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Introduction

Scientific aspects

Summary of the major scientific contributions of the SIRENA project

The SIRENA project constituted a major contribution within the field of the understanding of irradiation mechanisms in Zircaloy-based alloys (in particular Zr-Nb alloys). The list of publications and communications given in the next section show clearly that the project was a major advance. We will try here to briefly emphasise the main scientific achievements reached during the project lifetime. These major contributions are sorted by increasing time and space scales.

☑ *Ab-initio simulations*

In the framework of SIRENA, state of the art ab initio calculations have been performed in hcp Zr, on point defect properties, interaction with Nb, and also iodine effects. Extended defects have also been determined and in particular the *first* ab initio calculation of screw dislocation core in hcp Zr have been performed showing a spreading in the prismatic plane in agreement with experimental results.

☑ *Cascade displacements*

A large database has been constituted on cascade calculations in α -Zr. MD studies used for low and medium PKA energies, performed with a high number of simulations for each condition of temperature and energy, have revealed the wide variety of defect clusters that can be created in cascades. Mobile or sessile, two-dimensional or three-dimensional clusters of both vacancy and interstitial type can be formed.

For higher energies, a good parametrisation of BCA computations with MD simulations allowed to show that the number of Frenkel pairs predicted by full MD and by its binary collision approximation are in reasonable agreement. The BCA predicts a power law dependence on the PKA energy which is close to unity. This is also the trend predicted by MD although deviations from unity are found, these deviations increasing for decreasing PKA energies. Nevertheless, it is possible to parametrise the BCA by means of a suitable recombination radius in such a way that BCA and MD predictions do not diverge by more than a factor of 2 over the range of energies between 1 and 100 PKA energies.

☑ *Short-term evolution of defects*

The diffusion of defects produced during irradiation in hcp zirconium was studied through a kinetic Monte Carlo model. The input data for these simulations is based on molecular dynamics calculations. The effect of different parameters for the case of the accumulation of the damage: dose rate, grain boundary approximation, mobility of interstitials clusters (rate theory approximation), bias for interstitials and anisotropy of interstitials (from 1D to 3D motion of interstitials).

☑ *Long-term evolution of defects (Rate-theory)*

A model based on a cluster dynamics model based on rate equation theory was proposed in 2002 to describe the point defect agglomeration in metals under irradiation. This model is restricted to materials where point defect diffusion is isotropic and is thus not applicable to anisotropic metals such as zirconium. Therefore the rate-theory code was modified as so to account for anisotropic metals and in particular to hcp Zr.

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☑ *Dislocations / defects interactions*

A model has been developed to simulate edge dislocations of the $1/3\langle 11\bar{2}0 \rangle(0001)$ and $1/3\langle 11\bar{2}0 \rangle\{1\bar{1}00\}$ slip systems in α -Zr. It was used to model the interaction of a $1/3\langle 11\bar{2}0 \rangle(0001)$ basal edge dislocation with four typical vacancy and self-interstitial atom (SIA) clusters created by displacement cascades in α -zirconium. Details of the atomic mechanisms and critical breakaway stress of interaction of a $1/3(11\bar{2}0)\{1\bar{1}00\}$ prism-plane edge dislocation with clusters of self-interstitial atoms have also been studied by simulation.

☑ *Mechanics at the mesoscopic scale:*

The development performed in the framework of SIRENA allowed to provide the *first* Dislocation Dynamics code compatible with the hexagonal symmetry of Zr-alloys and the *first* investigation of the Orowan mechanism in dynamical conditions.

☑ *Iodine assisted stress corrosion cracking simulation:*

No real micro-mechanical modelling of the iodine assisted stress corrosion cracking was made before, although the work done within the project was highly inspired by the one performed by O. Diard during its PhD. The proposed methodology also proposes a simplified approach to model iodine-SCC in large-scale experiments.

List of Publications and Communications

The publications and communications are also published in the SIRENA directory of the PERFECT web-site, and accessible for granted people. The links below should also point to these publications on the web site.

