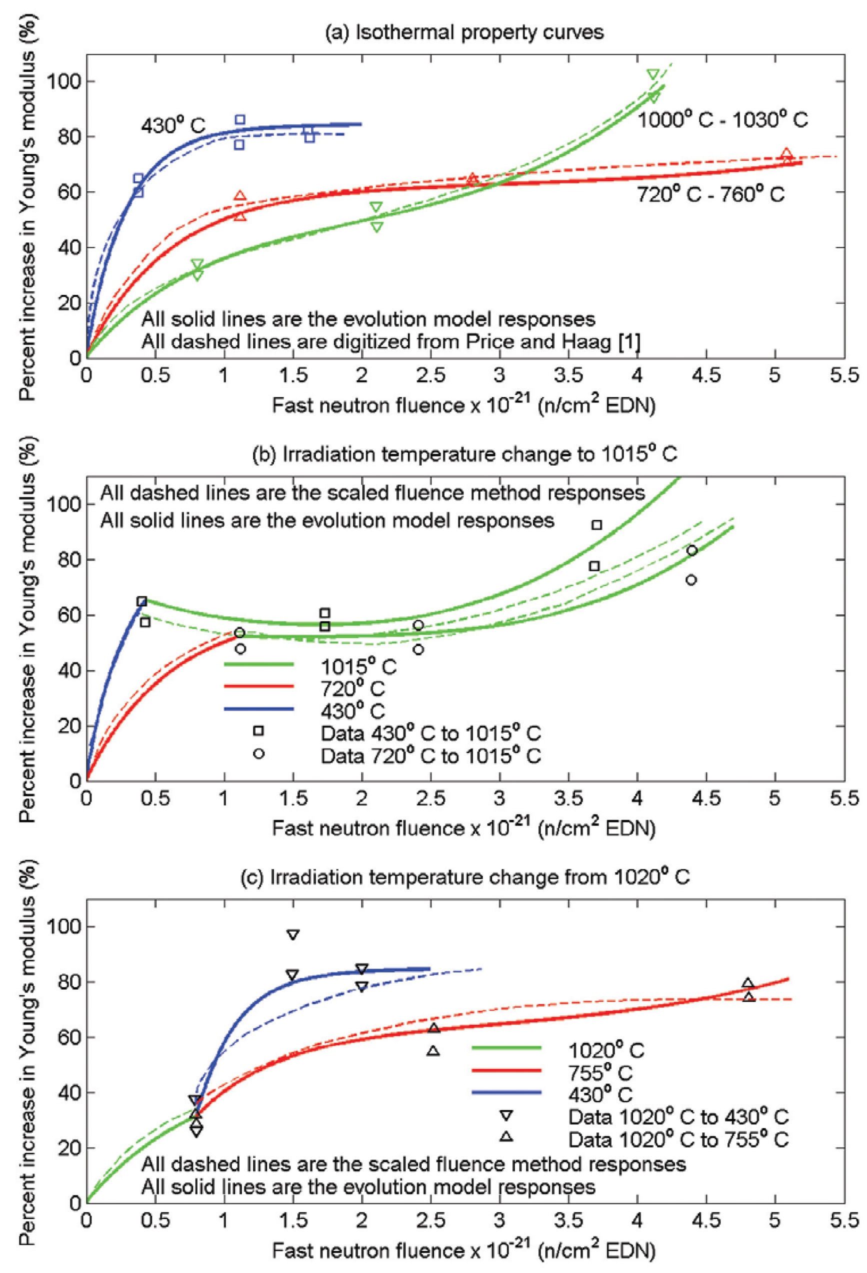

Figure 3: Young's modulus

THERMAL EXPANSION COEFFICIENT

Change in thermal expansion coefficient a is modelled as the sum of two independent mechanisms, i.e. $a = a_1 + a_2$, with

$$\frac{da_3}{d\gamma} = \theta_1 \,(1 - \frac{a_1}{a_{1s}}) \ \text{and}\ \frac{da_2}{d\gamma} = c_1 a_2^{\,c_2}$$

where θ_1, a_{1s}, c_1 and c_2 are temperature dependent material parameters. Results are depicted in **Figure 4**.

