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Theory-Based Models and Simulations of Materials for Fusion

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1. Introduction

Although experiment, theory, and computation are still at the core of the the scientific approach to knowledge, two new concepts have recently emerged: *models* and *simulations*. The definitions below are only intended to clarify the proposed initiative.

A *model* is a logical description of how a system (material, in our case) performs. For example, "enthalpy is linear in temperature" is a model. Most models are represented using mathematical expressions. Empirical models are collections of experimental observations fitted to mathematical expressions, such as (but not only) polynomial functions. When accurate, empirical models are valuable for technological applications. Theory-based models are built upon a theory developed within or across scientific disciplines (physics, chemistry,…etc). Theory-based models are expected to provide a deeper understanding of the nature of the properties and to have improved predictive character.

A *simulation* is the process of conducting experiments or running computer programs to reproduce, in a simplified way, the behavior of a system. Simulations describe the evolution of the system along a certain coordinate, most often the time. For example, a simulation of heat transport in a reactor material could involve the model described above to predict the temperature and enthalpy content of a specific materials volume, at different moments in time.

In this work we submit that both the models and the simulations must be subject to verification and validation and propose slightly different definitions of the concepts, compared with the Greenwald report [1, pp 162],: *Verification* is the process by which the fidelity of a numerical algorithm with respect to underlying mathematical representation of a model or simulation is established and the errors in its solution are quantified. *Validation* is the process through which the scientific community comes to accept that a particular model or simulation reliably predicts real world behavior. Most validation processes involve comparison with experimental data. Rarely, simulations are "weakly validated" against computational results.

2. Performance Gaps

In the Greenwald report, the need for controlling materials' properties is present in all themes. Theme A encourages the development of a set of computational models that are capable of predicting all important plasma behavior in various reactor regimes, while theme B wishes to design replaceable components that can survive the complex reactor environment. The report identifies several major gaps in the theory and control of materials properties. For example, in theme C, "Harnessing fusion power", the focus is on "understanding the basic materials science for fusion breeding blankets, structural components, plasma diagnostics and heating components in high neutron fluence areas". In other words, there is a need for theory-based models, coupled with experiments and computation. This is consistent with the TAP, EPACT, and BSAC reports.

In this context, success would be establishing the relationships between thermo-mechanical properties such as enthalpy, specific heat, thermal conductivity, and thermal expansion, and parameters such as temperature, composition, porosity, pressure, and irradiation level. Although there are models that account for “ono-to-one” relations, an important gap is the absence of comprehensive models that can relate multiple properties to multiple parameters. For example, there are several models of thermal conductivity of reactor materials as function of temperature but models that include composition as a parameter are quite rare.

Understanding the material microstructure evolution under irradiation and temperature gradients is another area of research in need of models and simulations to capture the effect of neutrons and ions on void and gas bubble formation, swelling, embrittlement, and corrosion. However, correlating thermo-mechanical properties to the neutron flux is a challenging endeavor. Since a certain flux can be associated with a variety of changes in the properties of the materials, depending on the history and damage mechanisms involved, solving for the irradiation level may lead to mathematically ill-posed inverse problems. On the bright side, the direct problems (change in properties versus irradiation level) can be solved using simulations.

In summary, the goal is to control the properties and phenomena in irradiated materials for fusion applications. To achieve this goal, we propose to develop theory-based models that enhance the understanding of materials properties, to perform simulations of irradiation effects on reactor materials, and to create and maintain an international knowledgebase of data, models, and simulation results.

3. Components of the proposed initiative

3.1 Develop theory-based, comprehensive models of materials properties.

We will build upon existing studies of irradiation effects on materials properties such as thermal conductivity, species diffusivity, and thermal expansion. Outstanding results have been already captured in empirical models and are successfully used in reactor design. However, the empirical models are only valid within the range of parameters used to develop them. In this initiative we propose to engage the scientific community in developing theory-based, comprehensive models that enhance the understanding of reactor materials properties and have validated predictive character.

For example, we propose to develop Quantum Mechanical models of point defect formation in irradiated materials and couple them with Statistical Mechanical models, to predict and control the composition and species diffusivity at various temperatures and fluxes. To address phase stability in reactor materials at the interface with the plasma and during transient regimes, we propose to develop Thermodynamic models of the Gibbs free energy of all phases that are at risk of undergoing phase transformations.

