RADIATION EFFECTS ON STRUCTURAL MATERIALS

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1. INTRODUCTION

The successful development of commercial fusion energy depends critically on advances in a number of key engineering technologies. Of these, developing structural materials that can withstand the grueling environment of fusion reactors is an area of primary importance. First-wall and blanket materials will operate in an environment that has never existed before and that subjects them to extreme conditions. For instance, materials will be exposed to high heat and particle fluxes from the plasma side; simultaneously, high energy neutrons will displace each lattice atom from its site several hundred times during the lifetime of the material. Additionally, several hundred parts per million of gaseous species (*i.e.*, hydrogen and helium) as well as transmutation products will be produced by nuclear reactions, and when the structure is conductive, large body forces resulting from eddy currents may also be produced during transient operation. Coolants will also subject the structure to mechanical loadings that invariably induce a three-dimensional stress state in the material. It is, therefore, crucial to recognize the complexity of the loading and environmental conditions to which the material is subjected.

Obviously, incremental engineering knowledge must be gained through the construction of scalable experiments and test devices. Present-day experiments can be used to give us an understanding of the phenomena that control materials behavior in a controlled environment. As a result of these "simple" experiments, we will be able to design more complex environments to simulate realistic fusion conditions.

Sound fundamental understanding of neutron irradiation effects on structural materials will enable the fusion design community to develop new materials to meet the optimum requirements of fusion reactor conditions. Theoretical insights into basic damage mechanisms are essential to the overall strategy for materials development. Theory has provided a reasonably organized framework by which materials behavior in the complex irradiation and thermal environment of

fusion reactors can be understood. Additionally, theory has provided valuable guidance to the process of selecting irradiation and material conditions, which can lead to a more rational approach to fusion materials development.

In order to confidently predict the performance of structural materials and, therefore, component lifetimes in complex blanket geometries, testing must ultimately be made in a prototypical fusion environment by exactly duplicating thermal, radiation, electromagnetic, and mechanical loadings. However, until prototypical fusion conditions are made possible, carefully planned simulation experiments by electrons, ions, and neutrons are used to guide materials development. The degree to which simulation experiments realize realistic fusion conditions is extremely dependent on sound theoretical understanding of the fundamental processes. Theoretical research has been utilized by the conceptual fusion-reactor design community to incorporate the often sketchy data base into phenomenological models, which are subsequently used for more accurate data extrapolations by design engineers.

At UCLA, our research at UCLA on modeling the effects of fusion neutron irradiation effects on structural materials covered a number of theoretical and materials engineering areas during the six-year period (January 1984 through February 1990). In Section 2, we summarize the range of research activities which were supported by two consecutive three-year grants from the division of Development and Technology of the Office of Fusion Energy. This Executive Summary will serve to give an overall perspective of our work. A number of papers and reports from our research group have appeared in the open literature. We organize these technical contributions in Section 3 under the following categories:

- Atomic Displacements
- Microstructure Evolution
- Materials Engineering, Mechanics and Design
- Invention of Low-Activation Steels
- Research Motivated by Grant Support

One of the important contributions of university research is the education of graduate students. We have been quite successful in this particular aspect, and an account of our graduate and post-graduate student participation is given in Section 4. Section 5 gives a complete list of publications which resulted from, or were motivated by these two grants.

2. EXECUTIVE SUMMARY

2.1. History and Objectives

A three-year research proposal entitled, "Radiation Effects on Structural Materials" was submitted to the Materials Branch of the Development and Technology Division of the Office of Fusion Energy in mid-1983. The project was subsequently approved for a three-year period starting in January 1984. The objectives of the proposed research were stated as the development of theoretical methodologies and insights in the following areas of radiation effects on structural materials for fusion applications:

1. Helium effects on the properties of austenitic and ferritic alloys;
2. Microstructure evolution under irradiation;
3. Radiation hardening of austenitic and ferritic alloy systems, and radiation embrittlement of ferritics;
4. Precipitation kinetics under irradiation, and in-reactor creep;
5. Development of design equations for critical materials properties.

The research was based on both mechanistic and phenomenological descriptions of basic radiation effects. Mechanistic approaches result in greater understanding of the basic underlying physical processes. On the other hand, phenomenological theories often lead to useful equations for data extrapolations and for design purposes. The following general achievements were expected from the proposed research:

1. To discover fundamental radiation-damage phenomena and to gain new insights into the underlying physical mechanisms;
2. To suggest carefully planned experiments in order to unravel the action of important damage processes;

3. To extrapolate present-day experimental data to anticipated fusion conditions;
4. To develop design correlations for the improvement of blanket design concepts.

A milestone chart of proposed research is shown in Figure 1.

This phase of our research was a balanced mix of fundamental radiation-damage studies and design-oriented investigations. Based on our success with this work, we proposed a continuation project for a subsequent three-year period (February 1, 1987 - January 31, 1990). The emphasis of the continuation proposal was on the fundamental aspects of microstructure behavior under fusion irradiation conditions.

The proposed research covered a number of areas within the broad framework of radiation-damage theory. The overall objective was to develop and apply new theoretical methods in order to enhance the understanding of radiation-damage phenomena in a fusion environment. Specifically, we proposed a continuation of our work utilizing non-equilibrium statistical mechanical methods to describe microstructure evolution during irradiation.

The majority of approaches for analyzing microstructure evolution have been based on deterministic causal description that were provided by rate theory conservation equations. However, the existence of a large number of interacting entities, on the order of 10^{30} atoms in a typical engineering solid, implies that the system's degrees of freedom are much larger than can be represented by individual equations. Such a situation naturally leads to fluctuations around a reference state. In this work, we concentrated mainly on the role of these fluctuations on microstructural development and evolution. First, fluctuations around a "critical" state can determine the extent of embryonic cluster nucleation. Second, as the clustering system evolves, fluctuations determine the "dispersion" or "spread" around the average state.

Fig. 1. Milestone chart for proposal on "Radiation Effects on Structural Materials"

The work we proposed as listed below addressed a number of related areas in radiation damage:

1. Numerical solution to the transient, two-dimensional Fokker-Planck equation for the self-consistent description of helium-filled cavity nucleation and growth;
2. Development of an analytical "moments" method for describing the evolution of probability density of interstitial loops;
3. Development of a new method to experimentally measure, for the first time, dislocation bias towards self-interstitials;
4. Monte Carlo numerical simulations of collision cascades in polyatomic media;
5. Dislocation system self-organization and the relationship to in-reactor creep;
6. Precipitate stability during irradiation.

A milestone chart, as originally proposed, is shown in Fig. 2. Research on collision cascades and dislocation creep seemed particularly promising. The Department of Energy agreed to grant UCLA a "no-fund extension" of the project until November 1990.

2.2 Highlights of Research Accomplishments

Research work sponsored by the original grant and its continuation resulted in a considerable number of publications that can be roughly grouped into five separate categories. Most of the published research (55 papers and numerous reports) was directly funded by the two grants over the six-year period. A number of published papers, however, were not directly funded by the grants, although the work was essentially motivated by the general themes established under this DOE sponsorship. We will highlight in this section the salient achievements of our research work.

Fig. 2. Milestone chart for continuation proposal on "Statistical Theory of Radiation Effects"

mass disparity between electrons and ions, only a small amount of momentum and energy is transferred in electronic collisions. Therefore, energy loss due to electrons on a moving ion can be considered to be a continuous process and may be fully treated through the use of the continuous electron-stopping power approximation.

Various theories were developed for the treatment of ion nuclear and electronic energy losses. Although the Thomas-Fermi potential is the most sophisticated model for treating nuclear collisions, its use requires cumbersome numerical calculations. In our work, we used continuous power-law-potential fits to the Thomas-Fermi model. For very low ion energies, we used the Born-Mayer potential. The collision integral was analytically solved by using the moment approximation, and accordingly, the power-law cross section was derived. For electronic stopping, the Biersack-Haggmark model, which combines both the Lindhard-Scharff low-energy and the Bethe-Bloch high-energy models, was adequate.

