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Critical Issues on Materials for Gen-IV Reactors

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FY08 LDRD Final Report
Critical Issues on Materials for Gen-IV Reactors
LDRD Project Tracking Code: 06-ERD-005
Magdalena Caro, Principal Investigator

Abstract

Within the LDRD on "Critical Issues on Materials for Gen-IV Reactors" basic thermodynamics of the Fe-Cr alloy and accurate atomistic modeling were used to help develop the capability to predict hardening, swelling and embrittlement using the paradigm of Multiscale Materials Modeling. Approaches at atomistic and mesoscale levels were linked to build-up the first steps in an integrated modeling platform that seeks to relate in a near-term effort dislocation dynamics to polycrystal plasticity.

The requirements originated in the reactor systems under consideration today for future sources of nuclear energy. These requirements are beyond the present day performance of nuclear materials and calls for the development of new, high temperature, radiation resistant materials. Fe-Cr alloys with 9-12% Cr content are the base matrix of advanced ferritic/martensitic (FM) steels envisaged as fuel cladding and structural components of Gen-IV reactors. Predictive tools are needed to calculate structural and mechanical properties of these steels. This project represents a contribution in that direction.

The synergy between the continuous progress of parallel computing and the spectacular advances in the theoretical framework that describes materials have lead to a significant advance in our comprehension of materials properties and their mechanical behavior. We took this progress to our advantage and within this LDRD were able to provide a detailed physical understanding of iron-chromium alloys microstructural behavior. By combining ab-initio simulations, many-body interatomic potential development, and mesoscale dislocation dynamics we were able to describe their microstructure evolution. For the first time in the case of Fe-Cr alloys, atomistic and mesoscale were merged and the first steps taken towards incorporating ordering and precipitation effects into dislocation dynamics (DD) simulations. Molecular dynamics (MD) studies of the transport of self-interstitial, vacancy and point defect clusters in concentrated Fe-Cr alloys were performed for future diffusion data calculations. A recently developed parallel MC code with displacement allowed us to predict the evolution of the defect microstructures, local chemistry changes, grain boundary segregation and precipitation resulting from radiation enhanced diffusion. We showed that grain boundaries, dislocations and free surfaces are not preferential for alpha-prime precipitation, and explained experimental observations of short-range order (SRO) in Fe-rich FeCr alloys. Our atomistic studies of dislocation hardening allowed us to obtain dislocation mobility functions for BCC pure iron and Fe-Cr and determine for FCC metals the dislocation interaction with precipitates with a description to be used in Dislocation Dynamic (DD) codes. A Synchronous parallel Kinetic Monte Carlo code was developed and tested which promises to expand the range of applicability of kMC simulations.

This LDRD furthered the limits of the available science on the thermodynamic and mechanic behavior of metallic alloys and extended the application of physically-based multiscale materials modeling to cases of severe temperature and neutron fluence conditions in advanced future nuclear reactors. The report is organized as follows: after a brief introduction, we present the research activities, and results obtained. We give recommendations on future LLNL activities that may contribute to the progress in this area, together with examples of possible research lines to be supported.

Introduction/Background

This LDRD takes advantage of the spectacular progress in the theoretical framework that describes materials and the continuous progress of parallel computing. The pioneer development of molecular dynamics studies of radiation damage, the development of the mesoscale Dislocation Dynamics methodology, as well as recently-gained expertise in multi-scale methods, coupled to the most powerful computers in the world, has placed LLNL at the forefront of the mechanical properties field. This LDRD on "Critical Issues on Materials for Gen-IV Reactors" represents a contribution in the same direction. Within this LDRD we developed the first steps of a parameter-free computational methodology that provided insights into the mechanical and thermodynamic behavior of alloys under irradiation by linking the relevant tools at the atomistic scale with the corresponding mesoscale models.

The requirements originated in the reactor systems under consideration today for future sources of nuclear energy. Structural components, fuel cladding, and reflector materials, are expected to undergo significant degradation under the high temperature and high neutron-flux of the life time of Generation-IV (Gen-IV) advanced nuclear energy systems. In future energy scenarios of nuclear energy programs supported by DOE, advanced reactors are envisioned to be highly efficient, with enhanced safety, minimal waste, and improved proliferation resistance. Fe-Cr alloys with 9-12% Cr content are the base matrix of advanced ferritic/martensitic (FM) steels envisaged as fuel cladding and structural components of these future reactors. Prediction of how these materials will perform under high exposures (radiation induced swelling, hardening and embrittlement) represents a challenge to the capabilities of present day available models. Multiscale modeling, i.e. modeling of materials at several interconnected length and time scales (together with experimental verification) is a powerful approach that can provide advanced materials solutions to this and other critical issues on materials for advanced reactors.