- [Atomic-Scale Simulation of Defect Cluster Formation in High-Energy Displacement Cascades in Zirconium](#)
Roman E. Voskoboinikov, Yuri N. Osetsky, and David J. Bacon, to be published in the Proceedings of the Symposium on Radiation Effects, ASTM International.
- [Defect diffusion in hcp Zirconium: A kinetic Monte Carlo approach](#)
C. Arévalo, M.J. Caturla and J.M. Perlado
- [Long-term behaviour of irradiated hcp Zr coupling Molecular Dynamics and Monte Carlo simulations](#)
Poster presented by C. Arevalo
- [Long-term behaviour of irradiated hcp Zr using Monte Carlo simulations](#)
Article presented by C. Arévalo, M.J. Caturla and J.M. Perlado at COSIRES
- [Simulation of Radiation Effects in Zr-Nb alloys: Application to stress-corrosion cracking behavior in iodine-rich environment](#)
FISA 2003 communication on SIRENA by S. Jumel, C. Domain, G. Monnet, J. Ruste, J.C. van Duysen, D.J. Bacon, R. Voskoboinikov, B. Devincere, A. Barbu, F. Christien, M. Perlado, C. Aravelo, M. Hou, D. Kulikov and P. Tägstrom
- [Dislocation study of prismatic slip systems and their interactions in HCP metals: application to Zr](#)
G. Monnet, B. Devincere, L.P. Kubin Acta Materialia 52 (2004) 4317-4328
- [Investigation of glide properties in hexagonal titanium and zirconium: an ab initio atomic scale study](#)
C. Domain, A. Legris Proceedings, IUTAM conference, Osaka 2003
- [Ab initio atomic-scale modelling of iodine effects on hcp zirconium](#)
A. Legris and C. Domain, Phil. Mag. 85 (2005) 589-595

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- [Ab initio atomic-scale determination of point-defect structure in hcp zirconium](#)
C. Domain and A. Legris, Phil. Mag. 85 (2005) 569-575
- [Posters R. Voskoboïnikov at "Dislocation 2004"](#)
3 posters presented by R. Voskoboïnikov at the "Dislocation 2004" conference
- [Interaction of edge dislocations with interstitial dislocation loops in \$\alpha\$ -zirconium](#)
Z. Rong, D.J. Bacon, Yu.N. Osetsky and R.E. Voskoboynikov. Poster presented at ICFRM-12, Santa Barbara, California, December 2005.
- [Investigation of precipitation hardening by dislocation](#)
Ghiath MONNET, Phil. Mag., Vol. 86, 2006, 5927–5941
- [Ab initio modelling of defect properties with substitutional and interstitial elements in steels and Zr alloys](#)
C. Domain, Journal of Nuclear Materials 351 (2006) 1-19

Detailed scientific contributions

EDF

DD contribution (G. Monnet)

The development performed in the framework of SIRENA allowed to provide the *first* Dislocation Dynamics code compatible with the hexagonal symmetry of Zr-alloys and the *first* investigation of the Orowan mechanism in dynamical conditions. It led to two publications as detailed in the following.

(i) Development of Dislocation Dynamics (DD) code compatible with the hexagonal symmetry

The crystallography of the hcp lattice traditionally makes use of the four Miller–Bravais indices. This representation is unfortunately not appropriate for DD simulations. It implies handling one additional index with respect to cubic notations and abandoning all the advantages of orthogonality for arithmetic computations. An alternative solution, which is compatible with the lattice-based approach, has been adopted. It makes use of the orthorhombic description of the hexagonal cell, for details see reference below. The basal plane is indexed as a (111) plane and the slip directions become $\langle 110 \rangle$, like in the fcc structure.

- G. Monnet, B. Devincre and L.P. Kubin, Acta Mater. 52 (2004) 4317.

(ii) identification of dislocation mobility law

A typical Arrhenius form suited for the kink-pair mechanism is used for representing screw dislocation motion. Following a method previously developed for the tantalum, use was made of the Kocks formulas for the activation free energy as a function of the effective stress. The parameters of this formulas were fitted using the plentiful experimental work of the Mills and Craig [Trans Metal Soc AIME, 242 (1968) 1881]. The non-screw segments have a much larger mobility than the screw ones. Their dynamics involves two unknown quantities: their mean free-flight distance and their velocity, which depends in principle on stress and temperature. For the sake of simplicity, the mobilities of the two types of segments were assumed to be proportional to each other, with a proportionality constant K. Simulations showed that a substantial change in the value of K does not alter the yield stress, which confirms that the latter is governed by the onset of screw dislocation motion.