Ion transport problems are generally treated by using either deterministic or probabilistic methods of analysis. The deterministic methods, however, can only deal with simplified problems. Applying the discrete ordinate multi-group treatment to ion transport is much more difficult than it is for neutron transport. The high anisotropy in nuclear collisions, recoil multiplication in slowing-down processes, and the need for group cross sections lead to considerable calculational difficulties. For our work, a probabilistic Monte Carlo method was developed to treat ion transport in polyatomic multi-layer solids. It is capable of simulating cascade damage in both bulk and surface radiation damage analyses. This code has been shown to be superior in both computing speed and versatility when compared with other equivalent Monte Carlo codes, and simulation results agree with those from either experiments or other codes.

2.2.1.1. Cascade-Diffusion Theory. In order to ascertain bulk radiation damage, TRIPOS is used to simulate displacement collision cascades. An immediate application of the results is for the treatment of stochastic diffusion of point defects in the so-called cascade-diffusion theory.

Our study shows that the δ -function cascade model used in earlier investigations by different authors yields singular point-defect concentration fluctuations. Therefore, non-zero cascade size has to be included in order to avoid this singularity which is unphysical. With the consideration of cascade strength and size, our results from the homogeneous cascade model show that the point-defect concentration fluctuations can be smaller by a factor of 5 than those from the point-cascade model. For high-energy collision cascades, our results show that the fluctuations from the uniform tree subcascade models are 2 to 3 times higher than those from the homogeneous cascade model. However, the results from both subcascade models are a factor of 2 to 3 times smaller than those from the point-cascade model (see Ref. (15)).

2.2.1.2. Precipitate Dissolution. Precipitate dissolution is a mechanism which degrades material physical properties, particularly the creep strength, during irradiation. We numerically simulated this dissolution by using TRIPOS. A collision cascade induced by a 14-MeV fusion neutron was able to totally destroy some of the small precipitates with a diameter of 15 Å or less but only 10% of the larger precipitates (30-Å diam) were destroyed by the same collision cascade. The average dissolution rate for 30-Å-diam precipitates has a maximum of 7% for an optimized separation of 100 Å (see Refs. [1,6]).

Recent experimental work [N. Sekimura, T. Zama, H. Kawanishi and S. Ishino, "Precipitate Stability in Austenitic Stainless Steels During Heavy Ion Irradiation," presented at 2nd Intl. Conf. on Fusion Reactor Mater. (Chicago, IL, April 1986)] at the University of Tokyo shows that precipitates greater than 200 Å are not dissolved for irradiation doses up to 100 displacements per atom by fusion collision cascades. Our work has also been extended by Muroga *et al.* [T. Muroga and K. Kitajima, "Computer Simulation of Precipitate Recoil Resolution by Energetic Collision Cascades," presented at 13th Intl. Symp. on Effects of Radiation on Mater. (Seattle, WA, June 1986)] at Kyushu University to explain the incubation dose phenomenon in the swelling of fusion reactor materials. We have also observed the preferential dissolution (sputtering) effect for the Monte Carlo-type precipitates.

A cascade slowing-down theory based on coupled diffusion equations was developed to determine the average dissolution rate of precipitates. Hard-sphere collisions and no electronic stopping were assumed. A Neumann series expansion was used to solve for the coupled diffusion equations and the results were similar to the "escape zone" concept proposed for the fission gas-bubble re-resolution effects. Planar and spherical precipitate models were shown to yield similar results. An empirical formula to determine the dissolution parameter as a function of precipitate size and PKA energy was also derived (see Refs. [1, 4 and 6]).

2.2.1.3. Surface Sputtering Analysis. The TRIPOS code was applied to the analysis of surface radiation-damage problems with sputtering of surface atoms as the main emphasis. The sputtering yield calculations from TRIPOS consistent with either experimental results or theoretical predictions from other codes, and analog TRIPOS code was a factor of 3 to 10 times faster than TRIM. Importance sampling techniques such as particle splitting and Russian roulette were used, which further enhanced the TRIPOS simulation speed by an extra factor of 3.

For light ions on gold, copper, and tantalum surfaces, TRIPOS results showed good agreement with results from experiments and/or TRIM. For helium ions on graphite and titanium surfaces, it was found that neither TRIM nor TRIPOS predictions were in perfect agreement with experimental results if unadjusted surface binding energies were used. However, good agreements from TRIPOS were obtained by adjusting the surface binding energies, indicating probably that other atomic surface phenomena can be dominant for these two surfaces in addition to the collisional effect (see Ref. [4]).

2.2.1.4. Preferential Sputtering and Associated Surface Evolution Phenomena. Surface evolution and preferential sputtering of compounds and alloys under ion bombardment was finally investigated. Results from earlier theoretical works using the EVOLVE and TRIDYN codes differed.

Results from TRIPOS were similar to those from TRIDYN, where an ion mixing zone resulting from light ion implantation was observed. However, for the case of 2-keV Ar on laminated AuPt, the results from TRIPOS show a 20-Å-thick altered layer, while those from EVOLVE show a 40-Å-thick layer. The disagreement is attributed to possible problems in the EVOLVE code for treating high-Z recoils. TRIPOS showed that these recoils generally remain at their point of generation while EVOLVE shows that these recoils travel a significant distance from their point of generation. On the other hand, simulations from TRIPOS show good agreement with the results from TRIDYN for 5-keV Ar on LuFe.

TRIPOS was also used to simulate the experiment of 150-eV ^3He on Cu-3%Au (G.L. Nelson and R. Bastasz, *J. Vac. Sci. Tech.*, 20 (1982) 498)]. Good agreement with experimental results was obtained. For fusion reactor first-wall and limiter coatings made of TiC, an enrichment of titanium atoms in the surface region is predicted by TRIPOS simulations. This result is in qualitative agreement with experimental observations.

Modeling of the surface seems to have an important influence on the results of theoretical studies and a major effort is needed to couple our analyses with theories predicting the surface topography, chemistry, and other surface atomic clustering processes. Such effort will yield valuable information on this important topic.

2.2.1.5. Cascades in Polyatomic Ceramics. The understanding of radiation damage phenomena in polyatomic ceramic materials is still at an early stage as compared to that in metallic structural alloys. The binary collision approximation was used in a Monte Carlo study of high-energy collision-cascade creation in MgAl_2O_4 . The study focussed on two aspects of cascade generation: cascade morphology and cascade stoichiometry. In the high-energy regime, typical fusion neutron cascades showed a tree-like morphology. To a large degree, instantaneous recombination occurs in the "stem" part of the cascade because of the closer separation of vacancy-interstitial pairs. Following this recombination phase, fusion neutron cascades tended to result in Frenkel pairs distributed on the "branches" of the tree in a zone extending over 100 to 200 nm. The

stoichiometry of displacements within the cascade was found to be substantially different from bulk stoichiometry, and was dependent upon the energy and type of primary knock-on atom (PKA) (see Ref. [5]).

2.2.1.6. Molecular Dynamics of Cascades and Sputtering. An empirical, composite interatomic potential was developed to describe interaction of energetic particles by pair potentials at high energies and many-body potentials at low energies. Molecular-dynamics (MD) studies of low-energy collision cascades were performed. The displacement threshold surface in copper was investigated and compared to experimental data. Our computer simulations showed good agreement with the experimental results of King and Benedek at 10 K.