Within this LDRD we developed the first steps of a unified approach to multiscale materials modeling for nuclear applications based on sound theoretical considerations. This unified approach consists of a parameter-free computational methodology that provides insights into the mechanical and thermodynamic behavior of alloys under irradiation by linking the relevant tools at the atomistic scale with the corresponding mesoscale models. We combined state-of-the-art computational tools with two developments, namely, i) binary alloy

potentials fitted to reproduce thermodynamic data and phase diagrams and ii) atomistic studies of dislocation hardening that allowed us to obtain mobility functions determine the dislocation interaction with precipitates with a description to be used in Dislocation Dynamic (DD) codes. Because of the gaps they have bridged and the new science they have provided, these developments have significantly added to the scientific effort in multiscale modeling applied to engineering materials in general and nuclear materials in particular.

We studied the Fe-Cr system because Fe-Cr alloys are the base matrix for both 9-12Cr ferritic/martensitic steels and ODS (Oxide Dispersion-Strengthened) Steels. Ferritic steels have an open (body centered cubic) crystalline structure and are ferromagnetic. Bonding in bcc metals have some covalent character that is not properly described in classic potentials, and additionally, point defect properties (like formation energies of the various interstitials) depend on the magnetic structure that is neither included in the potentials. Because of these complications, at the time we started our LDRD, practically all the modeling data generated for steels was produced for idealized pure Fe with atomic potentials that did not reproduce all the characteristics of the perfect system; in particular, they did not even have the allotropic bcc-fcc transition at high temperature. In recent years, ab-initio studies of interatomic bonding interactions have been performed in model systems, in pure iron, and Fe-Cr alloys. However, we are still far from the generation of a complete database on Fe-C, Fe-Mo, Fe-Ni that would be useful in predicting the microstructural evolution of steels in high-temperature Gen-IV radiation environments.

As we shall see in the sections that follow, the very successful approach developed by A. Caro et al. [1] was applied to the development of a semi-empirical interatomic potential for Fe-Cr. This interatomic potential was tested and compared with existing databases for defect production in a multi-parameter space and was able to reproduce the relevant existing literature. Molecular dynamics (MD) studies of the transport of self-interstitial, vacancy and point defect clusters in concentrated Fe-Cr alloys was performed for diffusion data calculations using Monte Carlo (MC) methods. Basic thermodynamics of the Fe-Cr alloy and accurate atomistic modeling were used to help develop the capability to predict hardening, swelling and embrittlement using the paradigm of Multiscale Materials Modeling. Approaches at atomistic and mesoscale levels were linked to build-up the first steps in an integrated modeling platform that seeks to relate in a near-term effort dislocation dynamics to polycrystal plasticity.

High scientific impact was obtained in our FeCr Short-Range-Order (SRO) studies where we were able to explain experimental observations of SRO in Fe-rich FeCr alloys, and where atomistic off-lattice Metropolis Monte Carlo simulations gave insight into the physical origin of the SRO behavior. As spin-off of this LDRD we mention the Synchronous parallel Kinetic Monte Carlo code that was developed and tested and which promises to expand the range of applicability of kMC simulations. An extension of this effort to radiation damage calculations is recommended.

In summary, the methodology that was set up has shown promising features for practical applications. We were able in several cases to reproduce experimental work done at the atomic level on binary FeCr alloys. The reason is that our model is based on a classical potential that captures the essentials of the energetics and thermodynamics of the FeCr system.

The extension of these investigations to multicomponent materials is straightforward and will be part of future studies as well as further experimental comparison and validation.

