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nuclear science and technology

Improvement of Techniques for Multiscale Modelling of Irradiated Materials

(ITEM)

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Final report

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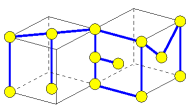


Contents

Objectives

The use of test reactors and hot cell facilities to study irradiated materials becomes more and more problematic. One way of partially solving this problem is to develop tools for computer simulation of radiation effects in materials, by applying multiscale modelling techniques. The development of such tools dedicated to the nuclear domain (called virtual test reactors: VTRs) began recently (1998), focusing on specific issues and using current simulation techniques. However, it is paramount to elaborate a new generation of techniques, which will allow the application field of VTRs to be enlarged within a few years. The objective of the ITEM Thematic Network was to ensure that these developments are performed rapidly and in a co-ordinated way in Europe. It was also a great opportunity for the European nuclear industry to lead such an international effort in the direction of its interest. Furthermore, the multiscale modelling approach is being aggressively pursued in the USA and in Japan. The network will allow Europe to exchange information at an equal level with these countries.

The network gathered 40 members and was organised into the following seven technical areas (TA):

- Website and Database Construction and Maintenance TA is in charge of setting up the EDAM database which will contain codes, physical parameters and any other information relevant to perform multi-scale simulation of materials.
- Radiation Damage Modelling TA has as objective to study the formation and evolution of radiation-induced defects in simple systems (e.g. clustering of point defects) at different time and space scales. The interaction between those defects and dislocations will also be studied.
- Simulation of Mechanical Properties of Single Crystals TA is aimed at solving issues concerning the simulation of single-crystal plasticity with dislocation dynamics codes.
- Polycrystal Simulation Methods TA has as objective to link atomic-level information about extended defects and microstructure evolution into new and/or improved mesoscopic and macroscopic multiscale models of the thermal/mechanical/radiation response of polycrystalline materials.
- Multiscale Modelling Applications TA is aimed at improving VTRs from the point of view of code-coupling efficiency and computing speed.
- Experimental Validation TA is in charge of identifying *ad hoc* mechanical testing and/or microstructure characterisation to validate step by step the simulation made with VTRs.
- Phase Stability and Kinetics of Phase Transformations in Alloys under Irradiation TA has as objective to assess new methods to study the stability of phases of alloys under irradiation.

In addition, ITEM members have been solicited to produce a document on best-practice guidelines for multiscale simulation. ITEM was also very helpful in establishing the university partner network for the PERFECT (Prediction of Irradiation Damage Effects on Reactor Components) IP proposal under the Sixth Euratom Framework Programme (Euratom FP6).

This report finalises the work and the results achieved within the ITEM network.

A. Context

The development of virtual test reactors (VTRs) began recently, in 1998, in the framework of a collaboration between several European organisations (the REVE project, involving EDF, CEA, University of Lille and University of Rouen in France; SCK-CEN and University of Brussels in Belgium; CIEMAT and Polytechnic University of Madrid in Spain; University of Liverpool in the UK) and was extended by setting up an international working group, with the collaboration of American and Japanese laboratories (International Group REVE: IGR). The work of this group focuses on simulation of irradiation effects on reactor pressure vessel (RPV) steels. In addition, the European Commission has accepted to support the RTD project SIRENA, devoted to simulate iodine-assisted stress-corrosion cracking in irradiated Zr-Nb alloys. All these programmes rely mainly on existing simulation techniques and do not try to develop new ones.

While these programmes are being carried on, it is paramount to prepare a new generation of simulation techniques, which will allow producing more quantitative and reliable VTRs in a few years. In Europe, many research groups, very different in nature (from university departments to national research laboratories and R&D divisions of large companies), are currently working on this new generation for many applications (nuclear and non-nuclear). However, they are not linked together by any formal structure to share experience, exchange codes or data, compare results and develop common techniques.

The ITEM Thematic Network is aimed at ensuring that developments critical for the improvement of VTRs are performed rapidly and in a co-ordinated way in Europe. Its objectives are:

– to share knowledge about existing computer simulation techniques for multiscale modelling
– to co-ordinate efforts, in order not to duplicate codes, routines and results, but, on the contrary, combining them for better efficiency
– to apply simulation techniques developed in other fields to the study of radiation effects
– to set up benchmarks, in order to compare existing simulation techniques
– to define and carry out, in collaboration with other partners, *ad hoc* experimental programmes to validate their simulation tools
– to identify realistic future developments and applications of multiscale modelling, inside and outside the nuclear domain, thereby identifying the directions in which to concentrate efforts.

B. Work programme

The work programmes of the seven technical areas (TAs) of ITEM deal mainly with recommendations, proposition of simulation methods and their improvements, establishment of links between different simulation methods as well as with simulations and experiments. The main points are described hereafter:

Website and Database Construction and Maintenance

- Setting up a website
- In order to favour the spreading of multiscale modelling activities in Europe, the Network creates a database (European Database for Multiscale Modelling, EDAM) containing the main data required to carry out multi-scale simulation of usual materials : such as inter-atomic potentials, migration and formation energies of point defect clusters, binding energies between defects and dislocations, parameters for dislocation dynamics, etc. At first, EDAM has to be filled in only with data provided by the mem-

bers. Later on, the main laboratories worldwide involved in multi-scale modelling will be invited to complement it with their data. The database will be freely available for any laboratory in the world on the network website.

Radiation Damage Modelling

- Proposal of a method to allow for electron-phonon coupling in simulation of displacement cascades.
- Identification of the mechanisms controlling the mobility and trapping of small interstitials clusters in pure elements (Fe (bcc), Ni (fcc), Zr (hcp) metals and covalent Si, etc.) binary systems (Fe-C, Fe-Cu, Zr-H, etc.) based on empirical potential or *ab initio* calculations.
- Recommendations on the application fields of different methods (kinetic Monte Carlo, rate equations) for simulating the long-term evolution of radiation-induced damage.
- Proposal to improve methods to allow for stress-effects and temperature gradients on the formation of irradiation-induced defects.
- Comparison of different methods to characterize at the atomic scale the interactions between dislocations and irradiation-induced defects. Recommendation on their application fields will be make. The network will also provide a consensual agreement on the best way to introduce temperature in these simulations.

Simulation of Mechanical Properties of Single Crystals

- An evaluation of the different possible approaches to treat boundary condition issues will be proposed, in order to widen the field of application of dislocation dynamics codes and improve their accuracy. The possibility to couple such simulations to Finite Element codes will be evaluated too, thereby linking the work with the activities of TA IV.
- Identification of the best method to simulate structural hardening in irradiated and non-irradiated materials.