The study of the collisional phase of low-energy cascade evolution showed the following: (1) The development of a replacement collision sequence (RCS), which leads to stable Frenkel pairs, is completed in about 0.1 ps. (2) The initial propagation of a RCS is much faster than the longitudinal elastic (sound) wave in copper and is even faster than the initial PKA speed, showing that cascades propagate through collective atomic motions. (3) The close agreement of our MD results with the experimental data on the displacement threshold surface indicates the usefulness of this composite potential for the simulation of low-energy ion-solid interactions (see ref. (8)).

The interaction between low-energy copper atoms and an atomically smooth [100] surface was investigated using an MD computational method. A newly formulated interatomic potential, which empirically combines the Ziegler universal potential at high energy and the embedded-atom many-body potential at low energies, was utilized in the study of near-surface cascade dynamics. The analysis included surface atom sputtering, and reflection and penetration of incident copper atoms. It was shown that the sputtering yields of low-energy Cu atoms on a [100] Cu surface are in general agreement with experiments and with other MD calculations using only pair potentials. It was shown in this work, however, that while pure pair-potential MD simulations show no reflection and Monte Carlo calculations give unrealistically large values,

our analysis demonstrated the physical transition from reflection to adsorption as the incident atom energy is lowered. Detailed mechanisms of sputtering, penetration, and reflection of atoms with energies in the range of 10-1000 eV were given.

2.2.2. Microstructure Evolution

It is now well-established that the mechanical and physical properties of materials can be controlled by changing the basic microstructure. Irradiation introduces atomic displacements, heat, and new transmuted atoms. Complex microstructural changes take place in irradiated materials. It is, therefore, central to the development of alloys for fusion conditions that an understanding of the basic mechanisms which govern microstructural evolution of structural materials during irradiation is established. The following is a brief summary of our work in this area.

Pulsed irradiation fluxes can cause alterations in the development of irradiated microstructures when compared to those resulting from steady irradiation. Theoretical analysis of irradiation damage development and examination of pulsed ion-irradiated microstructures have indicated conditions for expected effects from pulsing on fusion reactor materials. In pure metals, high instantaneous damage rates and pulse annealing periods comparable to defect relaxation times can cause significant pulsing effects. In addition, irradiation-affected phases in alloys are altered by pulsed irradiation compared to steady irradiation [10].

Theoretical and experimental evaluations of pulsed flux effects on radiation damage indicate that pulse compression for inertial confinement frequency and phase stability for magnetic fusion are important pulsed effects issues. Pulse compression, (*i.e.*, brief periods of high damage rate) increased mutual recombination of point defects and increased the interstitial clustering kinetics. On the other hand, pulse annealing periods allowed recovery of nonequilibrium defect states, irradiation microstructures, and radiation-modified phase changes.

Pulsed-irradiation compared to steady-irradiation experiments conducted at constant instantaneous damage rates have shown significant differences in irradiation response for alloys containing unstable phases. Stable alloys were generally insensitive to pulsed flux effects except at high temperature. Pulsing theories have shown that greater pulsing effects are expected for heavy ion-irradiation damage rates than for magnetic-fusion damage rates, and for low dose microstructures than for high dose microstructures.

One of the major uncertainties in understanding cavity nucleation and growth is the degree of stability of helium-vacancy clusters (HVCs) in an irradiation field. Such stability is a complex function of irradiation variables (damage rates, helium production rates, and fluence), as well as material parameters (sink density, temperature, and defect parameters). The goal of investigating the stability of HVCs is to understand and consequently to model cavity size distributions. Our research first investigated helium-vacancy binding energies, which were then used in analyzing the stability of HVCs under irradiation. The stability studies established the critical HVC size, *i.e.*, the helium:vacancy ratio that ensures growth under specified irradiation conditions. Using these models it is possible to understand the cavity size distribution of various simulation facilities. The fine cavity-size distribution seen in many high flux isotope reactor experiments can be explained by the favorable irradiation conditions, which lead to "spontaneous" nucleation of HVCs. In experimental breeder reactor-II experiments, on the other hand, the conditions for spontaneous nucleation of HVCs are not met, and nucleation is "delayed," and occurs by stochastic fluctuations [11].

Using a rate theory model, Ghoniem, Alhajji, and Kaletta [14] developed a solution to the problem of the rate of helium absorption at grain boundaries. In fusion reactor conditions, helium is expected to be uniformly generated inside the grains of structural materials. With the simultaneity of displacement damage production, helium atoms can be trapped in vacancies or vacancy clusters, inhibiting the migration of helium.

In this work [14], we showed reasonable agreement with available data on matrix helium-filled cavity nucleation and growth. This investigation demonstrated the effects of several physical mechanisms that are significant in interpreting experiments and furthering theory development. The following points were concluded:

1. The injection of helium gas into the solid, either by nuclear reactions or by implantation, cannot be separated from the question of vacancy mobility. It was shown that large helium concentrations lead to the immobilization of a large fraction of vacancies, leading to a "constrained" model of cavity growth provided that the cavities or clusters are immobile.
2. Helium gas re-solution due to the interaction of displacement damage with gas-filled cavities is a process of prime importance to cavity re-nucleation. At high re-solution rates, "dynamic nucleation" is a continuous process throughout irradiation.
3. Theoretical models and experiments are both needed to determine the effects of re-solution.
4. The external source of helium injection can be less important compared to internal helium sources to gas re-solution effects on gas arrival rates at grain boundaries.
5. During early irradiation, helium gas is trapped in small vacancy clusters. A large fraction of gas migrates to grain boundaries until matrix cavity nucleation is complete. When this is achieved, the majority of introduced gas resides in matrix bubbles, and a small percentage still arrives at grain boundaries.

Heavy ion irradiation accelerates the production of displacement damage in irradiated materials. Bullough and Ghoniem [13] developed exact analytical solutions to the time-dependent equations of point-defect diffusion to spherical cavities. In their work, they showed that the effective cavity sink strength increased with dose rate. Therefore, care must be exercised in high displacement-damage simulations, or microstructural sink strengths will be underestimated.

Collision cascade size and shape effects on point-defect diffusion during irradiation were studied in Ref. [15]. In contrast to the point cascade model of the cascade-diffusion theory of Mansur *et al.*, where cascades are mathematically modeled as δ -functions, we represent cascades as spheres and spherical shells. The dimensions of the vacancy cascade sphere, or the interstitial cascade shell correspond to the energy of the PKA. Subcascades are also studied at high PKA energies. It is shown that the δ -function representation of collision cascades overestimates the rms value of the magnitude of point defect fluctuation by a factor of 2 to 5, for large size cascades typical of fusion reactor conditions.

Our results showed that fluctuations in point-defect concentrations are sharply reduced as compared to those of the point cascade model if the cascade size effect is taken into account. For larger size cascades, the spherical cascade model predicts a lower magnitude of fluctuation in point-defect concentration. However, for cases where the damage rate is fixed and cascade strength and size are increasing, the decrease in point-defect concentration fluctuations is partly due to the homogeneous distribution of point defects within the cascade. Tree-like point-defect distributions in large cascades can be approximated either by a linear subcascade model or by a homogeneous subcascade model. These two models depict extreme configurations observed in Monte Carlo simulations of defect structures in large cascades. Defect concentration fluctuations based on these two subcascade models fell in between those based on the point and homogeneous cascade models. For the same conditions, the point-defect model gives a sharp increase in the magnitude of the defect concentration fluctuation, while the homogeneous cascade model actually predicts a decrease in the magnitude of this fluctuation. The actual behavior of the concentration fluctuation is expected to fall in between the results from the two subcascade models. For an anticipated fusion-reactor neutron spectrum, cascades tend to have sizes that correspond to defect concentration fluctuations around the plateau region for the subcascade models.