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(iii) constitution investigation of identification of dislocation mobility law

Development described before allowed to perform the first DD simulation of plastic deformation of Zr. The emphasis being on low temperature properties, a methodology was developed to control the mean-free path of the highly mobile non-screw dislocations. Several investigations were performed on the hardening that results from the interactions of dislocations gliding in different prismatic slip planes. The net result is that no junctions can be formed between intersecting screw dislocations, so that the work hardening coefficient drops to rather small values when temperature decreases due to stronger forest interactions and the continuous production of forest density by the easy motion of non-screw segments in many slip planes. Therefore, the low temperature stress-strain curves associated with prismatic slip in hcp metals are unique and combine features typical of both bcc and fcc crystals.

On the other hand, the strengthening generated by the irradiation-induced precipitation of Nb needles was also investigated, for more details see reference below. It was shown that at fixed strain rate the magnitude of the stress fluctuation depends on the value of the imposed strain rate coupled to the size of the simulated volume. An increase in the strain rate smoothes the stress curve and increases the critical Orowan stress. The strengthening by Nb precipitates in Zr-1% Nb alloy has been determined and compared to existing models. DD simulations show that the radiation-induced hardening related to the precipitation of Nb needles is close to 25%. This result clearly indicates that radiation-induced precipitation is not responsible for the large hardening of irradiated Zr-1% Nb alloys. DD simulation results show that most of theoretical models, overestimate the Orowan stress, even with respect to DD simulation carried out at large strain rates. A general superposition rule is proposed to account for the strengthening induced by different precipitate families.

- G. Monnet, Phil. Mag., 86 (2006) 5927.

Ab initio contribution [C. Domain (EDF) A. Legris (University of Lille)]

In the framework of SIRENA, state of the art ab initio calculations have been performed in hcp Zr, on point defect properties, interaction with Nb, and also iodine effects. Extended defects have also been determined and in particular the first ab initio calculation of screw dislocation core in hcp Zr have been performed showing a spreading in the prismatic plane in agreement with experimental results.

(i) Point defects in Zr and Zr-Nb system

Vacancy and the different self interstitial configurations have been characterised and formation energies have been calculated in hcp Zr. A new picture has been obtained. Contrary to previous results obtained using empirical potentials, we found that the octahedral configuration should be the most stable SIA, immediately followed by the basal octahedral and the basal crowdion, the three structures having very close formation energy. These results will change the diffusion properties and will affect the long term evolution of the microstructure under irradiation.

The interaction of Nb with point defects have shown a strong interaction of Nb with self interstitial, with a binding energy close to 1 eV, whereas no significant interaction are present between Nb and vacancies. This strong interaction of Nb with self interstitial should induce a fast diffusion of Nb present in solid solution under irradiation. Under irradiation the formation of Nb needles at the beginning of the neutron radiation is probably associated to this important Nb – self interstitial interactions.

- C. Domain and A. Legris, Phil. Mag. 85 (2005) 569-575
- C. Domain, Journal of Nuclear Materials, 351 (2006) 1-19

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(ii) Iodine effects in hcp Zr by ab initio

In order to elucidate possible mechanisms of stress corrosion cracking of nuclear power plant cladding material, we have investigated the iodine–zirconium interactions using ab initio atomic-scale calculations.

We show that for the gas pressure estimated during the reactor power transients, the reduction of the zirconium effective free surface energy induced by the adsorption of atomic iodine is significant (more than 80%). Furthermore, for given iodine partial pressure, the surface energy reduction for the basal planes is higher than for the prismatic ones, in agreement with the experimental observation of a cleavage along the basal planes. We have also estimated the iodine surface diffusion coefficient, and its high value (about $10^{-6} \text{ cm}^2 \text{ s}^{-1}$ at 600 K) indicates that iodine is mobile enough to follow the crack tip during the cracking experiments reproduced in laboratory conditions. Our results clearly rule out the influence of absorbed iodine during the cracking process, its equilibrium concentration being totally negligible.

- A. Legris and C. Domain, *Phil. Mag.* 85 (2005) 589-595

(iii) Screw dislocation properties in hcp Zr

Our *ab initio* determination of the stacking fault energies, elastic constants and structure of the screw dislocation core are in agreement with experimental observations. The prismatic stacking fault energy is lower than the basal one and the prismatic fault configuration is located at a local minimum of the gamma-surface excess energy.