Research Activities and Results

- **The FeCr phase diagram**

Ab-initio results have shown that FeCr formation energy has a change in sign from negative to positive as Cr composition increases above ~10%. Using our very successful approach that makes use of an interatomic potential that incorporates ab-initio results and the thermodynamic properties of the FeCr system, we were able to quantify the implications of the change of sign in the Fe-Cr heat of formation on the phase diagram [1]. The use of a recently developed parallel MC code with displacement allowed us to predict the evolution of the defect microstructures, local chemistry changes, grain boundary segregation and precipitation resulting from radiation enhanced diffusion [2]. We found that a significant difference appears in a region of temperature and composition that is relevant for the nuclear applications of this alloy. In particular, the solubility limit is finite at low Cr concentration, see Fig 1. Experimental results seem to confirm the validity of the location of the new solvus line. This result is of high scientific impact and shows that miscibility gap of the ferromagnetic phase of the FeCr solid solution as obtained from our calculations (solid red line). Also shown is the solvus as it appears in SSOL CALPHAD metallurgical database. Note the infinite solubility of Cr in Fe at low Cr compositions and low T. A few experiments have been done at low temperature. These experiments seem to confirm our findings, see [3] and [4].

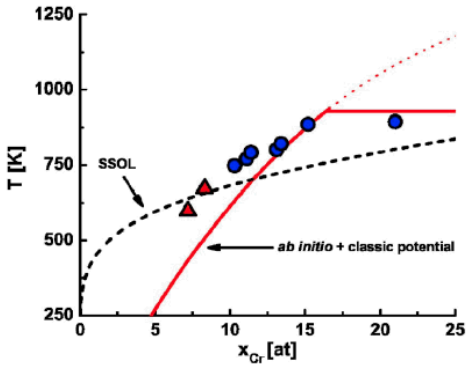

Fig.1: (Solid line) Low temperature and composition region of the phase diagram based on ab initio results generated using the recently developed Fe–Cr empirical potential; (dashed line) solvus from the metallurgical database CALPHAD; and experimental results from [3] (circles) and from [4] (triangles).

- **Point defect properties in FeCr alloys**

Our model brings the most reliable data on formation energies of a diversity of defects that appear in a solid solution in FeCr binary alloy. Data in the literature is usually limited to

vacancy and interstitial (mixed and self-interstitials) formation energies in pure elements. We obtained point defect properties as a function of Cr concentration [5, 6]. Vacancy formation energy decreases with respect to the linear interpolation, see Fig. 2. Below 6% Cr concentration, the vacancy formation energy (Efv) deviates from the line that links vacancy formation energies of pure elements, see Fig 2a.

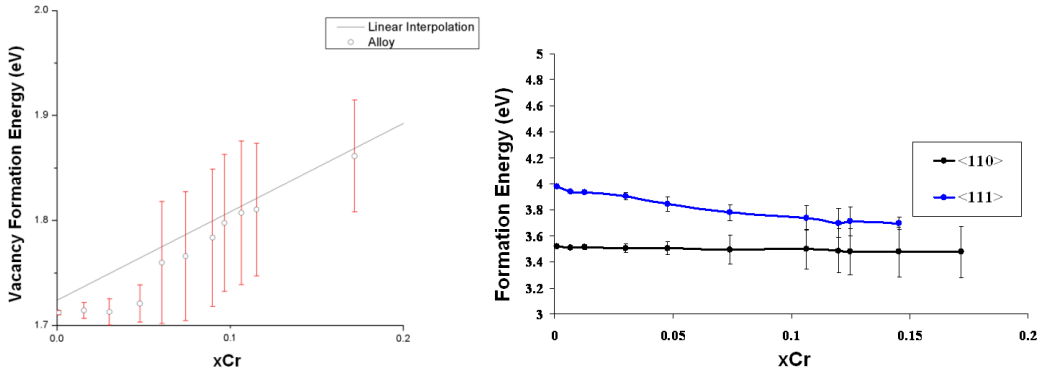

Fig. 2: a) Vacancy and b) self-interstitial formation energies as a function of Cr content in the FeCr sample.

As shown in Fig. 2b, no effect of Cr concentration on self-interstitials formation energies: <110> formation energies remain lower than <111> at all Cr concentrations and self interstitials <111> convert to the lower <110> during the simulation. We also calculated the formation energies of mixed interstitials and found that at Cr concentrations about 10%, all distinction between different types of interstitials disappears within the dispersion of the energy values. These results are of importance in understanding FeCr alloys swelling resistance since swelling seems to depend on interstitials mobility and has been shown to decrease with decreasing Cr concentration.