Modeling cavity nucleation at grain boundaries in structural alloys under the combined influence of helium and stress was the primary objective of our work in Ref. [16]. The role of

stress in cavity nucleation was analyzed by using an extension of classical theory, taking into account grain boundary sliding to describe stress concentration buildup and relaxation at particles and triple-point junctions. Helium clustering in the matrix is modeled using rate theory. The helium flux to grain boundaries is determined applying sink strength theory which takes into account the various competing clustering mechanisms in the matrix. Helium clustering on grain boundaries was also theoretically investigated using rate theory. The work agrees with experimental observations showing that irradiation results in grain-boundary bubble densities that are orders of magnitude larger than cavity populations observed in conventional creep experiments. It is shown that even if the total injected helium is as little as one part per million, it can result in grain-boundary bubble densities on the order of 10^{13} m^{-2} . Such cavity population exceeds typical grain-boundary cavity densities associated with creep experiments. Grain-boundary bubble densities are shown to reach steady state for injected helium amounts on the order of 10 parts per million.

Our time-dependent extension to classical nucleation theory has shown that, in the absence of irradiation, grain-boundary sliding is the driving force for grain-boundary cavity nucleation. When sliding is resisted by triple-point junctions or by hard particles at grain interfaces, sufficiently localized stresses are set up and immediately relaxed by diffusion or dislocation creep. The ensuing nucleation pulse was shown to be sensitive to the cavity shape and to the boundary inclination to the applied stress. Stress-induced cavity nucleation can, therefore, be statistical and dependent on the stochastic nature of sliding, and the distribution of irregularities on boundaries normal to the applied stress. It was concluded that, with a cavity shape factor on the order of 0.01 and surface normal to inclinations of only 15 to 20 degrees to the applied stress, a small number of such nucleation pulses is required to saturate all available nucleation sites. It was also shown that stress-induced nucleation is very rapid and that cavity life is spent mainly in the growth regime.

Under irradiation, the introduction of helium from nuclear reactions causes a dynamic helium flux to grain boundaries. This atomic helium flux drives another mode of grain-boundary

cavity nucleation; helium-vacancy clustering. The rate theory of helium clustering showed that this mode of cavity nucleation is much stronger than the stress-induced mode. With as little helium as 1 appm total, helium-nucleated grain-boundary cavity densities on the order of 10^{13} m^{-2} may result. This work and experiments on grain-boundary cavitation by helium are in basic agreement. The effective helium migration energy on the grain-boundary for such an agreement is on the order of the self-diffusion energy. Calculated grain-boundary bubble densities in the presence of irradiation are several orders of magnitude greater than cavity densities in the absence of irradiation. These quasi-steady-state densities are reached rather quickly at helium contents on the order of 10 appm. Our model also shows that, consistent with experiments, the saturation cavity density increases with increasing helium implantation rate.

An important parameter in the rate theory of swelling is the dislocation-loop bias factor, Z_l^1 , which is a measure of the rate of interstitial atom absorption relative to vacancy absorption at interstitial loops. The Fokker-Planck (F-P) equation was used to describe interstitial loop evolution, with a kinetic nucleation current boundary condition at di-interstitial atomic clusters. The majority of loop nucleation is shown to be finished after one milli-dpa, which allows the shape of the loop distribution function to be governed mainly by the drift (F) and dispersion (D) functions in the F-P equation. Since collision cascades contribute significantly to D , their effects must be suppressed by using low-energy ions or high-energy electrons to produce spatially homogeneous atomic displacements. Under these conditions, both F and D are shown to be proportional to the square root of the number of atoms in a loop. The proportionality parameters depend on material and irradiation conditions and are linearly proportional to Z_l^1 . The ratio, $F:D$, which resembles the Peclet number in fluid flow, can be used in a unique way to determine Z_l^1 without the usual complications of uncertainties in material and irradiation conditions. This is shown to constitute an internal variable measurement of the bias factor.

The moments solution to the F-P equation, with transient nucleation conditions, can be effectively used to measure the interstitial-loop bias factor, Z_l^1 . To take advantage of this solution, a number of experimental conditions must be satisfied. These conditions are: (1)

Irradiation doses beyond a short transient period of ~ 0.001 dpa and before loop unfaulting at several dpa's; (2) Sample temperatures low enough such that vacancy emission from loops does not significantly contribute to their growth (*i.e.*, below 450 - 500°C for Ni at a dose rate of $\geq 10^4$ dpa/s); (3) The use of low-energy ions or high-energy electrons to minimize the effects of collision cascades on the fluctuations in loop sizes during their growth.

Comparison between the current theory and experiments showed that a combination of the parameters Z_1^I , E_{2i}^b , E_i^M , and D_j/D_i can produce all observed features of interstitial loop evolution in ion-irradiated nickel. The best set of these parameters was found to be $Z_1^I = 2$, $E_{2i}^b = 1.19$ eV, $E_i^M = 0.55$ eV, and $D_j/D_i = 60$.

The dynamical evolution of a 1-D dislocation pile-up was numerically studied in Ref. [18]. By extending particle methods of computational statistical mechanics, criteria for accurate numerical simulation of the pile-up evolution were established. A combination of explicit integration of the equations of motion and dislocation freezing after 40 position oscillations gave a maximum error of 5% in the trajectory of the leading dislocation. Explicit integration preserves spatially oscillatory behavior and was shown to give accurate results. The evolution of the dislocation distribution function showed small density wave formation during the compression phase of the pile-up. Our work on the dynamics of dislocation pile-ups impacts the understanding of the development of localized plastic deformation ahead of cracks in ductile materials. This approach will be pursued for other micromechanical applications where continuum mechanics is incapable of treating localized plasticity.

The formation of inhomogeneous distributions of vacancy loops in irradiated materials was studied [19] in the framework of a dynamical model based on the rate theory of radiation damage. Dislocation structures are associated with dynamical instabilities due to the competition between defect motion and interactions. The dependence of the critical wavelength of the microstructures on material variables, such as the displacement-damage rate, network-dislocation

density, or temperature, was obtained. The postbifurcation analysis was performed in the weakly nonlinear regime where the selection and stability properties of 3-D structures were investigated.

The occurrence of pattern-forming instabilities seems natural for defect populations in irradiated metals and alloys. It mainly results from the different mobilities and bias in the migration of point defects to line defects, such as vacancy loops or network dislocations. We showed that structures with different symmetries may be simultaneously stable beyond the primary bifurcation. For example, when the diffusion and interactions of point defects are isotropic, the maxima of the vacancy loop density may correspond to either bcc lattices or planar arrays. Hence, these structures could be in nonparallel orientations, *i.e.*, with a structure different from the structure of the host lattice. On increasing further the displacement-damage rate, bcc lattices become unstable and a first-order-like transition should occur to planar structures. In the case of anisotropic interstitial diffusion, planar structures should be the rule. Hence, since the symmetry of the defect structures is a crucial issue in irradiated material, our analysis shows that a careful study of the post-bifurcation regime is needed to test the relevance of particular kinetic models to the interpretation of experimental observations.

Atomic clustering into circular planar disks is an important process responsible for interstitial-loop formation in the bulk of irradiated materials, and the evolution of atomic planes during thin-film growth. We developed a stochastic theory for the formation of planar-atomic clusters by atomic diffusion [20]. The theory accounts for transient coupling between master equations representing small-size atomic clusters and an F-P equation for larger ones. The F-P equation was solved self-consistently, together with the master equations by the moments method. Equations for the rates of change of atomic species and for the nucleation rate of atomic clusters were simultaneously solved with appropriate equations for the average size and various moments of the distribution function. An application of the theory was given by comparing the results of calculations with experimental data on interstitial-loop formation in ion-irradiated nickel.