Despite the limited supercell size and approximate boundary conditions used, screw dislocation cores in Ti and Zr show a clear spreading in the prismatic plane. The secondary spreading of edge character along the basal planes should control the lattice friction at low temperature. This first ab initio calculation of the core structure of screw dislocation is in agreement with the easier prismatic slip observed experimentally and shows that the prediction of the empirical potential found in the literature with a basal spreading is not suitable to describe properly the screw dislocation.

- C. Domain, *Journal of Nuclear Materials*, 351 (2006) 1-19

University of Liverpool

Work has been performed on two fronts, as follows.

Displacement cascades

A systematic study of damage in high-energy cascades in α -Zr with primary knock-on-atom (PKA) energy up to 25keV has been carried out by molecular dynamics (MD) over a temperature range from 100 to 600K. The high number of simulations for each condition of temperature and energy has revealed the wide variety of defect clusters that can be created in cascades. Mobile or sessile, two-dimensional or three-dimensional clusters of both vacancy and interstitial type can be formed. The population statistics of clusters of each type, and the fraction of vacancies and self-interstitial atoms (SIA) in clusters, were obtained and their dependence on the temperature and PKA energy were investigated. Both vacancy and SIA clusters can be mobile. However, depending on their type self-interstitial clusters exhibit one-dimensional, planar or three-dimensional motions, whereas vacancy clusters of only one type can glide and in one dimension only. We have also performed separate MD simulations of some SIA and vacancy clusters to study their thermal stability and possible transformations. These results were presented to the ASTM Symposium on Radiation Effects held in Boston, USA, in June 2004 and will be published in the Proceedings [1].

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Data for the defects created in all the cascades simulated (PKA energy 10-25keV and temperature 100-600K) have been compiled and copied to a CD deposited with the SIRENA Coordinator.

Atomic-scale simulation of dislocation-damage interactions

A model has been developed to simulate edge dislocations of the $1/3\langle 11\bar{2}0 \rangle(0001)$ and $1/3\langle 11\bar{2}0 \rangle\{1\bar{1}00\}$ slip systems in α -Zr [2]. The distribution of atomic displacements in the dislocation core shows that in the model used, the edge dislocation in the basal plane dissociates into two Shockley partials whereas the dislocation in the prism plane remains undissociated. The effective core radius and core energy have been estimated, and dislocation response to increasing applied shear stress studied to determine the critical stress for dislocation glide (Peierls stress). The model has now been used to investigate dislocation-obstacle effects in the two different slip systems, as follows.

The interaction of a $1/3\langle 11\bar{2}0 \rangle(0001)$ basal edge dislocation with four typical vacancy and self-interstitial atom (SIA) clusters created by displacement cascades in α -zirconium has been modelled [3]. A triangular cluster of SIAs lying within a basal plane adjacent to the dislocation glide plane is not absorbed by the dislocation but is pushed along by the leading partial. A 3-D SIA cluster lying across the glide plane is completely absorbed by the dislocation by creation of a super-jog. The dislocation also climbs by interaction with a prismatic vacancy cluster, but only half of the vacancies are absorbed in this case. For a cluster formed from a basal platelet of vacancies, the dislocation experiences a glide resistance, but both the line and cluster are fully restored after breakaway. Strain-stress curves and the critical stress for dislocation breakaway from the four clusters have been calculated.

Details of the atomic mechanisms and critical breakaway stress of interaction of a $1/3(11\bar{2}0)\{1\bar{1}00\}$ prism-plane edge dislocation with clusters of self-interstitial atoms have also been studied by simulation [4]. Four clusters typical of the primary state of radiation damage have been considered. A triangular cluster of 5 SIAs lying within a basal plane bisected by the dislocation glide plane is not absorbed by the dislocation but acts as a moderately strong obstacle. A 3-D SIA cluster lying across the glide plane is completely absorbed by the dislocation by creation of a super-jog, and is a weak obstacle. Interaction of the dislocation with glissile interstitial loops with perfect Burgers vector in one of the two orientations inclined at 60° to the dislocation glide plane shows that the process depends on the vector orientation. Both defects are strong obstacles to dislocation glide on the prism plane, but one, which initially forms a sessile segment on the dislocation line, is particularly strong. Strain-stress curves and the critical stress for dislocation breakaway have been calculated for all clusters.