Polycrystal Simulation Methods

- Comparison of atomic simulations of defect-defect interactions and identification of the elementary mechanisms and transport coefficients to be included in mesoscopic codes.
- Connection with different groups working on large-scale molecular dynamics simulations in order to identify a common simulation strategy.
- Elaboration of one or more reference mesoscopic simulation models to include different classes of coarse-grained defects (dislocations, grain boundaries, microcracks, displacement cascades) into one unified framework. The possible link with macroscopic (finite-element) codes, also in terms of new and/or improved constitutive relations, will be defined, in connection with the activities of TA III. The opportunity of exploiting parallel computing for mesoscopic modelling will also be discussed.
- Formulation of a reference multiscale model by examining and comparing existing macroscopic models of materials response to an external load (thermal, mechanical, radiation). Such a multiscale model will include all the relevant information obtained from the atomic- and mesoscopic-level simulations, and will be tested in one or more of its possible practical implementations, also in the framework of massively parallel computing, on one or more selected benchmark problems.

Multiscale Modelling Applications

- Identification of the VTRs of greatest importance and interest to concentrate efforts. This will be done by considering all the VTRs under development in Europe.
- Identification of advanced systems to properly couple both existing and newly developed codes. The aim of this task is to make sure that next generation VTRs will be more efficient from the computational standpoint.
- Introduction in the VTR chosen of the developments achieved within the other TAs.

Experimental Validation

- Identification of adequate experimental techniques suitable to give conclusive results comparable with computer simulation out puts.
- For selected cases, centres devoted to experimental activities and, if needed, also other centres, will perform planned experimental programmes for the validation of the simulation. Within the Network the results will be analysed and discussed. The effectiveness of the experiments in creating a feedback between theory, computer simulation and experimental observation will be evaluated.
- Consolidation of the knowledge on techniques capable of either transforming the experimentally measured magnitude into information directly comparable with the simulation, or predicting what type of response will the simulated object give when observed experimentally (simulation of the electron microscope image produced by a simulated defect, calculation of the positron lifetime in a simulated vacancy cluster, etc.). Such techniques exist but can be still improved and optimised, new ones could be developed.

Phase Stability and Kinetics of Phase Transformations in Alloys under Irradiation

- Development and parameterization of inter-atomic potentials, the study of the mobility of small interstitial clusters and the study of their interaction with dislocation.
- Development of modelling techniques for precipitation and order-disorder phase transformations in multi-component alloys. Various enhanced or induced phase transformation will be studied (precipitation, intergranular segregation, etc.).
- Development of new simulation models or techniques to deal with elastic effects, incubation time for precipitation under irradiation, heterogeneous phase transformations.

C. Main achievements

The construction of the ITEM network permitted gathering some of the main actors in the field of multi-scale modelling of materials and radiation damage simulation. Thus, a scientific European community has been built. A larger scope has been covered from atomic simulation (at different levels with *ab initio* molecular dynamics and atomic Monte Carlo) up to mesoscale and mechanic modelling.

This section describes the main achievements: workshops, setting up of the EDAM database, best-practice guidelines and preparation of the PERFECT proposal.

C.1 Workshops

In addition to the kick-off meeting and the first-year plenary meeting, three technical workshops have been organised related to the TAs II, III, IV and VII. During these successful informal workshops based on high-quality presentations, a large part of the time was dedicated to discussions.

Two workshops was organised jointly by TA III and IV in Todi and Dijon (the so-called “Colloque franco-italien sur la micromécanique des matériaux”). It brings two different scientific communities which are not used to meet in their regular scientific activities. These two communities are the plasticity one (interested in dislocation structure and properties and dislocation dynamics) and the mechanics one (interested mainly in polycrystal simulations). This has been a particular occasion for discussions about the possibility to carry out multi-scale simulation of the deformation of materials from the atomistic description, up to dislocations, and continuum mechanics.

These workshops were open to non-member colleagues of ITEM (with their own financial support), which has allowed to enlarge and enrich the discussions. It was also an opportunity for PhD students to learn about the fields of plasticity and mechanics.

TA II has organised a workshop on different simulation scales illustrated on model alloys. The following materials and systems have been discussed: description of primary defects in Fe-P (with some results obtained partially within the PISA European project) and Fe-C, defect production and interaction in Fe, Cu and Zr, long term damage evolution in Fe and FeCu.

TA VII has set up a workshop on the difficulties to simulate phase transformation in alloys (especially multi-component alloys) under irradiation. It was concluded, that the developed models can take advantage of the quantities determine by MD or *ab initio* for example (within WP2) and have to be linked with experiments.

Discussions during these workshops have put into evidence that it will be almost impossible to perform dedicated simulation developments or experiments within the ITEM context. Nevertheless, new results have been provided by exchanges between on going work within the framework of other research projects (such as REVE, SIRENA, PISA).

These discussions have constituted the preliminary work for the elaboration of the Euratom PERFECT proposal.

C.2 Deliverables

The table bellow summarises the final status of the different deliverables.

Among the 31 technical deliverables, 14 of them have been produced and are given in Annex to this final report, which correspond to about 50 % of the provisional work.

The deliverable list was very ambitious for several reasons. First of all, no work is supported by ITEM itself, which was known as the rule of the network. In fact, the construction of the database or the establishment of recommendations were not so easy to perform and were not straightforward. In fact, to obtain a consensus on some open questions was difficult and for some other points the answers were not known at this point.

These points are illustrated and developed by the following examples.

One of the items of the EDAM database was the empirical potentials and their assessment with the different physical properties predicted, such as defect formation energies, phonon dispersion curves, dislocation core structure. These data were not all available for the dif-

ferent a priori interesting empirical potentials, even for Fe, which was the material with the larger amount of effort in the material modelling scientific community. Furthermore, for Fe, some potentials have been published in 2003 and 2004, constructed with a new strategy: some *ab initio* calculations in particular for self interstitial stability were considered in the fitting procedure; which has conducted to Fe potential with right interstitial stability as well as a screw dislocation core in agreement with *ab initio* calculations and experimental observations for the first time. This comparison on Fe potential is the object of a joint review article that will be published in the special *Journal of Nuclear Materials* devoted to PERFECT.

The mobility and trapping of interstitial clusters in Fe (corresponding to the deliverable D5) is not yet solved, even with the large effort involved in PERFECT. The important progress has been obtained in PERFECT, with the establishment of new interstitial configurations which are sessile, contrary to the previous common opinion of glissile interstitial clusters which can migrate easily. These new sessile configurations will have important consequences on the modelling of damage accumulation which in fact will be exploited within the next PERFORM 60 European project. The sessile interstitial configuration work has been the object of a nice joint EDF-SCK-CEA paper published in 2008 in *Physical Review Letters*.

Another important point is the deliverables of the TA V on multi-scale modelling applications. The critical review and comparison of different methods for linking in a modular computational system different codes and for setting some recommendations for better computational performance has been the object of both the integration and the physics-modelling sub-project of PERFECT which has produced RPV2 and INTERN1. The comparison of the different methods, atomic kinetic Monte Carlo, object kinetic Monte Carlo, event kinetic Monte Carlo and rate theory, has been just finalised into a joint review article that will be published in the special *Journal of Nuclear Materials* devoted to PERFECT.