The nucleation phase of interstitial loops was shown to be very fast, and the transient period for loop formation is finished in about 0.001 dpa. The effects of three point-defect parameters on loop density and average size was studied by comparing theoretical calculations to experiments. An increase in the loop bias factor, Z_1^1 , was found to increase the average loop size but had a very small effect on the total loop density. An increase in the di-interstitial binding energy, E_{2i}^b , increased the loop density and reduced the average diameter in a significant way. For nickel, a value of $E_{2i}^b = 1.19$ eV reproduced available experimental data. The value of the effective self-interstitial migration energy had a dramatic effect on the total loop density and the loop average size. A value of $E_1^{me} = 0.55$ consistency with experimental data. This is an indication that interstitial migration is hindered by atomic traps.

The distribution function of circular-planar atomic clusters, when displayed as a function of the loop diameter, is non-Gaussian. The deviation from Gaussian behavior is caused by several factors. First, the continuous nucleation of small-size clusters introduces a component of small-size clusters. Second, if the dispersion and drift functions are size dependent, higher-order additional terms are introduced as correlations to the Gaussian distribution function. Third, the assumption that the stochastic process of atomic additions to a cluster results in an instantaneous circular disk produces a transformation of the stochastic process from size space to diameter space. This transformation introduces another distortion to the distribution function.

Applying the theory to interstitial-loop formation revealed several simplifying features that are consistent with experiments. The high mobility of single interstitials and large binding energy of a di-interstitial cluster result in rapid termination of the nucleation process and, hence, nucleation-related distortions to the distribution function are nearly nonexistent. A consequence of cluster growth by diffusional accretion of single atoms or by addition of small numbers of multiple atoms from cascades is a distribution function that is nearly Gaussian in size space. Higher-order non-Gaussian corrections to the moments of the distribution function tend rapidly to zero for large $\langle x \rangle$ (or long times). This is a result of the growth law used for individual atomic clusters. Viewed from a different perspective, in the limit of large $\langle x \rangle$ and assuming no

other growth mechanism to dominate (*e.g.*, coalescence), the thermodynamic limit is attained where the ratio of the system variance to the average size tends to zero in accordance with the law of large numbers.

Atomic agglomeration into interstitial loops under irradiation is affected by collision cascades. Comparisons of theoretical calculations and experiments indicated that the stochastic fluctuations in loop sizes caused by the net absorption of single interstitial atoms are not adequate to explain the wide dispersion in the distribution function. To be consistent with experimental observations, additional fluctuations because of cascades must be included.

Time evolution of non-equilibrium systems, where the probability density is described by a continuum F-P equation, is a central area of interest in stochastic processes. In our work (Ref. [21]), numerical solution of a 2-D F-P equation describing the growth of HVCs in metals under irradiation is given. First, nucleation rates and regions of stability of HVCs in the appropriate phase space for fission and fusion devices were established. This was accomplished by solving a detailed set of cluster kinetic rate equations. A nodal line analysis was used to map spontaneous and stochastic nucleation regimes in the helium-vacancy (h-v) phase space. Growth trajectories of HVCs were then used to evaluate the average HVC size and helium content during the growth phase of HVCs in typical growth instability regions.

The growth phase of HVCs was modeled by a continuum 2-D, time-dependent F-P equation. Growth trajectories were used to define a finite solution space in the h-v phase space. A highly efficient *dynamic remeshing* scheme was developed to solve the F-P equation. As a demonstration, typical HFIR irradiation conditions were chosen. Good agreement between the computed size distributions and those measured experimentally were obtained.

In Ref. [22], the evolution of helium-filled cavities during neutron irradiation was analyzed in terms of the stochastic theory of atomic clustering. The conventional separation of nucleation and growth was replaced by a self-consistent evolution model. Starting from kinetic

rate (master) equations for the clustering of helium and vacancies, helium mobility, HVC stability, and cavity nucleation and growth were all included in the model. Under typical fusion irradiation conditions (cascade damage and high helium-to-dpa ratios), the following is suggested: (1) Helium mobility decreases with the evolution of the microstructure. At quasi-steady state, it is mainly controlled by interstitial replacement of thermal desorption. (2) Gas re-resolution from cavities by cascades increases nucleation at high fluences. (3) The cavity size distribution is broadened because of cascade-induced fluctuations. (4) The majority of helium-filled cavities are in a non-equilibrium thermodynamic state.

In Ref. [23], new concepts were reviewed which replace the conventional separation of microstructure evolution analysis into nucleation and growth. Classical nucleation theory is inadequate under fusion conditions (high helium-to-dpa ratios) and the usual "mean field" approximation of microstructural growth cannot account for cascade effects. A comprehensive theory of microstructure evolution under fusion conditions was formulated based on non-equilibrium statistical mechanics. Dynamic re-resolution of helium gas in cavities was shown to cause continuous nucleation of helium-filled cavities. Microstructure evolution (*e.g.*, dislocation loops and cavities) was modeled by kinetic rate equations for small size features and by F-P equations for sizes larger than few atomic dimensions. Semi-analytical and numerical methods were developed for the analysis of microstructure evolution and the results were compared to experiments. The problem of spatial self-organization of microstructures under irradiation was described in terms of newly developed Ginzburg-Landau-type equation and the results were also compared to experiments.

2.2.3. Materials Engineering, Mechanics, and Design

Research at UCLA on materials engineering, mechanics, and design has been motivated primarily by conceptual design studies. In this regard, the thrust of our work has been on extrapolation of materials data to the operating environment of a fusion reactor. Strong

contributions from design studies have been made. The results of this area of research are therefore both fundamental and applied. A brief summary of research performed at UCLA in this area is given below.

In this paper, Ref. [24], we presented the results of our analysis of data provided by SANDVIK Steel Research Center for the high temperature properties of HT-9. We developed design equations for use in inelastic structural mechanics applications for the most important thermal creep parameters. Empirical correlations for creep rupture time and the complete description of elongation *versus* time were presented. A phenomenological description of steady-state creep was also developed. It was found that dislocation creep can explain the measured data.

The sensitivity of lifetime predictions for fusion-reactor blanket structures was investigated in Ref. [25] by applying the Monte Carlo numerical technique. A structural computer code, stress analysis including radiation effects (STAIRE), developed for the analysis of mirror fusion blankets, was developed and used as a deterministic model for the prediction of the lifetime of semicircular coolant tubes. Uncertainties in material variables were treated as probabilistic inputs to the STAIRE code and output distributions were obtained.

Irradiation creep rates were shown to be sufficient for relaxation of swelling-induced stresses under most conditions. In the absence of high stresses, the creep limit seems to be life-limiting, although this depends on the design-dependent swelling rate. In the case of the Mirror Advanced Reactor Study (MARS) blanket design, a lifetime of several hundred displacements per atom was shown to be highly probable.

The effects of radiation on the structural performance of fusion reactor structures is recognized as a major issue for the development of fusion reactor technology. Neutron irradiation changes the mechanical properties of structural components resulting in a general degradation of these properties. In addition to the mechanical loads (pressure and weight) and

the thermal strains, non-uniform inelastic strain fields are induced by radiation swelling and creep in fusion structures. In Ref. [26], we described a new computer code, STAIRES, (stress analysis including radiation effects). This code is based on standard beam theory for pipe-bends. The theory was modified in two areas: (1) consideration of the pipes' cross-section deformation as the radius of curvature changes; and (2) inclusion of inelastic radiation and thermal strains (swelling and creep). An efficient analytical/numerical approach was developed for the solution of indeterminate beam problems. As an application of the method, the stress distribution and deflections of toroidal blanket pipes in MARS were evaluated. Swelling strains were identified as a major source of stress and deformation in the proposed blanket design, and possible solutions to the problem were outlined.

Several methods for developing design correlations for ferritic steels were discussed in Ref. [27]. Equations describing swelling, embrittlement, and irradiation creep were reviewed. We developed design equations for use in elastic structural-mechanics applications for the most important thermal-creep parameters. Empirical correlations for creep rupture time and the complete description of elongation *versus* time were presented. A phenomenological description of steady-state creep was also developed.