These simulations were undertaken using energy minimisation to mimic static conditions ($T = 0\text{K}$) in order to provide a direct atomic analogy to modelling based on elasticity. The results of these three studies were presented at the international conference Dislocations 2004 held in France in September 2004 and will be published in the Proceedings [2-4]. In future work, it will be necessary to extend the simulations to (a) a range of obstacle size and spacing, and (b) temperature greater than 0K . Emphasis will be placed on the prism-plane dislocation because of its importance for plasticity in Zr and the fact that the obstacle strengths found in the modelling above are highest for the prism-plane slip system.

1. R.E.Voskoboinikov, Yu.N.Osetsky, D.J.Bacon, 'Atomic-scale simulation of defect cluster formation in high energy displacement cascades in zirconium', to be published in the Proceedings of the Symposium on Radiation Effects, ASTM International.
2. R.E.Voskoboinikov, Yu.N.Osetsky, D.J.Bacon, 'Core structure, dislocation energy and Peierls stress for $1/3\langle 11\bar{2}0 \rangle$ edge dislocations with (0001) and $\{1\bar{1}00\}$ slip planes in α -Zr', to be published in Mater. Sci. & Eng. A (Dislocations 2004 Special Issue).

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3. R.E.Voskoboinikov, Yu.N.Osetsky, D.J.Bacon, 'Interaction of $1/3\langle 11\bar{2}0 \rangle(0001)$ edge dislocation with point defect clusters created in displacement cascades in α -zirconium', to be published in Mater. Sci. & Eng. A (Dislocations 2004 Special Issue).
4. R.E.Voskoboinikov, Yu.N.Osetsky, D.J.Bacon, 'Self-interstitial atom clusters as obstacles to glide of $1/3\langle 11\bar{2}0 \rangle\{1\bar{1}00\}$ edge dislocations in α -zirconium', to be published in Mater. Sci. & Eng. A (Dislocations 2004 Special Issue).

Université Libre de Bruxelles

This study was the opportunity to make several steps in the understanding of radiation damage evolution in Zr.

As far as displacement cascades are concerned, it was shown that the number of Frenkel pairs predicted by full MD and by its binary collision approximation are in reasonable agreement. The BCA predicts a power law dependence on the PKA energy which is close to unity. This is also the trend predicted by MD although deviations from unity are found, these deviations increasing for decreasing PKA energies. Nevertheless, it is possible to parameterise the BCA by means of a suitable recombination radius in such a way that BCA and MD predictions do not diverge by more than a factor of 2 over the range of energies between 1 and 100 PKA energies.

Further work is presently in progress, using the BCA, to study cascade morphology distributions on a statistical basis. This is necessary in order to predict the clusters of vacancies and interstitials as formed as a consequence of displacement cascades representing the initial conditions for the long term evolution of damage.

It may be anticipated that vacancies and interstitial will cluster with minimal energy configurations. Although we don't know yet the cluster size distribution resulting from individual cascades and of sets of individual cascades, it is possible to determine the formation and binding energies of vacancy clusters as a function of their size, and this is what was done in the second part of this contract.

In the same line, a procedure was developed for the calculation of the formation energies of point defect clusters and corresponding vacancy binding energies in Fe-Cu system. This newly developed procedure is used in the present work for the calculation of vacancy binding energies to different types of vacancy clusters in hcp Zr. An uncertainty is found with obtaining the most stable configurations and therefore with finding correct formation energies. However this uncertainty seems to be more pronounced for big clusters where the approximation procedure may conveniently be used. Besides energy calculations, some information on the clusters configurations is obtained: MMC leads to 3D vacancy clusters independently of initial configuration. As a result of MMC, clusters have faceted structures, with well-defined (0001) and $(10\bar{1}1)$ facets.

The displacement fields around different types of dislocation loops were calculated. It was found that it is necessary to apply some special annealing procedure in order to let atoms close to the loop rearrange correctly.

The fact that the best minimal configuration energies found are associated with the most isotropic configurations is intuitively no surprise as spherical configurations minimise the surface to volume ratio and hence, surface excess energies. However, experimental observations essentially report about dislocations loops. Although transmission electron microscopy does not allow imaging small vacancy clusters, nor, probably, the smallest dislocation loops without ambiguity, we paid particular attention to them. Over the whole range of sizes considered (up to 700 vacancies), binding energies are higher in three dimensional clusters than in two dimensional arrangements of vacancies.