List of deliverables						
N°	**Designation**	**Initial date of the delivery**	**Nature**	**Dissemi-nation**	**Responsible**	**Status**
D1	Network website	Month 6	O	CO	Domain	Done
D2	European Database for Multiscale Modelling (EDAM)	1 : Month 12 2 : Month 24	Da	PU	Domain	Partially done
D3	Intermediate and final progress reports for TA I	Every year	Re	CO	Domain	This final report
D4	Method to allow for electron-phonon coupling in displacement cascades	Month 24	Me	PU	Bacon	Evaluated – unnecessary, but method available
D5	Model to explain the mobility and trapping of interstitial clusters	Month 36	Me	PU	Bacon	Almost done
D6	Recommendation on methods for long term evolution of irradiation-induced damage	Month 36	Me	PU	Bacon	Done
D8	Method to allow for stresses and temperature gradient in the simulation of radiation damage	Month 24	Me	PU	Bacon	Partially done
D9	Recommendation on methods to characterise interactions between dislocations and defects	Month 36	Me	PU	Bacon	Done
D10	Intermediate and final progress reports for TA II	Every year	Re	CO	Bacon	This final report
D11	Dislocation dynamics method capable of ac-counting for complex boundary-value prob-lems	Month 36	Me	PU	Devincre	Done
D12	Method to simulate structural hardening	Month 36	Me	PU	Devincre	Almost done
D13	Intermediate and final progress reports for TA III	Every year	Re	CO	Devincre	This final report
D14	Definition of atomistic simulation models for defect-defect interaction	Month 12	Me	PU	Cleri	Done
D15	Comparison of results from atomistic simula-tions of defect-defect interaction	Month 24	Da	PU	Cleri	Done
D16	Definition of a reference atomistic simulation model for polycrystal plasticity	Month 12	Me	PU	Cleri	Done
D17	Specifications for a community parallel MD	Month 12	Me	PU	Cleri	SUPRESS

	code for very-large-scale polycrystal simulations					
D18	Recommendation on mechanisms to be included in mesoscopic simulations.	Month 24	Me	PU	Cleri	Almost completed Unified with D19
D19	Definition of integrated methods for mesoscopic simulations	Month 24	Me	PU	Cleri	Almost completed Unified with D18
D20	Comparison of results from different mesoscopic methods for polycrystal plasticity and evolution	Month 48	Da	PU	Cleri	
D21	Specification of a multiscale macroscopic model including microscopic information	Month 24	Me	PU	Cleri	Postpone to month 48
D22	Comparison of results on benchmark problems simulated at the macroscopic level with the multiscale model	Month 48	Da	PU	Cleri	
D23	Intermediate and final progress reports for TA IV	Every year	Re	CO	Cleri	This final report
D24	Critical assessment on the importance of different materials for the present and future interest of the nuclear industry and the degree of knowledge of radiation consequences on them	Month 36	Me	PU	Perlado	Not done
D25	Critical review/comparison of different methods for linking in a modular computational system different codes and recommendations for better computational performance.	Month 36	Me	PU	Perlado	Not done
D26	Comprehensive model for sequential application of multiscale models to a specific material.	Month 48	O	PU	Perlado	Not done
D27	Comparison study of experiments and modelling, and recommendations for further improvement of VTR performances.	Month 48	Me	PU	Perlado	Not done
D28	Intermediate and final reports for TA V	Every year	Re	CO	Perlado	This final report
D29	Identification of the weak points of the multiscale modelling techniques, on which to focus efforts	Continuous assessment	Da	PU	Malerba	

D30	Recommendations on the best way of validating multiscale modes through experiments	Month 48	Me	PU	Malerba	Done
D31	Complete set of experimental results validating computational results produced by the Network	Month 48	Da	PU	Malerba	Transferred to PERFECT
D32	Recommendation of desirable improvements of computational techniques used to compare experiment and simulation results	Month 24	Re	CO	Malerba	End ITEM And in PERFECT
D33	Development of a new computational technique for experiment/simulation comparison or high optimisation of an existing one	Month 48	Me	PU	Malerba	End ITEM And in PERFECT
D34	Intermediate and final for TA VI	Every year	O	PU	Malerba	Almost done
D35	Method to study alloying effects on the mobility of interstitial clusters	Month 12	Me	PU	Soisson	
D36	Recommendation on methods to simulate the long -term evolution of radiation damage in multicomponent alloys	Month 24	Me	PU	Soisson	Done
D7	Consensual agreement on the best way to deal with phase stability under irradiation	Month 36	Me	PU	Soisson	Done
D37	Method to study alloying effects on the interaction between dislocations	Month 12	Me	PU	Soisson	Done
D38	Intermediate and final progress reports for TA VII	Month 36	Me	PU	Soisson	This final report
D39	Newsletters	Every year	Re	CO	Domain	Not done
D40	Annual reports and cost statements	Every year	Re	CO	Domain Et al.	Partially done
D41	Mid-term report	Month 24	Re	CO	Domain	Final report

C.3 EDAM database

The website (http://item.edf.fr) has been built and it supports the EDAM database. The construction of the latter was not as fast as expected, due to some delay in the organisation of the way to enrich it. Its access was restricted to ITEM members only. EDAM was enriched by the TACs in order to be proposed and discussed with all members by the end of 2003 during the end year 2 plenary meeting.

It was observed after these discussions that the enrichment of the database is not a straightforward task unfortunately. The data were not ready on shelves to be integrated in EDAM.

Furthermore, the issue of the use of the database was an open question. To gather data is a good point of course, but the data are produced by some codes and/or have to be used by some other codes.

C.4 Best-practice guidelines for multiscale simulation

A common work to write best-practice guidelines for multiscale simulation of irradiation effects has been started. A first draft has been written by some members of the network and will be enriched by the other ones in 2004. This document contains recommendations to carry out correctly multiscale simulation of irradiation effects. It deals with errors and uncertainties and proposes test cases for benchmarking. It follows the work performed within the thermo-hydraulic community, in the framework of the European ECORA project.

C.5 Preparation of the PERFECT proposal

ITEM has helped to build the PERFECT proposal. ITEM meetings started the identification and analysis of key issues to solve to simulate the behaviour of structural material under irradiation. They also pointed out where simulation and modelling can contribute. ITEM has permitted to establish a network of material science laboratories which will partly contribute to future PERFECT project.

The organisation of the ITEM network in technical areas has also been a skeleton for the organisation of the PERFECT project.
The database has been transformed to the different platforms developed which include both database, as well as the different simulation codes.

ITEM meetings and discussions have been a good opportunity to exchange with the different members, in order to better know their expertise field, facilities and possibilities. It constitutes precious information for the definition and distribution of the different tasks in PERFECT, as well as the choice of the partners.

Furthermore, the ITEM website has been used to gather and share some information and documents for the construction of the PERFECT proposal.

D. Dissemination and exploitation of the results

The website (http://item.edf.fr) is a key element for dissemination and use of the results. General presentations of the network and a members list are accessible to everyone through it.

Access to the database and presentations made during the different workshops are restricted to the members. This access permits to look for details information and to learn about other simulation methods or experimental techniques. It should promote interaction between the different simulation communities and the experimental ones.