Creep processes, due to irradiation and thermal fields, have generally been assumed to relax stresses resulting from the loading of structural components. However, in order to determine failure modes and mechanisms, a global inelastic structural analysis is required. We developed the STAIRES computer code to meet this need. This code is based on a modified beam theory for the self-consistent determination of stresses and deflections in beams of circular cross section. The work was applied to the lifetime analysis of the MARS blanket modules. The objective of the work in Ref. [28] was to assess the global (3-D) impact of both irradiation and thermal creep strains on the stress resulting from thermal and swelling strains.

A pin-type fusion reactor blanketed using γ -LiAlO₂ solid tritium breeder was designed [29]. Tritium transport and diffusive inventory were modeled utilizing the DIFFUSE code. Two

approaches were used to obtain characteristic LiAlO_2 grain temperatures. DIFFUSE provides intragranular diffusive inventories which scale up to blanket size and the results compared well with a numerical analysis, giving a steady-state blanket tritium inventory of 13 g.

Start-up transient inventories were modeled using DIFFUSE for both full and restricted coolant flow. Full flow gave rapid inventory buildup while restricted flow prevented this buildup. Inventories after shutdown were modeled and it was found that reduced cooling had little effect on removing tritium but preheating rapidly purged inventory.

DIFFUSE provided parametric modeling of solid breeder density, radiation, and surface effects. Massive inventory and marginal tritium release resulted from 100% dense pins. Only large trapping energies and concentrations increased inventory significantly. Diatomic surface recombination was only significant at high temperatures.

Our theoretical model, presented in Ref. [30], described high-temperature helium embrittlement as a sequence of four steps. First, helium clustering in the matrix was described by the conventional rate theory. This was coupled to rate equations for the transport of single helium atoms to grain boundaries in the second phase. The third step was concerned with the influence of helium and stress on the nucleation of cavities at grain boundaries, with particular emphasis on the role that precipitates and triple-point junctions play in the nucleation process. Finally, various growth modes of grain boundary cavities which lead to fracture by inter-linkage of equally spaced grain-boundary cavities were investigated [30]. A description of this comprehensive model was given, with emphasis on the growth and inter-linkage of grain boundary cavities under the effects of irradiation and applied stress. A comparison between the model predictions and recent experimental creep rupture data was given. The model proposed a new explanation of the creep rupture behavior of martensitic steels as opposed to austenitic steels. Vacancy source limitation at grain boundaries resulting from dislocation interactions was identified as the primary reason for the retarded growth of grain-boundary cavities in martensitics.

Mechanical interaction between the solid breeder material and its cladding during power cycles is an important consideration in the design of solid breeder blankets. The analysis presented in Ref. [31] gives a design tool for material choices and lifetime prediction for breeder pins. The UCLA solid-breeder blanket design was evaluated and operating conditions were suggested. The material model for the pellet included linear thermoelastic behavior and swelling. The cladding was assumed to be thin and to exhibit swelling and creep. Two alternate breeder/cladding material pairs were analyzed ($\text{Li}_2\text{O}/2.25\text{ Cr-1Mo}$ and $\text{LiAlO}_2/\text{9-C}$). While high swelling excludes the $\text{Li}_2\text{O}/2.25\text{Cr-1Mo}$ design, it was found that in the $\text{LiAlO}_2/\text{9-C}$ case, compatibility of thermal expansion between the breeder and the cladding (as well as low swelling of the breeder) resulted in less than 0.5% total plastic strain after one year of operation.

The bowing of circular-solid breeder pins was studied using standard beam theory in Ref. [32]. Deformations caused by thermal gradients, swelling gradients, and gravitational forces were included in the investigation and swelling was found to cause the most severe pin bowing. The bowing of beryllium multiplier rods was found to be insignificant when swelling is not considered. In all cases, it was found that adding internal supports can reduce the rod deflections to acceptable levels without increasing the stresses beyond design limits.

The formation of dislocation cells and subgrain structure is of great significance to understanding high-temperature deformation of many solids. Experimental observations on dislocation patterns, and cellular structures in particular, were reviewed in Ref. [33]. The basic features of such structures were discussed, and the conditions allowing dislocation patterning behavior were described. Theoretical formulations that attempt to model this phenomenon were reviewed, with emphasis on recent dynamical computer simulations [34].

Singular thermal stress fields in bonded viscoelastic quarter planes were studied with the use of viscoelastic analogy [35]. The order of the singularity was shown to depend on the material properties, indicating that it will vary with time in viscoelastic materials. This was studied in detail for Maxwell materials, and it was shown that the order of singularity generally

increased with time. This evolution of the singularity can, for certain combinations of material properties, lead to initial increases in the stress levels near the edge of the interface before relaxation occurs.

Solutions for thermal stress singularities in finite bonded strips were sought in Ref. [36] by using an eigenfunction expansion in the neighborhood of singularity. The coefficients in the resulting series were determined by satisfying the boundary conditions on surfaces far removed from the singularity either pointwise or in an integrated sense. The latter of these techniques was found to be more reliable. The accuracy of the solution was checked by comparing it to a semianalytical solution for thermal stresses in bonded quarter plane, which was derived by using the Millin transformation. It was shown that the eigenfunction approach provides accurate solutions for the leading term in the series, thus capturing the essence of the thermal stress fields near the edge of the interface. The far-field solutions, however, are found to feature excessive inaccuracies, which are attributed to numerical errors.

A relevant design data base is needed for structural components in near-term and commercial fusion devices. A high-flux, high-fluence fusion-neutron test facility is required for testing the failure mechanisms and lifetime-limiting features for first-wall, blanket, and high-heat-flux components. In Ref. [37], we described the key aspects of the fusion environment that influence the response of structural and high-heat-flux components. In addition to test capabilities for fundamental radiation-effects phenomena, *e.g.*, swelling, creep, embrittlement, and hardening, it was shown that the facility must provide an adequate range of conditions for accelerated tests in order to study the limitations on component lifetime due to the interaction between such fundamental phenomena. In high-heat-flux components, testing the failure mechanisms of duplex structures was shown to require maintenance of an appropriate temperature gradient in the 14-MeV neutron field. Thermal stresses were shown to cause component failure, particularly when the degradation in the thermal conductivity and mechanical properties by irradiation were considered. Several factors were discussed for assessment of the failure modes of the first-wall and blanket structures: displacement-damage dose and dose rate, the amount of

helium gas generated, the magnitude of irradiation and thermal creep, prototypical temperature and temperature-gradient distributions, module geometry, and external mechanical constraints.

A simple dislocation model for creep in engineering materials was constructed [38] in order to predict high temperature deformation under arbitrary time-dependent stress and temperature histories. The model also has the advantage of being compatible with the rate theory of radiation damage, which allows radiation effects to be included. The basis of the model was the generation and immobilization of dislocations at subgrain boundaries, the recovery of the static dislocations at the boundaries, the dynamics of nucleation and growth of subgrains, and the evolution of the dislocation density of the boundaries. The effects of solutes and hardening precipitates were included. Example calculations were given for the martensitic steel, HT-9.

A new methodology in computational micromechanics, dislocation dynamics (DD) was introduced in Ref. [39]. Dislocation dynamics was developed to examine the dynamic behavior of dislocation distributions in solid materials. Under conditions of externally applied stress, dislocations exhibit glide with a velocity proportional to the power of the applied stress and climb motion with a velocity that is a function of the applied stress and temperature. These motions result from long-range force fields comprising both externally applied stress and long-range interactions between individual dislocations. Short-range reactions were represented as discrete events. The DD methodology was to be differentiated from particle methods in statistical mechanics (*e.g.*, molecular dynamics and the Monte Carlo method) in two respects. First, DD was developed to study the dynamical behavior of "defects" in the solid. Second, the small number of dislocations allows for a complete dynamical representation of the evolution of dislocations in the material medium without the requirement of statistical averaging. The purpose of the DD methodology was to bridge the gap between experimentally observed phenomena and theoretical descriptions of dislocation aggregates, particularly the evolution of self-organized dislocation structures under temperature, stress, and irradiation conditions.