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In the third part of this work, we showed that such arrangements are not necessarily the best stable and that artificial local overheating leads to rearrangements of two-dimensional configurations into stacking faults arrangements known for hcp materials.

Binding energies need to be re-examined in the light of such rearrangement.

Particular attention is paid to the strong strain fields around dislocation cores configurations since they are certainly of large influence on the diffusion of interstitials and vacancies in their vicinity. This diffusion is the main factor governing the growth kinetics of vacancy loops.

UPM

Work During Year 3 (2004)

We have studied diffusion of defects produced during irradiation in hcp zirconium through a kinetic Monte Carlo model. The input data for these simulations is based on molecular dynamics calculations (David Bacon and Roman Voskoboinikov)

1. Database of displacement cascades created by recoils from 10 to 25 keV obtained by Molecular Dynamics (MD) simulations have been used as initial damage state in the metal. They have been followed for times of hours and a fixed temperature of 600K. We have firstable focused on the evolution of single cascades, and studied the stability of those clusters formed in the MD for long times, as well as the possibility of growing of defects. All calculations were done at 600K. We have computed the number of defects escaping recombination as a fraction of those produced in the cascade, and therefore the number of defects that would interact with the microstructure.
For calculations of cascade ageing, the size of the computational box was 1000x1000x1000 nm³. The starting defect microstructure was introduced in the centre of the kMC computation box according to the spatial configuration obtained by MD simulations. Then the system was annealed during 1000 s at 600K, and the number of defects able to reach the edges of the kMC computational box were counted to determine the escape fraction. In order to have a good statistics, we performed 100 annealing runs for each cascade using a different series of random numbers and then calculating the average escape ratio, the recombination ratio between vacancies and interstitials, the defects surviving the bulk and the average clusters size for these remaining defects.
These calculations helped us to understand the long term behavior of cascade damage, before going into the accumulation of damage under fission conditions.
2. Using 25 keV cascades studied in (1) we have studied the evolution of the microstructure during irradiation under fission environment conditions (damage accumulation): dose rate of 10⁻⁶ dpa/s, 600K, 100x100x100 nm³ simulation box and final dose of 0.1 dpa. Periodic boundary conditions were used in this case. We have introduced 1 dimension motion for the diffusion of SIAs and interstitials clusters (anisotropy). We have also considered grain boundary approximation of 1 μm (if one SIA makes one million jumps without find another defect dissapear of the system).
3. Effect of different parameters for the case of the accumulation of the damage:
 - Effect of dose rate
 - Effect of the grain boundary approximation

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- Effect of the box size
 - Effect of mobility of interstitials clusters (rate theory approximation)
 - Effect of a bias for interstitials
 - Effect of the anisotropy of interstitials (from 1D to 3D motion of interstitials)
4. First approach of electron irradiation simulation (Validation of the code)

CEA/DEN/DMN/SRMP

The work dealt mostly with the Task 4.3 and 5 : Rate equation modeling of the point defect clusters and Nb precipitation in ZrNb alloys.

A model based on a cluster dynamics model based on rate equation theory was proposed in 2002 to describe the point defect agglomeration in metals under irradiation. This model is restricted to materials where point defect diffusion is isotropic and is thus not applicable to anisotropic metals such as zirconium.

Work completed in 2002:

In order to introduce to introduce the Nb zirconium precipitation under irradiation, we merge in a first step the code developed for the simulation of point defect cluster evolution in the isotropic case with a cluster dynamic code devoted only to precipitation. We tested and validated this new code able to describe the precipitation under irradiation taking into account the microstructurale changes on the well document problem of the precipitation of copper in ferritic alloys under irradiation

Work completed in 2003:

- Following the approach proposed by Woo, we extended the model to the case where self-interstitial diffusion is anisotropic. The model was as a first step applied to the loop microstructure evolution of a zirconium thin foil irradiated with electrons in a high-voltage microscope. First, the inputs were validated by comparing the numerical results with experimental results given by the literature. Further calculations were made to evidence the effect of the thin foil orientation on the dislocation loop microstructure under irradiation. The result is that it is possible to reproduce for certain orientations the "unexpected" vacancy loop growth experimentally observed in electron-irradiated zirconium. This effect is direct linked to SIA diffusion anisotropy.

