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KINETIC THEORY OF RADIATION EFFECTS*

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The kinetic theory of radiation effects based on defect and microstructural reactions is assessed. In particular, consideration is given to the role of supercomputing in this area. The transparencies used in the presentation contain all of the technically detailed information that was presented, as well as salient points of opinion and discussion in highlight form. The aim of the present short summary is to supplement and explain my appraisal rather than to repeat all specifics that are covered there. How the kinetic theory has been applied to radiation effects in fusion reactor materials is described in order to provide background and sufficient perspective to consider specifically the role of intensive computing. A more complete background is available in reference [1].

Cascades, in which displaced atoms are generated, are formed on a time scale of about 10^{-13}s. The kinetic phenomena that bridge the gap between this realm and changes in macroscopic properties of technological significance span much longer time scales. The interstitials created may be removed at sinks by diffusion in times as short as 10^{-6}s, while the corresponding vacancies require a time scale ranging from about 10^{-3}s to 1s, depending sensitively on the temperature. The wholesale buildup of extended defect microstructure that results from such reactions, including dislocation loops, dislocation network, cavities, precipitates and segregated regions requires time intervals measured in units of 10^{6}s. Changes in properties resulting from these processes include swelling, creep, phase instability, hardening and embrittlement.

To help achieve the quantitative and mechanistic understanding of these processes, the kinetic theory of radiation effects has been developed in the DOE basic energy sciences radiation effects and fusion reactor materials programs, as well as in corresponding efforts in other countries. This discipline grapples with a very wide range of phenomena and draws on numerous sub-fields of theory such as defect physics, diffusion, elasticity, chemical reaction rates, phase transformations and thermodynamics. The theory is cast in a mathematical framework of continuum dynamics.

Issues particularly relevant to the present inquiry can be viewed from the standpoints of *applications of the theory* and *areas requiring further progress*.

Applications of the Theory

Three primary activities can be identified: understanding mechanisms, alloy design for radiation resistance, and numerical predictions and extrapolations. In relative terms, the first two areas historically have not been and are not anticipated soon to become computing-intensive. Mechanistic

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understanding is built up by combined theoretical and experimental work. Mathematical formulation is achieved based on models of physical processes thought to be relevant to the details of phenomena in question, such as swelling, creep or embrittlement. Theoretical analysis of approximate or limiting cases, together with simple calculations typically are carried out. Mechanistically oriented irradiation experiments, often on simple materials under highly structured conditions are performed in conjunction. In the course of this work the theory plays both leading and supportive roles.

After some understanding is demonstrated, possible beneficial manipulations of materials or irradiation parameters are sometimes readily apparent. With further explorations, these ideas may be developed into principles for alloy design for radiation resistance. The principles can be valuable even without precise quantitative predictions. Simply knowing what outcome to avoid or which directions to pursue in terms of alloying additions, for example, may be very powerful in practice. A successful example of this is alloy design for swelling resistance based on the theoretical concepts of critical radius and critical number of gas atoms. The theory and experimental work surrounding the critical quantities is illustrated in detail in the transparencies. Some of the most swelling resistant alloys available have been developed on this basis [2].

The third area, computed numerical predictions or extrapolations from known results to conditions where no experimental data are available, is also an important activity. It is here that more intensive computing is often required. Between five and ten years ago it is my impression that precise predictions were often mentioned and generally accepted as the main goal of theoretical modeling. I believe that this is too narrow a point of view and that the motivations mentioned above, i.e., understanding mechanisms and alloy design are now accepted as equally important. Attempting precise numerical extrapolations certainly has its place in reactor engineering and design, for example, in assessing lifetime and lifetime-limiting phenomena, and in devising engineering accomodations. Numerical extrapolations have no substitute for specific complex alloys subjected to arbitrary operating conditions, where the final outcome of irradiation cannot be predicted by simple calculations, even granting that we may know the multiple mechanisms operating and understand each in the context of single variable experiments. The structure and approximations of a recently developed composite model, together with examples of its capability to describe experimental results is covered in the transparencies [3].

Areas Requiring Further Progress

Again we may identify three separate considerations: physical theory, experimentally measured input parameters, and computational power. My assessment of the current situation is that the required continuing development of the theory and the state of experimentally measured input parameters presently control progress in the kinetic theory of radiation effects.

Computational power is not limiting overall. However, in certain specific areas such as that mentioned above and others to be noted below, advances in or better use of existing power will translate into gains.

The present stage continues as one of identifying the most important physical processes in different materials in various irradiation regimes, and in achieving their mathematical formulation and physical understanding. Yet, as shown in a classic example [4], a validated theroetical model can still produce vastly different results or even opposite answers to a question, when parameters are not well known. These parameters include a large array such as "fundamental" properties of point defects including migration energies, as well as related "derivative" properties such as bias for swelling or creep, for example. The example referred to above concerns the range of reported experimentally measured migration energy for vacancies in pure nickel. Using the extremes in the reported range to predict swelling, with all other parameters held constant, the theory not only gives swelling predictions that differ by orders of magnitude but describes the material as being in different physical regimes, so that other predicted properties are also affected. In practice such problems are dealt with by measuring swelling itself, for example, under certain conditions. For consistency with the theory, this then forces restrictions on the possible values of certain *combinations* of parameters, such as bias, vacancy migration energy and point defect generation rate, for example. Only combinations in this range are subsequently used for calculations, even though the individual parameter values remain uncertain.

Aspects of the general theory of point defect clustering were covered in the presentation. Several approaches to solving the clustering problem are available. Most are based on further analysis of the discrete clustering equations in terms of systematic approximations and limits. However, in principle the discrete system of equations can also be solved directly with no further mathematical analysis. The full solution of such a set of equations, whose numbers run into the hundreds of millions, requires capabilities beyond forseeable levels of computing power. The gain in accuracy and insight over formulations currently in use is a subject of debate. Therefore, a strictly discrete clustering approach is a computing-intensive application where the incremental gain must be weighed in terms of the resources required.

Another application that is computing-intensive is the cascade diffusion theory. This formulation removes the usual limitations of temporal and spatial homogeneity in the conventional kinetic theory and considers the consequences of point defect production in discrete cascades. In order, to describe the point defect concentration in a small region, discrete cascades produced at all prior times and everywhere in the material are accounted for. This generalization is found to be crucial for some phenomena, such as irradiation creep. A new mechanism of irradiation creep, cascade-induced creep, emerges from this work. Cascade-induced creep is not recognized, by definition, within the formalism of conventional kinetic theory. Upon numerical evaluation the process turns out to provide a significant component of irradiation creep.

To summarize, intensive computational power has a limited, but nevertheless important, place in the kinetic theory of radiation effects. One of the fundamental reasons is that the kinetic theory is based on continuum dynamics. It is therefore intrinsically less computation-bound than formulations based on molecular dynamics, for example. Even within its own scale of computational intensity, it is expected that advances in and better use of existing computational power will not by themselves guarantee accelerated progress overall. Continued advances in the theory and improved knowledge of basic materials parameters are prerequisite to greater benefits from computational power. However, specific areas may benefit from increased computational capability. Examples of these include: (1) numerical computations using composite models for engineering applications, which cover complex materials under arbitrary irradiation conditions, (2) cascade diffusion theory calculations that go beyond homogeneous continuum dynamics, and (3) approaches toward more direct solutions of the discrete clustering equations.

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