The dynamic organization of dislocations into spatially heterogeneous substructures was demonstrated by applying the principles of dislocation dynamics that were outlined in Ref. [39]. This work was continued in Ref. [40], where it was shown that the formation of persistent slip bands is a consequence of the competition between dipole formation and annihilation of dislocations of opposite Burgers vectors in the absence of temperature-enhanced climb recovery under cyclic stress conditions. Planar arrays, which were also uniaxial structures, were shown to arise from enhanced dislocation multiplication and the formation of stable dipole configurations along a slip plane at lower temperatures where climb was unimportant. Biaxial dislocation systems experience additional degrees of freedom compared with uniaxial systems because of available motion along additional slip systems. It was demonstrated that for a system of orthogonal slip directions at high temperatures in which climb and glide motion were competitive, dislocation cellular structures formed as a result of immobile dipole and junction formation and by the internal elastic strain energy minimization caused by long-range self-shielding. It was shown that the internal elastic strain energy is reduced by the self-organization process. However, the short-range nonlinear processes (*i.e.*, dipole and junction formation) were shown not to allow absolute elastic energy minimization.

Thermal and swelling stress fields in bonded structures were sought in Ref. [41] by using a model consisting of two thin, rectangular strips perfectly bonded along one surface. Existing results for stresses in the bulk, based on beam theory, were presented and their limitations were discussed. Plane elasticity was used to derive general solutions for the stress fields near the edge of the structure, in many cases yielding logarithmic or algebraic singularities. Methods for coupling these general edge fields to the stresses in the bulk were discussed, and the techniques were applied to the materials and loading conditions relevant to fusion components. The impact of swelling and creep on both the order of the singularity and on its intensity was shown.

The sensitivity of lifetime predictions of fusion structures with limited materials data base was studied in Ref. [42].

In Ref. [43], we presented an engineering analysis for the design of the first wall/blanket system for the TITAN reverse-field-pivot conceptual fusion reactor. The geometry of the first wall was dictated by the surface heat flux, the coolant temperature, and the maximum allowable structure temperature. We found that a reasonable design could be found up to 4 MW/m² heat-flux wall load.

The thickness of the blanketed tubes was determined by the internal heat generation rate, a minimum coolant bulk temperature set by the requirement on thermal efficiency, as well as the temperature limit on the structure. The radius of the tubes was given by the required structure fraction.

The aspect ratio of the rectangular channel design was determined by the pressure stress concentration at the corners. The wall thickness was limited by the heat generation rate and fluid bulk temperature. These two constraints defined the allowable range of designs. Further analysis addressed the effect of poloidally varying coolant temperature and the effect of the irradiation environment.

Naughton, Ghoniem, and Lin [44] developed a micromechanical model for the effects of irradiation on fatigue crack initiation. The model was able to explain the ductility-dominated low-cycle fatigue regime, as well as the strength-dominated high-cycle fatigue regime.

In Ref. [43], Ghoniem and Amodeo developed a method for computer simulation of the behavior of individual dislocations. The equations of motion of individual dislocations were simultaneously solved by using extensions of dynamical particle-simulation methods [i.e., molecular dynamics, Langevin dynamics, and the Monte Carlo methods]. The evolution of 1- and 2-D patterns was illustrated by computer simulation of dislocation dynamics. In 1-D patterns, criteria for accurate numerical simulation of dislocation pile-up evolution were

established. The potential for using specialized numerical and computational techniques to reduce the demands on existing computers was discussed. The work was completed in Ref. [46], where a rapid algorithm for dislocation dynamics calculations was developed.

2.2.4. Research on Low-Activation Steels

In 1983, the idea of developing a low-activation steel for fusion applications emerged at UCLA. We then contacted the Department of Energy requesting support for its development. However, funding limits and priorities did not allow dedicated support for this idea. Since our research on radiation effects and fusion materials has mainly been funded by the grants outlined in this report, we were fortunate to be able to pool the available resources and develop the first known low-activation steel in the world, UCVS-1. A patent on this steel, and on several others which were developed in collaboration with Hanford Engineering Development Laboratory, was granted on November 11, 1986 (U.S. Patent No. 4622067). We summarize our efforts on ferritic alloys in fusion applications below.

Proposed fusion reactors may enjoy significant advantages regarding public safety and waste disposal over current fission reactors. Neutron activation of the structural materials can be minimized by the appropriate choice of alloys. Unfortunately, commercially developed alloys for high-temperature applications become activated with neutron absorption, leading to sometimes very long decay chains. The work reported in Ref. [47] discussed the results of a new "low activation" ferritic alloy, UCVS-1, developed at UCLA. This alloy, which contains vanadium instead of molybdenum for high-temperature strength, showed very promising combinations of strength, ductility, and low long-term radioactive products. It was shown in this paper [47] that the strength and ductility of UCVS-1 are comparable to 2-1/4 Cb-1 Mo up to 400°C, achieving significant advantages with regard to safety and radioactive waste disposal.

The patent disclosure (Ref. [48]) relates to ferritic alloys, and specifically to development of low-activation bainitic and martensitic stainless steels. The United States Government has rights in this invention pursuant to Contract No. DEAC06-76FF02170 between the United States Department of Energy and Westinghouse Electric Corporation.

Ferritic alloys are required for structural usage in the development of commercial fusion systems, where the residual fuel and wastes will themselves have negligible residual radioactivity. For purposes of this disclosure, "low activation" shall be defined as a radiation level below 1 Ci/m³ after waste disposal and burial for 100 years.

Low activation characteristics have not been vital in the development of structural materials for use with nuclear fission reactors, since the high levels of long-term radioactivity that persist in the spent fuel generated by a fission system far overshadow the amount of radioactivity in the surrounding structure. Most research and development with respect to long-term radioactive levels has been directed to the fuel components rather than to the machine structure.

The invention of this steel is a result of a study designed to develop bainitic and martensitic stainless steels with low-activation characteristics for structural applications in fusion reactors. The objective was to identify low-activation ferritic alloys, and specifically low-activation bainitic and martensitic stainless steels, which had strength properties capable of being utilized in fusion reactor structural components.

To achieve the objectives, the ferritic alloy having a bainitic or martensitic microstructure consists primarily of chromium (2.0 to 13.0% by weight), vanadium, tungsten and/or tantalum (0.3 to 1.5% by weight), carbon (0.075 to 0.30% by weight), manganese (0.1 to 15.0% by weight), and silicon (0.05 to 1.00% by weight). The remainder of the alloy is iron. The resulting alloy is characterized by low-activation properties and is devoid of subversive amounts of elements that materially interfere with this characteristic. In general, other elemental additions to the alloy should total less than 0.5% of its total weight. The alloy content of nitrogen,

niobium, molybdenum, nickel, and copper should be maintained below maximum total weight percentages which have been developed theoretically from known characteristics of these elements when exposed to nuclear particle bombardment as follows: nitrogen, less than 0.33% by weight; niobium, less than 0.000029% by weight; molybdenum, less than 0.003% by weight; nickel, less than 0.9% by weight; and copper, less than 0.12% percent by weight. If any one of these elements is present at the prescribed limit, none of the others may be present.

Ferritic/martensitic alloys are being developed for structural applications in fusion reactors. Within the ferritic/martensitic class of alloys, compositional and heat treatment variations are performed to optimize alloy properties for specific applications. The environmental conditions in fusion reactors pose a new challenge for ferritic/martensitic alloy optimization. Examples of the unique features of fusion designs include high surface- heat loads, magneto-forces, liquid-metal coolants, neutron radiation effects, etc.