- **Heterogeneous precipitation in FeCr alloys**

Our studies on non-equilibrium processes in heterogeneous systems in the presence of defects (point defects and solute clusters) and external potentials (dislocations, grain boundaries, cracks, surfaces) lead to a finding of significant science impact: the unexpected behavior found for the precipitation of a' Cr-rich solution, i.e. a rejection of Cr from grain boundaries. We found that in the cases studied of binary alloys with max 15% Cr content at 750 K (~475 ^{o}C) there is no thermodynamics driving force for precipitation of the Cr-rich phase at grain boundaries. Fig. 3 shows a polycrystalline sample with an average grain size of 5 nm. We observe a multiplicity of configurations of grain boundaries, triple and higher order junctions. Blue dots are Fe atoms sitting at boundaries, red dots are Cr atoms. Fe atoms at perfect bcc positions are not shown. A surprising effect can readily be observed: Cr does not precipitate at any boundaries. Instead all a' precipitates are in the interior of the grains, avoiding contact with the grain boundary network [7].

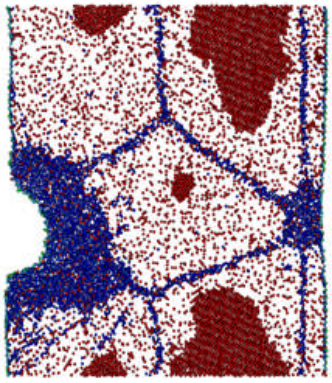

Fig 3: Polycrystalline sample with average grain size of ~ 5 nm (Cr atoms in red) showing Cr does not precipitate at boundaries: a' precipitates are at the interior of the grains, avoiding contact with the grain boundary network.

Quantitative description of heterogeneous precipitation is the next step in this study. Note that evidence of grain boundary Cr depletion has been reported experimentally [8], see Fig. 4, presumably due to a kinetic effect (vacancies migrating preferentially via the Cr sites).

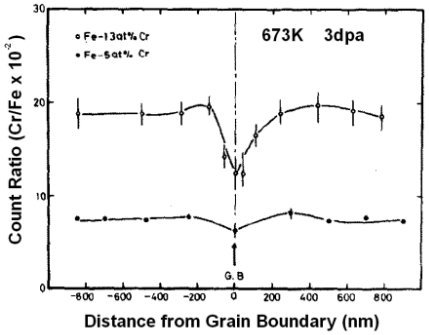

Fig. 4: Concentration profile of Cr in Fe at and near a grain boundary as a function of distance from the grain boundary taken from [8]

These results are relevant in Gen-IV studies because 7-12%Cr FM steels are preferred candidates for cladding, wraps and inner components in future nuclear reactors. These steels show good mechanical properties and remarkable resistance to swelling but they suffer from radiation hardening and embrittlement below 400 oC, even at moderate doses. Both atomistic simulations and experiments show precipitation of a' phase in alloys containing more than 15%Cr when subjected to temperatures in the range of 350-550 ^{o}C.

- **Precipitation in FeCr alloys in the presence of free surfaces and the origin of corrosion**

Precipitation and segregation in FeCr alloys as a function of Cr content were investigated underlying the controversy regarding the origin of corrosion resistance in these alloys [9]. It is well known, that the addition of Cr to Fe creates a Cr oxide layer that passivates the surface enhancing its corrosion resistance. However, ab-initio results favor Cr free surfaces. Calculated and experimental surface energies for pure Fe and pure Cr were compared. Experimentally, it is found that Cr has less average surface energy than Fe. Ab-initio results show the opposite behavior. Our large scale off-site Monte Carlo simulations show consistency with ab-initio results indicating that kinetic or thermochemical effects that are not incorporated in the simulations may be at the origin of this behavior. We investigated FeCr alloys in the solid solution and found that free surfaces are depleted in Cr and that this is a monolayer effect, see Fig. 5.

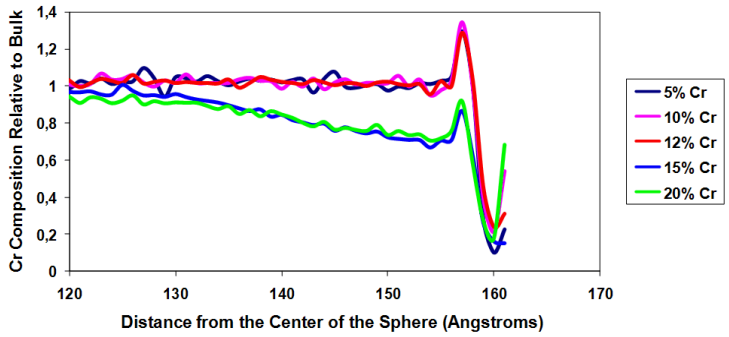

Fig. 5: Cr within different FeCr alloys showing Cr depletion is present at the surface of the sample in all cases.