To account for all the important materials properties and reactor phenomena, models and simulations must cover a wide range of space and time scales, starting with the nucleus and the atomic electronic structure (nm) all the way to the reactor components (meters), and from defect formation (pico-seconds) all the way to the operating characteristic times (months, years). Fig. 1 shows some of the theoretical and computational methods used for model development and simulations in materials [2]. The information is transferred between scales via characteristic parameters such as density, energy, temperature, or grain size distribution. In practice, meso-scale and continuum methods are often “atomistically informed”, in the sense that some of the parameters in the meso-scale method are optimized against the output of atomistic calculations.

Model development is not an exercise in mathematics. In fact, most models are developed by experimentalists. Modeling involves strong collaboration between experimentalists, theoreticians, and computer scientists. We will partner with scientists at irradiation facilities, such as FFMF and IFMIF, in designing experiments for model development and validation.

3.2 Perform simulations of irradiation effects on materials.

The Greenwald report recognizes that several important interactions, such as the effect of neutrons on the sintering of ceramics, are unknown [1, pp 62]. We propose to perform atomistic, meso-scale, and continuum simulations of irradiation effects in reactor materials, to predict and control point defect formation, microstructure evolution, He embrittlement, corrosion, and phase changes. For example, we will advance the meso-scale simulations of He effects on the microstructure of reactor materials [3].

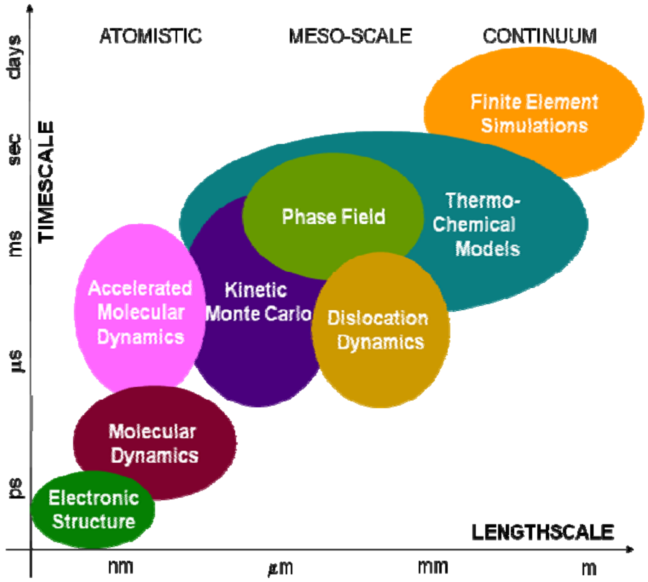

Fig. 1 Multi-scale theoretical and computational methods [2].

From a computational point of view, there is a tremendous opportunity to expand the investigation space by using high performance computing. Today, the top 500 supercomputers in the world can reach speeds over a teraflop per second. Already, in the USA, the European Union and Japan, neutron diffusion calculations, as well as reactor safety and security simulations, are performed on such resources. We propose to develop innovative code design and advance algorithms to run the components of the multi-scale methods on a national network of high-performance computers.

The predictive character of the simulation capabilities will be tested using experimental characterization. Facilities such as IFMIF, the Materials Test Station (MTS), and the Fusion Fission Materials Facility (FFMF) at LANL will enable damage levels similar to the reactor environment and will contribute to validation of models and simulations.

3.3 Develop and maintain an international knowledgebase of data, models, and simulation results.

Taking into account the fusion by-products and the chemical reactions in the reactor materials, it becomes necessary to study systems with a large number (>10) of components. This non-trivial task involves a well defined plan and careful, international coordination of research projects. Several European and Asian countries have already started this type of studies in conjunction with the development of databases for materials properties for nuclear energy applications. Besides maintaining a close collaboration with the existing databases, we propose to create, update, and maintain an international “knowledgebase” that includes experimental data, models (mathematical expressions), and simulation results (tables, graphs, diagrams), all linked to publications and web sites. The knowledgebase will have a friendly user interface and will use advance query techniques capable of retrieving numbers, text, and images.

REFERENCES

[1] Priorities, Gaps and Opportunities: Towards A Long-Range Strategic Plan for Magnetic Fusion Energy, A Report to the Fusion Energy Sciences Advisory Committee, October 2007.
[2] M. Stan, J. C. Ramirez, P. Cristea, et al., J. Alloys Comp., **444–445** (2007) 415–423.
[3] S.Y. Hu, M. I. Baskes, M. Stan and C. Tome, Appl. Phys. Let., **90** (2007) 81921-81923.