Reference [49] summarizes information relevant to the selection of alloy types to fusion applications. Four types of alloys were considered: HT-9, 2-1/4 Cb-1 Mo, Nb-stabilized 2-1/4 Cb-1 Mo, and the low-activation vanadium alloy UCVS-1. The important metallurgical variables and heat treatments influencing various structural phases (ferritic, bainitic, and martensitic) are discussed. Relevant mechanical property data is summarized to illustrate the definition of possible ranges of operating temperatures of these alloys for fusion applications. Since liquid metals, such as Li or LiPb, were considered to be candidate coolants and tritium breeders, we presented an assessment for liquid-metal compatibility with ferritic/martensitic steels. Radiological properties for both accident and radioactive waste disposal were then presented with emphasis on some of the unique possibilities with this class.

The Mirror Advanced Reactor Study (MARS) developed a high temperature blanket for the alternative applications of high efficiency electricity production or process heat for synthetic fuel production. The blanket had two radial zones. The choice of material for the metallic structure was a critical factor in the design. We selected HT-9 ferritic steel because of its

excellent physical and mechanical properties; resistance to neutron-induced void swelling and helium embrittlement, and compatibility with lead-lithium. The MARS reactor was designed for a 5-MW/m² wall loading and experienced a first wall damage rate of 69 dpm/full power years. Thus, we required a combination of design flexibility and material properties that would allow reliable operation to over 200 dpa. Through the use of HT-9, we were able to design a high performance blanket for a tandem mirror reactor that appears capable of long life operation (see Ref. [50]).

Our research on ferritic/martensitic alloys is summarized in Ref. [51]. The relevant design data are presented in a manner which defines the operation design windows for this class of alloys.

2.2.5. Research Motivated by Grant Support

The experience that we gained in developing theories and models for microstructural evolution has been helpful in a closely related area of research; that is the study of surface atomic clustering. Although no direct support was obtained from the grants reported here, collaborative efforts with Dr. Charles Stone (supported by DOE Magnetic Fusion Energy Technology fellowship), and Dr. Martin Vicanek (supported by a NATO grant) resulted in the publication of four papers (Ref. 52-55). For these papers, we developed rigorous models of surface atomic clustering under conditions of bombardment by thermal or energetic particles. The work is important to a number of applications, among which is the re-deposition process of surface atoms in the environment of a plasma edge (as in divertors or limiters).

3. PARTICIPATION BY GRADUATE STUDENTS, POST-DOCTORAL FELLOWS, AND VISITING SCIENTISTS

During the six year period covered by the grant (January 1984 through January 1990), one Masters and eight Ph.D. degrees were completed under the supervision of Professor N. M. Ghoniem. Two of the earned Ph.D. degrees were not supported by the grant, two others were partially supported, and one postdoctoral fellow was partially supported for approximately three years after earning his Ph.D. All Ph.D. and M.S. graduates, with the exception of one, are either U.S. citizens or permanent residents of the United States. Two of the former Ph.D. students hold academic positions; one is an associate professor and the second is an assistant professor. Other former students hold technical positions in national labs, universities, or are employed in the private sector. A brief description of former graduate students and of our distinguished visiting scholars is given below.

Ph.D. Degrees

1. **Jamal Alhajji:** "Theoretical Modeling of the High Temperature Helium Embrittlement in Structural Alloys," June 1985; Associate Professor of Mechanical Engineering, University of Kuwait.
2. **Shahram Sharafat:** "Theory of Helium Transport, Clustering and Cavity Evolution in Structural Materials Under Irradiation," March 1986; Development Engineer, University of California, Los Angeles.
3. **Philip Shang-Chih Chou:** "A Monte Carlo Approach to Ion Transport in Solids and Its Applications in Bulk and Surface Damage Analysis," June 1986; Research Engineer, Taiwan.

4. **James P. Blanchard:** "Analysis of Singular Stress Fields in Duplex Fusion Components," June 1988; Assistant Professor of Nuclear Engineering, University of Wisconsin; recipient of an NSF Presidential Young Investigator Award, 1990-1995.
5. **Robert Amodeo:** "Dynamic Simulation of Dislocation Pattern Formation in Metals During High Temperature Monotonic and Cyclic Deformation," June 1988; Research Engineer, Xerad, Inc., Santa Monica, CA.
6. **Rodger Martin:** "Simulation of Charge Generation and Transport in Semiconductors Under Energetic Particle Bombardment," March 1990; Research Scientist, Oak Ridge National Laboratory, Oak Ridge, TN.
7. **George Orient:** "Analysis of Steady-State Propagating Cracks in Creeping Metals," (co-advisor, Prof. Russ Westmann), April 1990; Research Engineer, Rockwell Science Center, Los Angeles.
8. **Charles Stone:** "Modeling Thin-Film Formation by Energetic Atom Deposition," March 1991; Research Scientist, General Atomics, La Jolla, CA.

M.S. Student

1. **Timothy Naughton:** "Micromechanics of Fatigue Crack Initiation Under Irradiation," (co-advisor, Professor T. H. Lin), 1986; Research Engineer, Edwards Air Force Base, Mojave Desert, California.

Visiting Scientists

1. **Dr. Isabil Abril:** Physics Department, University of Alicante, Spain, 1988; Atomic collisions in solids.
2. **Dr. Christian Abromeit:** Hahn-Meitner Institute, Berlin, Germany, 1989; Radiation stability of alloys.
3. **Dr. Daniel Walgraef:** University of Brussels, Belgium, 1987-1990; Spatial ordering of microstructures.
4. **Dr. John Gittus:** Director General, British Atomic Forum, United Kingdom, University of California Regents Lecturer, 1989; Dislocation creep.

4. LIST OF PUBLICATIONS

Research publications supported by the grant have mainly been the result of M.S. or Ph.D. dissertation work for students supervised by N. M. Ghoniem, or the result of joint collaborations between N.M. Ghoniem, post-doctoral fellows, and visitors to UCLA. The work is published in first-rate refereed journals or proceedings of technical meetings. The publications are listed here under five coherent categories, as summarized in section 2.

4.1. Published Research of "Atomic Displacements"

1. P. S. Chou and N. M. Ghoniem, "An Approximate Analytical Calculation of Precipitate Dissolution Rate Using a Slowing Down-Diffusion Theory for Charged Particles," *Nucl. Instr. and Meth.*, B9:209-217, 1985.
2. P. S. Chou and N. M. Ghoniem, "Collisional Aspects of Preferential Sputtering Using the Monte Carlo Method," *J. Nucl. Mater.*, 141-143:216-220, 1986.
3. J. P. Blanchard, N. M. Ghoniem, and S. P. Chou, "An Approximate Solution to the Scattering Integral for General Interatomic Potentials," *J. Appl. Phys.*, 61:3120-3123, 1987.
4. P. Chou and N. M. Ghoniem, "Applications of the Monte Carlo Code TRIPOS to Surface and Bulk Ion Transport Problems," *Nucl. Instr. Meth. Phys. Res.*, B28:175-184, 1987.
5. N. M. Ghoniem and S. P. Chou, "Binary Collision Monte Carlo Simulations of Cascades in Polyatomic Ceramics," *J. Nucl. Mater.*, 155-157:1263-1267, 1988.
6. S. P. Chou and N. M. Ghoniem, "On Precipitate Dissolution Using the Cascade Slowing-Down Theory," *Nucl. Instr. Meth. Phys. Res.*, B42:145-148, 1989.
7. S. P. Chou and N. M. Ghoniem, "The Effects of Many-Body Interactions on Point-Defect Generation," *J. Nucl. Mater.*, 176, 1990.
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