In Fig. 6, surface Cr composition is reported versus bulk Cr composition at different distances from the surface. The surface of the solid solution is always depleted in Cr.

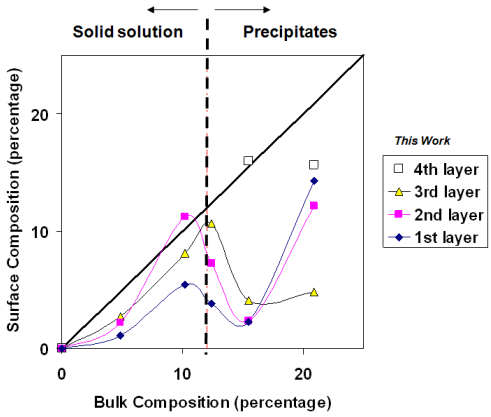

Fig. 6: Cr content in the bulk and at the surface is evaluated for different layers inside the FeCr sample. Cr depletion is present at the surface of the sample in all cases.

The precise origin of the enhanced corrosion resistance in FeCr alloys is still unclear. Further investigations that consider kinetic effects are foreseen. These might lead to a better understanding of the physical mechanism responsible for corrosion resistant properties.

- **FeCr order behavior and intermetallic phases at small Cr concentrations**

We investigated the presence of short range order in FeCr alloys [10]. Our recent advances in the development of Fe-Cr interatomic potentials and the availability of suitable simulation techniques (semi-grand canonical Monte Carlo) provided the possibility to explore the atomistic details of this processes. We studied the SRO evolution in a mixture of two phases and the influence of the kinetics of alloy decomposition on the time evolution of the SRO parameters. We found SRO parameter becomes more negative with increasing Cr concentration. As we decrease the temperature from 900 K to 100 K, the curves approach the theoretical lower limit for the SRO parameter (dashed line in Fig. 7). The SRO parameter reaches a minimum between 8 and 12% Cr, the location of which is only weakly dependent on temperature.

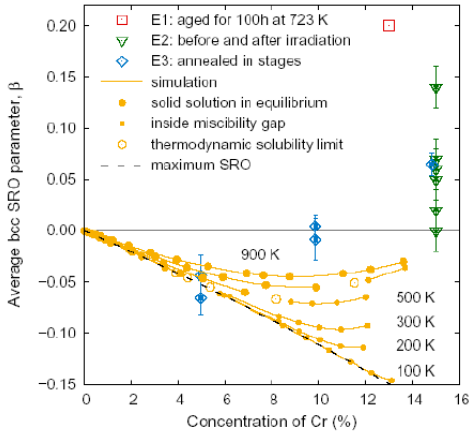

Fig. 7: (Solid Line) Dependence of SRO parameter on the total Cr concentration. Circles show simulation data. The dashed line represents the maximum possible order. E1: experimental data from [11], E2: experimental data from [12], and E3: experimental data from [13].

These results are of high scientific impact because they explain experimental observations of short-range order (SRO) in Fe-rich FeCr alloys [11-13]. The results of atomistic off-lattice Metropolis Monte Carlo simulations give insight into the physical origin of this behavior.

Density-functional theory (DFT) was used to demonstrate that there are several intermetallic phases at small Cr concentrations and that some of these phases correspond to an effective long-range attractive interaction between the Cr atoms. For the first time, simulations showed the presence of several long-range ordered structures that represent ground state phases at 0K in Fe-rich Fe-Cr alloys. At 3.7% Cr, a structure was identified with embedding energy E ~ −206 meV/Cr atom, see Fig. 7. This structure, marked in Fig. 8 as S1, is 49 meV/Cr atom below the infinite dilution limit. Embedding energies below the infinite dilution limit imply the presence of effective long-range attractive interactions between the Cr atoms which are the result of many-body effects.