E. Conclusions

The ITEM network has successfully started with the setting up of the EDAM database and with very fruitful technical workshops. So far, the network has difficulties to launch new research programmes but has started exchanges and coordination between existing ones. A broad multi-cultural community dealing with numerical simulation of materials has been built up.

The network created has allowed building the PERFECT project. Most of the partners of PERFECT were gathered within ITEM. ITEM has been a think tank for PERFECT.

Enrichment of the database EDAM is one of the key actions in order to have a high-quality European database useful for the material science community. EDAM will be improved by agreement among all network participants.

EDAM has been a prototype of data management for part of the PERFECT platforms. In addition, PERFECT (as well as SIRENA) will deliver complementary data to the database.

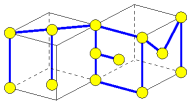
Best-practice guidelines for multiscale simulation have been written by some members of the network. In 2004 they were enriched by the other ones.

Looking back, the success of the ITEM European network was to build a scientific community on radiation damage modelling in Europe, which allowed realising the Euratom PERFECT project. This project permitted to successfully build a first set of multi-scale modelling tools for radiation damage for reactor pressure vessels and internal structure of nuclear power plants. PERFECT has been pursued within a new integrated project, PERFORM-60, in order to continue and improve these developments based on the work previously performed.

In conclusion, the importance of ITEM has been proven by the continued development within the PERFECT and PERFORM-60 EU projects.

ANNEX

Deliverables



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

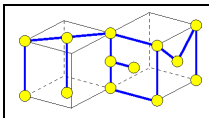
D1: Network website

Author: C. Domain
Date: 20/10/2004
Version 1

The network website has been completed. Its address is: http://item.edf.fr

It contains:

The description of the network
The work packages
The list of tasks
The list of members, with a description of their expertise and their coordinates
The list of meetings organised by the network, with the schedules, minutes of the meeting and presentation when available
Links to various material science websites
Links to some material science and radiation damage conferences



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D2: European Database for Multiscale Modelling (EDAM)

Author: C. Domain
Date: 20/10/2004
Version 1

Database construction

The database EDAM has been organised in different items corresponding to the different simulation scales and experimental validation:

Ab initio
Cohesive models
Primary damage – cascades
Medium term evolution – atomic kinetic Monte Carlo
Long-term evolution – kinetic Monte Carlo and cluster dynamics
Mesoscopic simulations
Polycristal simulations
Experimental irradiations
Codes
Links

The EDAM database has been located on the ITEM website: http://item.edf.fr/edam

The database is protected by login and password:

Login: item
Password: edam2001

Database contents

The structure of the database has been illustrated by some data from EDF, *ab initio* data, some cascade debris obtained by molecular dynamics, and some kinetic Monte Carlo parameters.
Several parameter sets used for dislocation dynamics have been gathered by WP III.

The database contains also several links to material science public web pages and databases (properties of elements, crystallographic structure, article database related to interatomic potential).

Database evolution

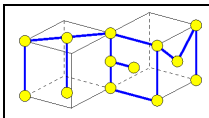
The evolution of the database with data from the members was unsuccessful, and almost not data were received from the members.

Members have already their own source of information, access to electronic journals, or direct search on the network (Google for example) is so powerful to get the information they look for.

In addition, each one has is own way to organise is collected data under their preferred tools and form. Thus a global database within data at the various scales is actually difficult to handle, and such database will be difficult to maintain because of the quick evolution of this field.

Thus, a database collecting more data seems not to be realistic.

And the website and database purpose should be more restricted to collect information on the life of the network: meetings, minutes of the meetings. Actually, the website with all the minutes of the meetings, as well as a large proportion of the member presentations given at the technical meetings contains lots of information and knowledge.



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D7: Consensual agreement on the best way to deal with phase stability under irradiation

Author: F. Soisson
Date: 20/10/2004
Version 1

This deliverable deals with phase transformations under irradiation (precipitation/dissolution of precipitates, order/disorder transitions, amorphisation/recrystallisation, etc.) and with the long-term evolution of composition fields in alloys under irradiation (segregation phenomena). Studies on alloying effects of long-term radiation damage, especially of point defects and point defect clusters are considered in deliverable D36. A first attempt to define a consensual agreement on these two topics can be found in ref. [1] (a more detailed version is in preparation).

1. Rate theories (RT) and mesoscopic kinetic Monte Carlo (KMC) simulations

Rate theories or Clusters Dynamics methods [2] and Mesoscopic KMC (Object [3] or Event [4] KMC) consider only special objects (point defects, solute atoms or clusters), rather the complete composition fields. As a consequence, they are mostly useful to study radiation damage in pure metals and dilute alloys (see D36). However in simple cases, precipitation kinetics can be modelled (ref. [2] for copper precipitation in iron).

Because of there low computational cost, it could be extremely useful to extend these methods to dilute multi-component systems, but this would require a better thermodynamic description (e.g. of the formation energies of multi-component precipitates).

2. Atomistic KMC

Most of the AKMC methods are based on rigid lattice approximations. In order to get a physical kinetic pathway, realistic diffusion properties must be reproduced (i.e. realistic jump mechanisms, migration barriers, correlation effects, etc.) [4]. Point defect jump frequencies can be computed according to various energetic models (e. g. constant pair interactions [4,5] or semi-empirical models [5,6]).

By comparison with RT and MKMC and because of its atomic nature, AKMC gives a better description of the diffusion and thermodynamic properties. It can also provide a detailed description of the micro-structural elements (e.g. precipitates, interfaces, etc.). It does not require *a priori* assumptions on the possible phases or objects which can be formed: in

some multi-component systems (FeNbC [7] or AlZrSc [8]) unexpected transient non-equilibrium phases have indeed been observed.

In the 1990s, AKMC simulations of phase transformations mainly focused on the competition between ballistic mixing and acceleration of diffusion, which drives many order/disorder processes under irradiation [9, 10]. Recently, other specific irradiation phenomena (such as point defects formation, recombination, annihilations at sinks) have been included in AKMC simulations to study radiation-induced segregation and precipitation kinetics in alloys [5].

An important limitation comes from the rigid lattice approximation. First attempts have been made to include long-range elastic fields in AKMC on rigid lattice, e.g. to study their effects on the kinetics of heterogeneous precipitation on dislocations [11]. AKMC with EAM potentials and relaxations of atomic positions (both at stable and stable-point positions) have been performed to study diffusion properties of Au-Ni and Ni-Al alloys. They involved a full computation of the attempt frequencies in the frame of Vineyard's theory. However, these techniques still appear to be too time consuming to simulate phase transformations kinetics, especially under irradiation. First simulations of precipitation kinetics during thermal ageing, with relaxation of the stable atomic positions, have been performed [12]. Attempt frequencies and saddle-point binding energies can be fitted on experimental data. This method is still in development at Augsburg University, and will be applied to alloys under irradiation in the framework of Perfect Programme.