Work completed in 2004:

- In a second step, the model was used to calculate the macroscopic straining induced by the point defect elimination on various sinks. We were especially interested in modeling the anisotropic growth of zirconium single crystals. By adjusting certain input parameter of the model, it is possible to reproduce the growth acceleration observed at high fluences.

Work completed in 2005:

- Introduction of the anisotropic diffusion in the code considering the precipitation under irradiation. Application to the precipitation of Nb in ZrNb alloys under irradiation.

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Publications:

- Modeling of copper precipitation in iron during thermal ageing and irradiation
F. CHRISTIEN, A. BARBU, J. Nucl. Mat., 324 (2003) 90-96
- Effect of self-interstitial diffusion anisotropy in electron-irradiated zirconium. A cluster dynamics modeling.
F. CHRISTIEN, A. BARBU Submitted to J. Nucl. Mat.,
- Application du modèle d'agglomération de défauts ponctuels en dynamique d'amas aux matériaux anisotropes
F. CHRISTIEN, A. BARBU, Document Technique DMN DMN/SRMP/NT/2004-011/A

Management Aspects

SIRENA was the first European project aiming at predicting the mechanical behaviour of an irradiated material using a chained multiscale approach. Moreover, few work was done at start of the project on the irradiation of Zr-Nb alloys, by comparison for instance with RPV steels. In particular, the adaptation of the common tools used for study of irradiation effects to the crystallographic structure of Zr alloys as well as the anisotropy of diffusion of the irradiation defects lead to huge developments in the different codes. But the other aspect of this scientific challenge was that many uncertainties were linked to the management of the project.

As an example, the used Zr-Nb potential for MD simulations could not account for both cascade simulations and dislocation / defect interactions. A supposedly better potential was obtained during a PhD but it had been accessible only at the end of the project. A choice had to be made in 2004: either continue with the current potential although it has many limitations, or wait for the improved potential. In order to unlock the situation, the work in late 2004 and 2005 was done with the same (old) potential.

The other main difficulty that slowed down the advance of the SIRENA project was the settlement, start and running of the PERFECT project. As a matter of fact, SIRENA was a kind of model pattern for the definition of the PERFECT project, although both projects were related to different materials. But the scientific community involved in SIRENA was also naturally involved in PERFECT as the scientific topics were very close. The huge amount of work required by PERFECT unfortunately gave less time to the participants to achieve the SIRENA tasks.

To be honest, the work-packages and tasks definitions of SIRENA were also tremendously underestimated in terms of man-power. The proposed goal of the project at start was no more than to provide a chained tool for prediction of the irradiated behaviour and iodine-assisted stress-corrosion cracking of Zr-Nb alloys, which is roughly the same thing than PERFECT should provide but with an effort of 30 participating organisations and a budget far more important! As pointed out above, the fact that this project was the first to try to provide such a tool can be an excuse to this, as the community had little or no experience on such projects. This is also why the dimension of PERFECT was much larger from the beginning.

As an example, as in 2004 nothing was done on the mechanical work-package of SIRENA, EDF took the decision to have a detached person from the CNRS to work on it in 2005. This was the only way to achieve the deliverable D6 to D8.

Finally, the transmission of the project between S. Jumel and S. Bugat in 2004 was too short and many documents were lacking, especially from the financial point of view. As the history of reversals was hard to retrieve, it took some delay to perform to the final reversals.

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Conclusions and prospects

As a conclusion, a lot of effort has been done in the understanding of the long-term irradiated microstructure of zirconium alloys, and the transition towards mechanical properties has been achieved, although the developments done would need more experiments in order to be validated.

However, as mentioned previously, the complete chain starting from neutron spectrum and ending by the simulation of iodine—assisted stress corrosion cracking is not done yet, from a software point of view. As decided during the last plenary meeting, all informations obtained during the project (cascade database, articles etc.) are gathered on the PERFECT web-site in a specific area. It is proposed in a further work to use the software platform developed during the PERFECT project and to adapt it to the aims considered for Zr alloys. All potential needed information are available, however this would require a certain amount of work.

Moreover, we have seen that the chosen potential used for dislocation / defects interaction and for cascades simulations is not the most accurate one. The interatomic potential developed by N. Poletz during its PhD will have to be characterised, in order to know if it is more suitable. However, if so, the whole chain (and in particular the computation of interaction strengths between dislocations and defects) of SIRENA would have to be run again.