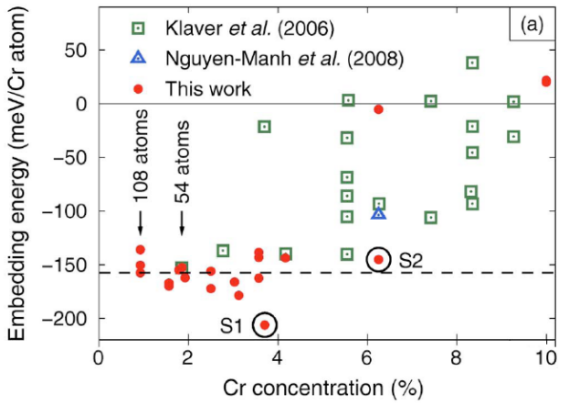

Fig. 8: Calculated formation energies plotted as embedding energy per Cr atom E [meV/Cr atom]. The structure with the lowest formation energy per Cr atom is marked by S1. In this structure the Cr atoms occupy a bcc sublattice three times as large as the underlying Fe bcc lattice.

In the course of this investigation other structures were found: For concentrations larger than 3.7% Cr, the structure with the lowest energy E ~-145 meV/Cr atom equivalent to a formation energy of -9.1 meV/atom (see S2 marked in Fig. 8 above and Fig. 9 below).

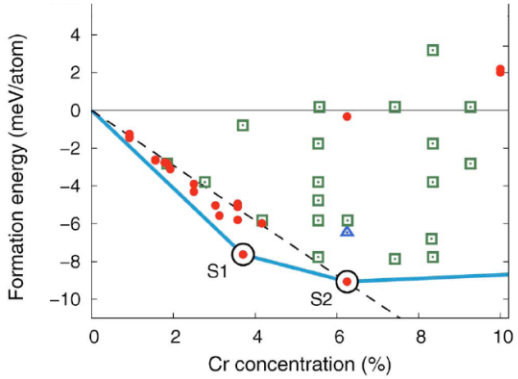

Fig. 9: Calculated formation energies plotted as formation energy per atom. The most stable intermetallic phases, S1 and S2 are connected by thick solid lines. For compositions which fall on these lines, the system decomposes into a two-phase mixture. For concentrations above 6.25% Cr, the thick solid line connects S2 with pure Cr.

The scientific impact of this investigation is the observation of embedding energies below the infinite dilution limit establishing in this way that there are effective long-range attractive interactions between the Cr atoms. This is the first time that this behavior is captured [14, 15]. The structures found in this study complete the low temperature–low Cr region of the phase diagram. We recommend further studies to elucidate the physical origin of this phenomenon.

- **Dislocation mobility functions in FeCr and dislocation dynamics**

Dislocation mobility functions 'transfer' atomistic information to DD meso-scale methodology; they are the critical link between atomistic and mesoscales. Dislocation mobilities for screw dislocations in Fe and Fe-9Cr were obtained using the same potentials as for the heterogeneous precipitation studies. The study was done using molecular dynamics (MD), using the methodology developed in [16]. The results for pure Fe are shown in Fig. 10. Note that obtaining data for pure Fe and Fe-9Cr is difficult. Simulations are noticeably slower than for FCC materials, due to the particular characteristics of screw dislocations in ferritic systems. In this investigation we established the first steps in the connection of atomistic and mesoscale level through mobility laws in pure Fe and in the FeCr solid solution.

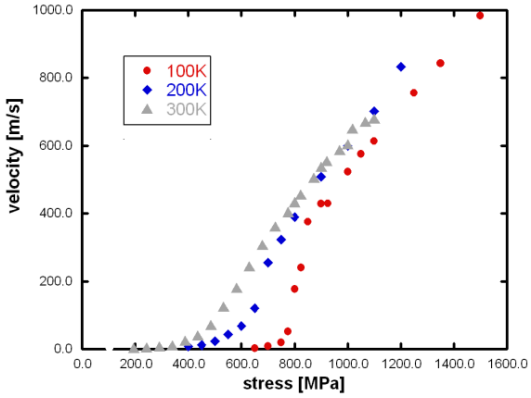

Fig. 10: Mobility in BCC iron as a function of the applied stress for temperatures up to 300K.

Additionally, we extended the capabilities of the atomistically-informed dislocation dynamics for FCC metals developed earlier [21]. In particular, we obtained loading curves for dislocation/stacking-fault tetrahedra (SFT) interactions in FCC Cu. A schematic representation of dislocation-SFT and dislocation-precipitate interaction is shown in Fig. 11. We studied the interaction of screw, mixed, and edge dislocations with SFTs from several angles and heights, and we characterized the strength of these SFTs as a function of the reacting geometry. We find that the SFT is relatively softer when the impinging dislocation is pure screw [17-19].