THERMAL CONDUCTIVITY

Thermal conductivity κ is modelled similarly to Young's modulus as

$$\frac{dx}{d\gamma} = \theta_1 \,(1 - \frac{\kappa_i - \kappa}{\kappa_{3s} - \kappa_s} + \frac{C}{\kappa_i - \kappa}) \ \text{with}\ \frac{dC}{d\gamma} = a_1\, C^{a_2}$$

where θ_1, κ_s, a_1 and a_2 are temperature dependent material parameters and is a temperature independent initial condition. Results are depicted in **Figure 5**.

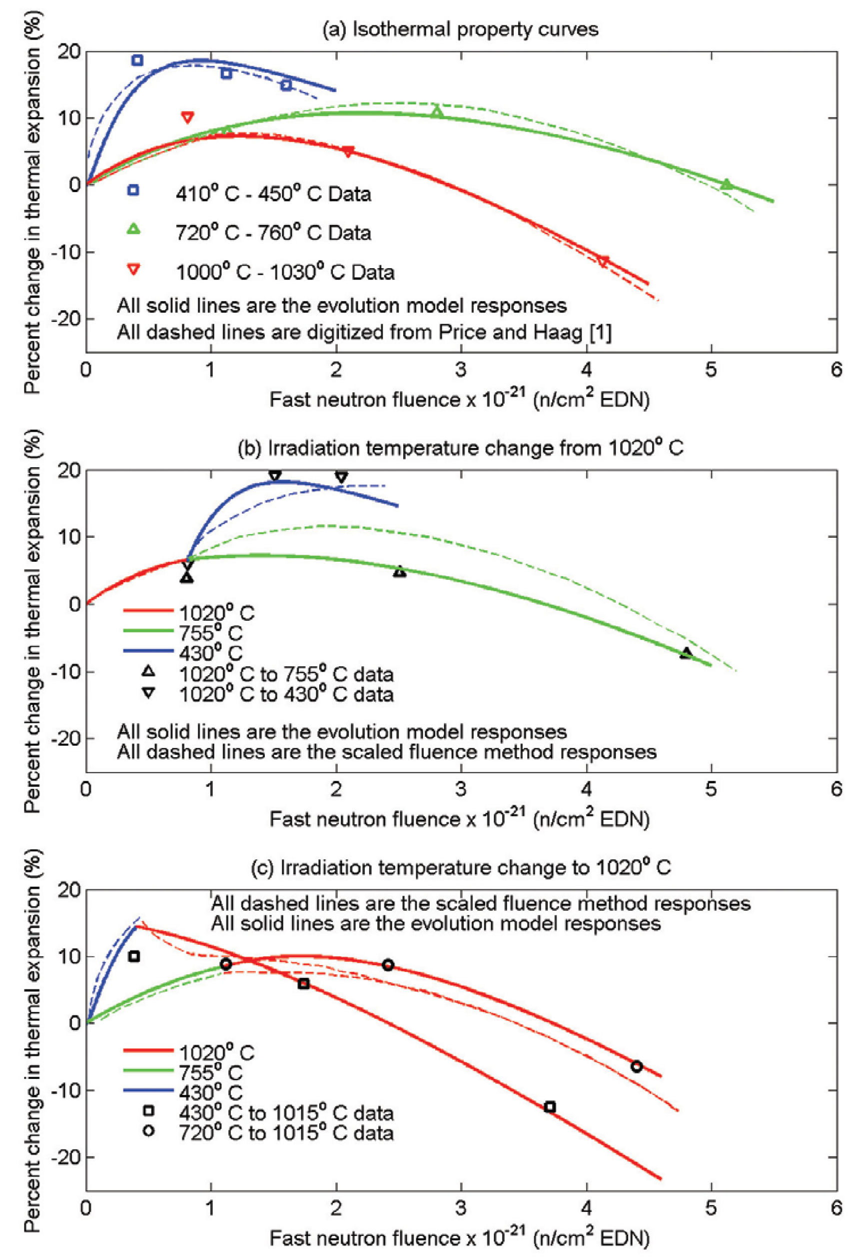

Figure 4: Thermal expansion coefficient

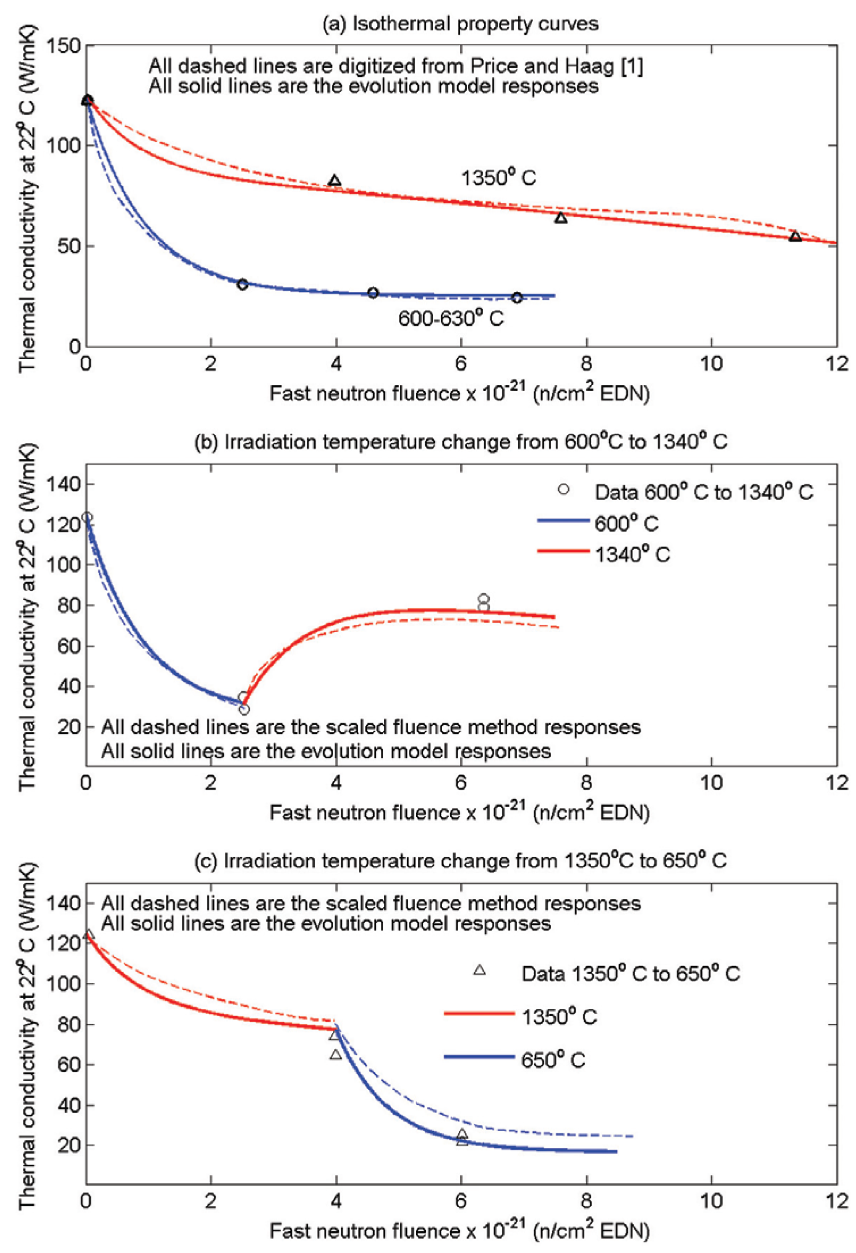

Figure 5: Thermal conductivity

CONCLUSIONS

It is demonstrated that path dependent material properties can be modelled using simple state variable evolution equations, if every irradiation temperature is assigned a different set of evolution equation parameters. Analytical forms for the temperature dependency of evolution equation parameters should be investigated in future.

REFERENCES

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[3] PS Follansbee, UF Kocks, A constitutive description of the deformation of copper based on the use of the mechanical threshold stress as an internal state variable, Acta Metallurgica, 36(1), pp. 81-93, 1988.