3. Mean-field kinetics

A Cahn-Hilliard approach has been applied to binary alloys under irradiation. It starts from continuity equations for the various chemical components [11]. It takes into account the thermal diffusion (enhanced by point defect super-saturation), ballistic mixing and coupling between point defects and solute fluxes. Linear stability analysis of compositional fluctuations and derivation of an effective free energy functional give the dynamical phase diagram under given irradiation conditions. Positives and negatives shifts of the phase boundaries are possible. By comparison with other methods, it is almost immediate and gives important analytical results. The main drawback is that it seems for the time being limited to binary alloys.

As for AKMC, Mean-Field Kinetics on rigid lattice start from an atomistic description of diffusion. But they deal with averaged concentrations on lattice sites and the activation energies of point defect jumps are computed using various mean-field approximations [15,16]. These methods give an accurate description of thermodynamic and kinetic properties, they can be easily applied to concentrated and multi-component systems, and they can take into account irradiation effects. Furthermore they are usually more rapid than AKMC simulations. They have been successfully applied to radiation-induced segregation phenomena in austenitic steels [15,16]. However thermal fluctuations are not taken into account in these deterministic approaches: they cannot be used to simulate kinetics of nucleation processes. Moreover, Mean-Field Kinetics are still in development to include diffusion correlations effects [16], which are naturally taken into account in AKMC simulations.

4. Amorphisation/recrystallisation

Irradiation effects on martensitic transformations have been observed in Ni-Al and Ni-Ti alloys. These systems show a pronounced shift of the martensitic transformation temperature

after high-energy irradiation. The case of Ni-Al alloys has been investigated using molecular dynamics simulations [17].

5. Conclusions and perspectives

The previous methods are clearly complementary tools. MKMC and rate theories are especially suitable for dilute alloys, AKMC and mean-field kinetics on lattice for multi-component and concentrated alloys. The main advantage of KMC simulations is that they include time and space correlations, however they are more time consuming than mean-field techniques. A common challenge will be to give a better description of elastic interactions. The coupling with *ab initio* calculations, in order to get more reliable data on diffusion properties, will be very important. Typical examples have been given by *ab initio* studies on the dumbbell migration in pure iron [18, 19], or vacancy migration in iron-copper [20, 21].

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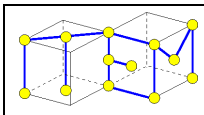

ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D11: Dislocation dynamics method capable of accounting for complex boundary-value problems

Author: B. Devincre
Date: 20/10/2004
Version 1

3D simulations of dislocation dynamics (DD) have been identified, in the last few years, as one of the key ingredient of multiscale material modelling. Their objective is to fill the gap between the atomistic and fully continuum studies, in conjunction with theoretical modelling. Hence, they are the necessary piece of a coarse graining process between atomistic simulations (simulations with a real predictive character, but working at a very small scale) and continuous models (engineering tools including many phenomenological aspects).

Three-dimensional DD simulations do not yet have a very long history. They have emerged in the 1990s, as a consequence of the increased computing power available to materials scientists. DD simulations essentially compute the properties of dislocation populations based on the elastic theory of dislocations. Their lower limit of validity in terms of length scale is then set by the breakdown of linear elasticity near dislocation cores, at a few inter-atomic distances. The largest length scale of interest is that of the representative volume element for the problem under examination. There is no definite value set for this quantity, which can go from a few nanometres in thin epitaxial layers to several tens of microns, or sometimes more, for the mean free path of dislocations in single crystals. A particular feature of DD simulations, which is not currently found in other simulations methods, resides in their explosive character. The dislocation density increases by orders of magnitude during plastic flow, which makes the times per step more and more demanding in terms of computing load as plastic strain increases. The evolution of DD simulations has, therefore, been closely related to that of the currently available computing power and to the code algorithmic efficiency.

In 2001, the ability to account for complex boundary conditions was identified as a key point for the future development of DD simulations. Within the context of ITEM, 3 axes of researches have been developed:

Periodic boundary conditions

Periodic boundary conditions (PBC) are a standard trick for modelling if one wants to restrict a simulated reference volume. In short, the problem in DD simulations is the following. Dislocations glide in a periodic array formed by a simulation cell and its replicas. Every time a portion of dislocation line crosses a boundary between two cells, which it does simultaneously in all cells, it emerges in all cells at the equivalent position on the opposite boundary. A balance of fluxes is then established through all the internal interfaces of the simulated volume. However, the application of PBCs to linear objects is known to lead to spurious self-interactions. In the case of dislocations, portions of loops may self-annihilate with replicas having emerged after a certain number of boundary crossings. Self-annihilation may reduce the mean free-path of dislocations; this can have drastic consequences that have not been considered so far in the context of DD simulations. A too short effective mean free-path affects the density of mobile dislocations and their storage rate and, hence, both the arrangement of the microstructure and the strain hardening properties. In the last Three years several methods that have been developed in order to control this artefact. These methods apply to DD simulations in which, like in real crystals, the slip plane spacings obey crystallographic relations.

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Surface, interface and interphase boundary

Over the years, different methods have been developed to calculate the state of mechanical equilibrium in a dislocated finite body. More recently, the questions, are this methods useful and how can they be implemented in DD simulation was a mater of debate. In the context of ITEM, works have been initiated to test and improve existing solutions. Such solutions are based on the “superposition method” and the “discrete-continuous model” (DCM). Although the underlying physical problem is the same, and therefore also its mechanical solution, these methods follow different strategies. As a consequence, it is not always clear how and where

exactly they differ or are similar. Our purpose was at the end to establish domain of application.

In terms of CPU, the comparison of the DCM and the superposition method is usually in favour of the last one. Indeed, the DCM requires a more detailed meshing (i.e. more elements with many nodes and Gauss points) and, therefore, larger computations. Also, the superposition method requires only data transfer between the DD and FE codes at the boundary elements of the mesh, whereas, the DCM imposes data transfer everywhere. From a practical viewpoint, the implementation of DD-FE coupling based on the superposition approach is easier to realise, but this last point may depend on the FE code that is used.

From a theoretical point of view, the two approaches are perfectly equivalent with one exception; calculations in an elastically anisotropic medium can be realised much more easily using the DCM approach. Indeed, for the superposition solution to be efficient, analytical forms are required for the displacement field of dislocation segments and for anisotropic media a general solution does not exist. In contrast, elastic anisotropy is easily taken into account with the DCM by only changing one input of the DCM calculation: the tensor of elastic moduli of the considered material. As a result, computing times are virtually the same for isotropic and anisotropic simulations.

To obtain the stress at an arbitrary position in the simulated body, Fes are using shape functions, which interpolate the stresses calculated at Gauss points. A basic hypothesis of the classical FE method imposes that shape functions are continuous within the elements. Since the dislocation fields vary as the inverse of the distance to the line, the resulting singularities at the dislocation line cannot be exactly accounted for. An immediate solution to this problem consists in refining the mesh. Alternatively, it as been shown than for each existing methods, one can substrate analytical forms for dislocation stress field at short distances. This virtual additional solid force can be regarded as a constitutive trick reducing as much as possible field singularities when needed.