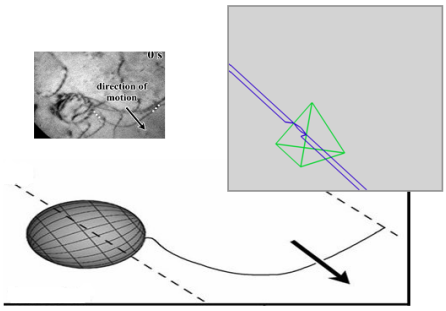

Fig. 11: Determination of the strength of dislocation obstacles leading to hardening: a) a micrograph showing the experimental finding b) dislocation-SFT interaction in an FCC sample c) a simplified schematic representation of the interaction of a dislocation with a precipitate in an FeCr sample.

The loading curve for a screw dislocation in Cu is shown in Fig. 12. The stress fraction is reported as a function of the normalized height showing that the strength of a SFT is a function of the glide plane height. This is an example of our ability quantified the dislocation-SFT interaction in FCC materials. The same methodology can be applied to BCC metals and FeCr alloys.

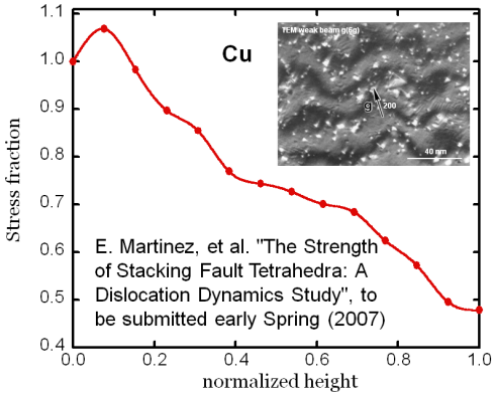

Fig. 12: Loading curve for a screw dislocation in FCC copper. a) Experimental micrograph showing the presence of Stacking-Fault-Tetrahedra SFT in Cu (white spots) b) Results of the simulation showing the SFT strength as a function of the glide plane height.

- **Kinetic Monte Carlo**

Our research in computer simulation of mechanical property changes in FeCr alloys focused on two outstanding issues in kMC simulations: the parallelization of kMC, which is very cumbersome and exceedingly difficult and the possibility of modeling heterogeneous systems and processes. Kinetic Monte Carlo (kMC) has traditionally been the technique of choice due to its ease of implementation and wide range of applicability. However, kMC algorithms only treat motion of particles in perturbation free environments and cannot reach the parameter range of number density and size distribution of species relevant to neutron irradiation conditions considered in this project.

Within this LDRD, a new approach to heterogeneous pkMC has been developed that is able to include interactions with grain boundaries, dislocations, etc. The recently developed pkMC is parallel and overcomes the difficulties typical of 'serial' codes and promises to expand the range of applicability of kMC simulations [20]. Note however, that parallelization of kMC is difficult due to the intrinsic asynchronicity of discrete events. The approach used in developing pKMC is a generalization of the standard n-fold kMC method, and is trivially implemented in parallel architectures. Its validity and parallel performance was tested by solving several pure diffusion problems (i.e. with no particle interactions) with known analytical solution, see Figures 13, 14.

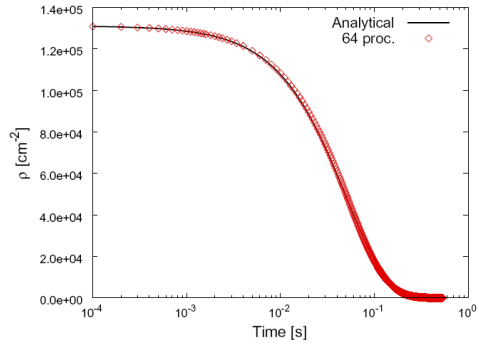

Fig. 13: Comparison between the analytical solution (continuous line) and a parallel run with 64 processors (open diamonds) for the problem of simple diffusion with no particle interactions and absorbing boundaries.

The algorithm simulates the right kinetic evolution, and is based on a perfectly synchronous decomposition of the computational box.