Lastly, the existence of elastic inclusions in the simulated body impose additional computations to the superposition approach and makes it less attractive by comparison to the DCM scheme, since the latter is transparent to this problem. Studies dealing with this important aspect were published recently.

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Simulation code optimisation and improvements

As mentioned in the introduction, numerical performance of DD simulations is an essential issue. This is why, in addition to the two above objectives defines at the beginning of ITEM, the more general question of code optimisation was explicitly discussed.

In short, two important ideas came out of the discussions:

– Present and future 3D -DD simulation code must be parallelized to run on cluster architecture. This technical aspect is a necessary in order to tackle the technical challenge associate to DD simulation. Most of the problem of interest suppose than one can run simulation with more than a million of dislocation segments. Those calculations cannot be run on a conventional workstations. Today, all the groups involve in ITEM and running 3D-DD simulations have parallelized (partially or totally) their code.

– Alternatively, it was proposed that reduction of dimensionality can be an alternative for many problems. This is why it was proposed to build up 2D-DD simulations were all the constitutive rules are tested by comparison with the results of 3D simulations. Hence, one can run simple and dedicated 2-D simulations with real predictive properties. Demonstration of this approach has been made for the problems of forest hardening and Hall-Petch effects in FCC materials.

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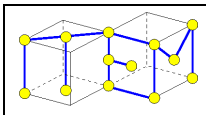

ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D12: Method to simulate structural hardening

Author: B. Devincre
Date: 20/10/2004
Version 1

Following conventional textbook presentations, the problem of hardening has been differentiated in four parts, each corresponding to specific mechanisms and properties. One must realise that the contribution of ITEM contractors to this general problem can only be partial and was mainly devoted to the question of the existing mesoscopic simulation improvements. Our ultimate goal is, of course, a better comparison of simulation results to experiment in order to improve the general understanding of this complex phenomenon.

Impurity and solution hardening

In the last years, a kind of consensus was made regarding impurity and solution hardening. The length scale of DD simulation being much larger than atomic spacing, DD simulations cannot account directly for chemical effects and the latter must be introduced at a mesoscopic scale with the help of phenomenological equations fitted either on experimental or atomic simulation data. A typical Arrhenius form initially suited for representing dislocation motion by a kink-pair mechanism appears to do the job in many cases (G. Schoeck, Phys. Stat. Sol. 8, 499, 1965; U.F. Kocks, A.S. Argon, and M.F. Ashby, Prog. Mat. Sci., Vol. 19, p. 1, 1975). Nevertheless, each material may exhibit very different properties and the thermodynamic justification of such approach must always, *a priori*, be verified.

Articles:

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Precipitation hardening

This problematic is of first importance regarding alteration of mechanical properties induced by irradiation. This is why such aspect was discussed in connection with the results of 'Radiation Damage Modelling' workshop group in ITEM. Several methods have benne developed in the 1970s to study this problem. Efficient 3D simulations of dislocation dynamics in large volumes and during large time scales gave access to a deeper insight into this problem. Most of the progress made during the last years is connected to the improvements made in the boundary value problems in DD simulations (see deliverable D11 of ITEM). In short, more sophisticate calculations are today reproducing results, which look the same as those obtained in the 70s with simple line tension models. Nevertheless, 3D –DD simulations have nowadays a real predictive character and can account for non-planar effects, like precipitates bypassing with cross-slip.

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Forest hardening

In a given slip plane, the main obstacle to dislocation motion arises from junction formation with a forest of non-coplanar trees. Theoretical and experimental estimates indicate that the resulting forest hardening is responsible for most of the work hardening. Whereas the critical stress for breaking a single junction can be calculated within some reasonable approximations (with MD and DD simulations), estimating the macroscopic average strength resulting from all types of junctions is not a simple exercise. Indeed, one has to account for a spectrum of obstacle strengths that depends on a number of geometrical parameters. Actually, dislocation

theory does not provide any general answer to this question of composition of obstacle strengths which is an open field investigated by DD simulations in the last years.

Main progresses made by the groups involved in the ITEM network on this subject are in summary: The simple Taylor relation accounts for most of the yield and flow stress in pure fcc metals. No such correlation is found between stress and the primary density, that is the density of forest obstacles responsible for the self-interaction, at least during monotonic deformation tests. Indeed, during the cyclic deformation of single crystals, very large densities of primary dislocations can be accumulated and the situation is quite different. The logarithmic drift of the pseudo-constant alpha in the Taylor equation is a signature of short-range interactions involving line tension effects that is essentially junction formation. Due to their mainly elastic nature, these interactions are not much sensitive to temperature, strain rate and core effects. The spatial distribution of the forest density undergoes significant changes along a stress-strain curve. The reason why the Taylor relation holds irrespective of these changes and is only sensitive to the average forest density is not well understood. Results of DD simulations are now transferred in the form of constitutive laws and they provide physically justified inputs for Finite-Element simulation.

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Interface hardening

Dislocation slip confinement at surface, interface or Grain boundary is also an essential mechanism of hardening. It is connected to the complex question of size effects in plasticity and it appears to be an emerging subject since it is in relation with the development of nanomaterials, MEMS, thin films technology, ultrafine-grained polycrystals, etc. The possibility to

consider those questions with DD simulations is directly connected to the improvements made in DD methodology regarding the question of boundary value problems (see deliverable D11 of ITEM). In the last years, work as been made to show that DD simulation can successfully reproduce all the complexity observed experimentally. The next step, still to be made, is really the interpretation of simulation results in order to propose models useful for material design.

Articles:

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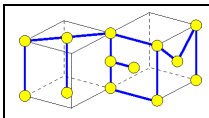


ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D14: Definition of atomistic simulation models for defect-defect interaction

Author: F. Cleri
Date: 20/10/2004
Version 1

1. Introduction

The description of microstructure evolution under external forces, e.g. temperature and stress, is a central subject of materials science. By materials microstructure we intend any extended defects beyond point-like ones: line defects (dislocations, disclinations), two-dimensional (grain boundaries, phase boundaries) and three-dimensional defects (inclusions, precipitates, voids, microcracks). All such defects can occur into different conditions as a function of temperature, stress, strain and strain-rate. Notably, non-point-like defects are not in thermodynamical equilibrium, and can transform into one another under the action of both the external forces and the internal driving forces. The macroscopic material behaviour resulting from such a complex interaction is that of a continuous flow (albeit very slow in most cases) and encompasses deformation, recovery and different stages of recrystallisation.

Macroscopic deformation results from a complex interplay of microscopic phenomena under strongly non-equilibrium conditions, making new experiments more likely to add new problems instead of solving existing ones. Clearly, much work is yet to be done also on the theoretical side, given that after the introduction of the concept of dislocation about seventy years ago we are still lacking a fundamental theory of the plastic response.

Most mesoscale-level microstructure models (such as vertex-tracking models, Potts model, phase-field model) describe the evolution of the system without making reference to explicit length and time scales: these must be provided by atomic-level simulations. More generally, the basic input ingredients of any such model, e.g. interface mobility, bulk and interface diffusivity, interfacial energy, as well as the elementary kinetic mechanisms, e.g. boundary migration and sliding, dislocation patterning, dislocation-grain boundary interaction, and so on, have an *atomic-scale* origin. In order for the mesoscopic model to be genuinely predictive, all such quantities must be generated from appropriate atomistic modelling. In the following we will outline the basic philosophy and some results of a coupled atomistic-mesoscopic strategy.

2. Atomistic models of extended defects and their interaction

We start from the hypothesis that the nucleation, motion and interaction between extended defects is at the basis of the mechanical response of materials and the key to modelling microstructure evolution. At the mesoscopic level we distinguish between two classes of elementary events during microstructure evolution: *geometric* and *topological* events.

The class of geometric events includes, e.g., grain-boundary migration and diffusion, grain rotation, void growth and shrinking, dislocation glide and climb, etc.: all such events are characterized by the topological invariance of the microstructure, i.e., the interwoven network of extended defects changes in shape but not in connectivity. Grain boundaries can shrink or elongate, grains and dislocations can grow or shrink, but each microstructure element preserves the number and ordering of its neighbours. Such geometric events are typically related to atomic diffusion, either in the bulk or along surfaces and interfaces, and are thermally activated.

On the other hand, *topological* events imply a drastic change in the number and connectivity of the microstructure. For example, if we focus on grain boundaries in 2-D, the only such events possible are the so-called *T1* and *T2* transformations, namely four-grain switching and disappearance of a three-sided grain, respectively (see Fig. 1). After each *T1* event two grains in the microstructure gain one side, while the other two loose one side. After several *T1* events, some grains will be left with only three sides: for them no further *T1* can take place since a two-sided grain is both a physical nonsense and a mathematically singular object. Then, the three-sided grain continues to shrink diffusively down to a critical radius, below which it disappears with a *T2* transformation, leaving a single triple junction behind itself (see Fig. 1).

Whenever a set of evolving dislocations is considered aside of the grain boundaries, the transformation of a dislocation wall into a grain boundary (and the opposite event as well) also fall into this class, since a new set of triple junctions is thereby generated or destroyed and the defect network topology is changed.

A topological event represents a *singularity* for any macroscopic continuum description. However, at the atomic scale all such events occur continuously (eventually overcoming an energy barrier) and in competition with the geometric (diffusive) events. Ideally, *T1* and *T2* topological events take place only at triple junctions while diffusive events involve grain-boundary atoms. While diffusive processes have been already studied in some detail, at least for a few relevant cases, almost nothing is known about the former. Such important parameters as the cut-off distances below which a *T1* or *T2* event takes place, are completely unknown at the atomic scale since they crucially depend on the (equally unknown) triple-junction atomic structure and energetics.

3. The problem of boundary conditions

The key issue in the atomic-level description of a system under an externally applied mechanical load, i.e. under a given state of macroscopic stress, is to ensure that the border conditions of the simulation cell properly represent the type and magnitude of the external load.

This problem is closely connected with the suppression of system-size effects such that the far-away stress and strain fields surrounding the region of interest, e.g., one or more dislocations or microcracks, converge to the proper linear-elasticity limit for any given state of loading.

Since any practically realisable atomistic system is of very small size, real-world extended systems are usually represented in molecular dynamics (MD) simulations by means of periodic border conditions (BC) applied to the box enclosing the atomistic system. Periodic BC may, however, induce spurious effects due to the fact that the atoms in the box interact with each other and with all their periodic replicas. For long-range fields, such as the elastic field of a dislocation, which decays as r^{-1}, or that of a microcrack, which decays as $r^{-1/2}$, this approach leads to the so-called problem of the image forces, namely the defect fictitiously interacting with itself infinite times, leading to a divergence in the total energy. In the recent literature this problem has been usually circumvented by studying particular clusters of defects, e.g. a dislocation dipole or quadrupole with properly arranged Burgers vectors, such that the long-range stress fields approximately cancel out. Clearly, one should aim at a more general framework in which, moreover, consistency with macroscopic continuum mechanics is ensured.

The problem of simulating an atomistic system in a well-defined state of *homogeneous* stress was boldly solved by the so-called Parrinello-Rahman (PR) formulation of constant-stress MD. The PR method is a special type of periodic BC in which the total stress (a Cartesian tensor) acts as a nine-component constraint determining the dynamic evolution of the size and shape of the (periodic) simulation box. However, in a discrete system the total stress can be obtained only as a sum over some 'atomistic' stress tensor, which is derived by breaking down the total stress into the contributions of equivalent atoms. By contrast, defects such as dislocations or microcracks tend to concentrate the stress field, thus making the system elastically inhomogenous. Consequently, the PR method is suitable only for a homogenous system.

Alternate forms of BCs have thus been devised to deal with extended defects in atomistic systems under a mechanical load: (a) *constant-displacement* or fixed-boundary BC, in which the border atoms are held in the strained configuration or, equivalently, periodicity is preserved across the border for the whole duration of the simulation; (b) *constant-traction* BC, in which periodicity is removed all around the borders and the equivalent forces necessary to preserve the state of deformation are computed and applied to the border atoms during the simulation. The above classes of BC correspond, respectively, to the displacement-boundary value (or Dirichlet) and to the stress-boundary value (or Neumann) formulations of continuum mechanics problems, in which either displacements or stresses are prescribed along the system borders.

The group of F. Cleri (ENEA, Italy) has developed a general atomistic simulation scheme to apply a general external load to a finite-size, non-periodic atomistic system while reproducing the loading conditions of an infinite continuum. Such a scheme, valid also at finite temperatures, is based on the definition of an atomic-scale *surface traction* perfectly equivalent to its continuum-mechanics analogue. The surface traction is applied as a constant external force to the free (i.e., non-periodic) borders of the atomistic system, hence the denomination of "constant-traction BC". As an additional benefit, the constant-traction BC under zero external load represents a practical way to embed an intrinsically non-periodic atomistic system, e.g. a dislocation or a triple junction, in a virtually infinite medium.

The method can be applied to any atomistic system enclosing one or more defects (dislocation, grain boundary, etc.). The region containing the defect(s) must be large enough to rule out interaction effects between the heterogeneity and the system borders. The system borders are considered free during the simulation. A force will be applied to the free borders, to be calculated from the foregoing procedure. In practice, the constant-traction MD method works in two separate steps: (1) the modulus of the average missing force is obtained in a separate bulk calculation at finite temperature, during which the atomic force across any dividing plane $\{hkl\}$ across which periodicity was removed can be calculated; (2) the surface traction is applied during the subsequent simulation to each border atom with a constant modulus corresponding to the given value of T and directed as the opposite of the instantaneous resulting force on each and every atom in the system, $\boldsymbol{f}_i$.

This method has been adopted as the basic tool for studying defect-defect interaction. In the following we describe a few examples of its application.

For more details see F. Cleri, *Simulation of mechanical loads in molecular dynamics simulations*, Phys. Rev. B 65, 014107 (2002)).