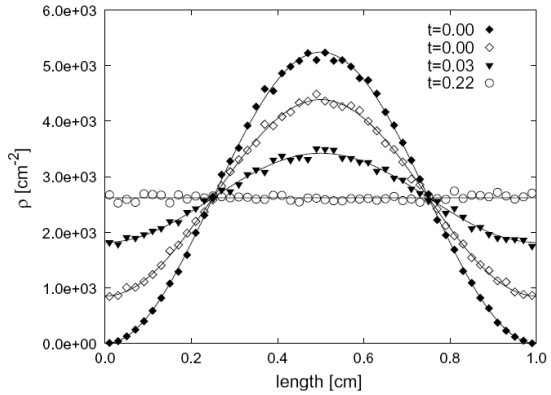

Fig. 14: Comparison between pkMC for 16 processors and the analytical solution of the time evolution of the spatial density profile for the case (ii) of diffusion without particle interactions and periodic boundary conditions.

Also diffusion-reaction systems with known asymptotic behavior were studied. We found that, for large systems with interaction radii smaller than the typical diffusion length, boundary conflicts are negligible and the global kinetic evolution agrees with the expected analytical behavior. A follow-up effort is being done to extend pkMC algorithm to radiation damage calculations. These efforts will come fundamentally in the form of updated reaction tables, and the extension of the method to 'object' Monte Carlo, i.e. the treatment of complex defect species as objects that behave as a single entity.

Exit Plan

We are now part of new LLNL directions, still pointing to materials discovery, synthesis and performance prediction through coupled predictive simulation and experiments. The computational approach that we developed within this LDRD will be incorporated in the simulation of radiation damage in multicomponent materials and help investigate helium

effects in FeCr alloys. This is important in view of LLNL activities relative to the recently approved SI on "Deep-Burn Materials" and LIFE fission-fusion engine project. The research performed within this LDRD has contributed to further LLNL modeling capabilities to the forefront of this field. This LDRD inspired several investigations that served to prepare new proposals recently submitted to DOE. As experimental methods improve, atomic scales that were not attainable before are at the reach of our hands today. At the same time computer simulations are able to model larger systems. Spectacular findings are expected in this field in the coming years.

It is important to note that the formalism that has been developed can be extended to binaries (Fe-C and Fe-He) and ternaries (Fe-Cr-He and Fe-Cr-C) with an approach that is reliable and has been shown to reproduce experimental results. Quantitative description of heterogeneous precipitation is still needed as well as the investigation of kinetic effect (vacancies migrating preferentially via the Cr sites). Our investigations in this LDRD have focused on FeCr equilibrium properties (SRO, precipitation, intermetallics, etc). To do this we used ab-initio results and the recently developed composition dependent interatomic classical potential coupled with a very successful approach that takes account of the thermodynamics of the FeCr system. In our studies we used molecular dynamics (MD) and our variance constrained Metropolis Monte Carlo (MC) that deals very efficiently with millions of atoms in a parallel environment. We were able to study FeCr alloys properties inside the miscibility gap revealing FeCr properties at the range Cr content and temperatures of interest in Gen-IV nuclear applications.

Extension of this work to time dependent processes by the development of massively parallel kinetic Monte Carlo simulation codes and their application to ternary alloys (FeCrHe - FeCrC - FeCrNi) is strongly recommended. Further investigations on the origin of corrosion resistance in FeCr alloys call for simulation developments that account for kinetic effects.

Our investigations established that there are effective long-range attractive interactions between the Cr atoms in FeCr alloys. This is the first time that this behavior is captured. The observation of embedding energies below the infinite dilution limit is of high scientific impact and we recommend extensive studies to elucidate the physical origin of this phenomenon.

The first steps in the description of the interaction process between partial dislocations and stacking fault tetrahedron (SFT) using Dislocation Dynamics (DD) was established. The connection with the atomistic scale was enabled using dynamic simulations of SFT-dislocation interaction therefore linking atomistic and mesoscopic scales. The extension of this methodology to the case of BCC metals and dislocation-precipitate interaction in FeCr alloys is foreseen. Studies furthering this effort are recommended.

Finally, we have developed a novel parallel kinetic Monte Carlo algorithm that promises to access time and length scales as-of-yet unexplored in kMC simulations. An extension of the pkMC code to radiation damage calculations is envisaged. The application of this powerful method to time evolution of FeCr systems will contribute to the progress in the understanding of kinetic effects that are so difficult to describe today.

Acknowledgements

The PI of this project gratefully acknowledges Dr. A. Caro for his contribution in the investigation of physical phenomena of increasing complexity and in the formulation of state-of-the-art methodologies that help gain fundamental understanding of materials strength and failure.

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