4. Example 1: Triple junctions and their interaction

As a first example, we quote a study of the properties of isolated triple junctions and their interaction in originating the *T1* and *T2* elementary events, jointly carried out by F. Cleri and co-workers at ENEA Casaccia and L. Colombo and co-workers at the University of Cagliari. The particular triple junction chosen in this first study was the multiple-twin Σ3-Σ3-Σ9 in Si, schematically shown in Fig. 2a. The crystals B/C form a {221}{221} (so-called Σ9) grain-boundary, while A/B and A/C form two non-equivalent {111}{111} (or Σ3) twin boundaries. In general, due to the very low degree of spatial symmetry in triple junctions the translational invariance is broken in one or two directions. In the case of Σ3-Σ3-Σ9, the system is periodic in the direction of the polar axis <110>, namely the x-direction in our reference system. The missing periodicity in the y- and z-directions was accurately supplied by constant-traction BC, which ensures the embedding of the system in a truly infinite Σ3-Σ3-Σ9 tricrystal. The atomistic configuration of the Si tricrystal was constructed firstly by cutting away a triangular sector from the configuration of the Σ9 boundary, as shown schematically in Fig.2; the empty region was filled with a portion of a crystal cut and rotated so as to generate two non-equivalent Σ3 boundaries. The resulting structure was equilibrated at about T=1000 K and then quenched down to T=0 K by means of molecular dynamics simulations. Directional bonding is Si was described with the Stillinger-Weber interatomic potential. We obtained excess energies, volumes, and stresses per unit length of several triple-junction configurations: we demonstrated quantitatively that a triple junction (see Fig. 3) is a true line defect, in many respects similar to a disclination defect.

For more details see: S. Costantini, P. Alippi, L. Colombo and F. Cleri, *Triple junctions and elastic stability of polycrystalline silicon*, Phys. Rev. B 63, 045302 (2001).

The study of the interaction between triple junctions as giving rise to topological changes in the Si polycrystalline microstructure was then started (see Fig. 4). In particular, the atomistic

mechanism underlying the *T2* topological event was studied. The objective was to calculate the critical size below which the three-sided grain becomes unstable and to identify the mechanism through which the instability sets in. The initial geometry is still the Σ3-Σ3-Σ9 triple junction of Fig. 3, into which a cylindrical grain of increasing size (radius between 2 and 4 a_0) was inserted; such a small grain preserves a rather curved boundary due to the strong tension that establishes with the surrounding grains. Each simulation started at T=0 K. The temperature was gradually increased in steps of 200 K from T=0 K up to 0.8 of the Si melting temperature, T_m=1685 K. At every step the constant-traction to the borders was re-computed, the lattice parameter suitably rescaled and the system was equilibrated for about 6 ps. Preliminary results indicate that the critical radius r_C is between 3 and 4 a_0. The instability mode is a progressive disordering of the inner grain, initiating from the boundary, until the grain has become alike to an *amorphous* particle. After amorphisation has taken place, the particle crystallizes back by rapid growth of the adjacent grains, restoring the original Σ3-Σ3-Σ9 triple junction.

It is important to stress that atomistic simulations of the *T2* process (and of the *T1*, still under elaboration) can provide an absolute length scale to mesoscopic models, whose only scale-dependent quantities are represented by the cut-off radius for each kind of topological event. Concerning the absolute time-scale, the whole process of amorphisation plus recrystallisation takes place over times of the order of a few tens of picoseconds: consequently, the *T2* process must be considered *instantaneous* from a macroscopic point of view and practically with a zero energy barrier, i.e. the triple-junction interaction poses no additional barrier to grain-boundary migration. Since junctions among higher-energy boundaries than twins and low-angle tilts in Si tend to be disordered and amorphous-like. Then, such a conclusion can be generalized to any kind of triple junction in Si. The observed feature of amorphisation of the inner grain is, however, specific to Si and it is quite possible that for other systems, e.g. metals and metallic alloys, the instability mechanism does not involve amorphisation. In such cases it is possible that, for some grain-boundary combinations, triple-junction interactions could represent an energy barrier to boundary migration.

For further details see: F. Cleri, G. D'Agostino, A. Satta and L. Colombo, *Microstructure evolution from the atomic scale up*, Comp. Mat. Sci. 23, 20 (2002)

5. Example 2: Interaction between a running micro-crack and a set of grain boundaries

Grain boundaries are usually considered a major source of degradation of the electric, thermal, and mechanical properties of polycrystalline semiconductors. In particular, GBs can represent a source of intrinsic fragility, being in general less strongly bound than bulk atomic planes. Intergranular fracture, i.e. the propagation of a crack along the GB plane between two grains, has been repeatedly investigated, from both a continuum mechanics and an atomistic point of view. In this study, concerning again polycrystalline silicon as a model system, it was of interest the eventual role played by a triple junction facing a crack front advancing in the grain boundary plane.

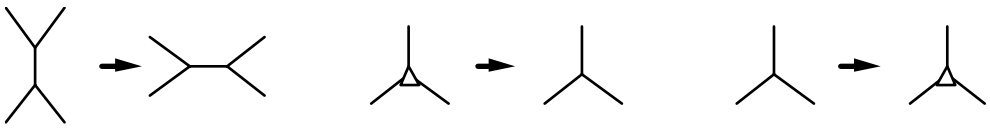
The (non-linear) elastic effect of the external loading on the triple junction is perfectly compatible with the picture of an additional elastic stress field superimposed over the elastic line tension of the triple junction (disclination-like) structure. A first series of MD simulations at *T*

= 0 K was then performed to evaluate the effect of an external stress on the triple junction energy and structure, again using the constant traction BC method for molecular dynamics simulations. For relatively small values of the deformation as measured in the far field (up to ± 5 %), the atomic structure of the triple junction is unchanged, i.e. no plastic deformation arises as a consequence of stress relaxation. The stress map around the triple-junction line retains the typical dipolar, disclination-like shape.

The microcrack was then placed a microcrack in the Σ9 grain boundary plane and applied an increasing load, to set the crack tip in motion towards the triple junction. The sequence of snapshots in Fig. 5 provides a qualitative picture of the interaction between the triple junction and the crack tip stress fields. The intergranular portion of crack propagation clearly has a brittle nature, the crack surfaces left behind the moving crack tip being flush with the typical steps of the vicinal {221} surface. When the crack tip approaches the triple junction it slows down, and eventually transforms into a more ductile behaviour, by breaking bonds along the {001} plane, i.e., the bisector of the {111} and {11-1} GB planes. The fracture surfaces in this second portion of the crack path are much rougher, and display a clear tendency to faceting towards {111} planes.

Although no dislocations are emitted from the crack tip, the increased surface roughness and reduced crack tip speed mark a sort of brittle-ductile transition. However, the relatively small size of the simulation box in this case prevented us from further observing the steady-state propagation regime in the ductile region.

For more details see: A. Satta, E. Pisanu, L. Colombo and F. Cleri: *Microstructure evolution at a triple junction in polycrystalline silicon*, J. Phys.: Cond. Matter 14, 13003 (2002)



T1 T2 anti-T2

Figure 1

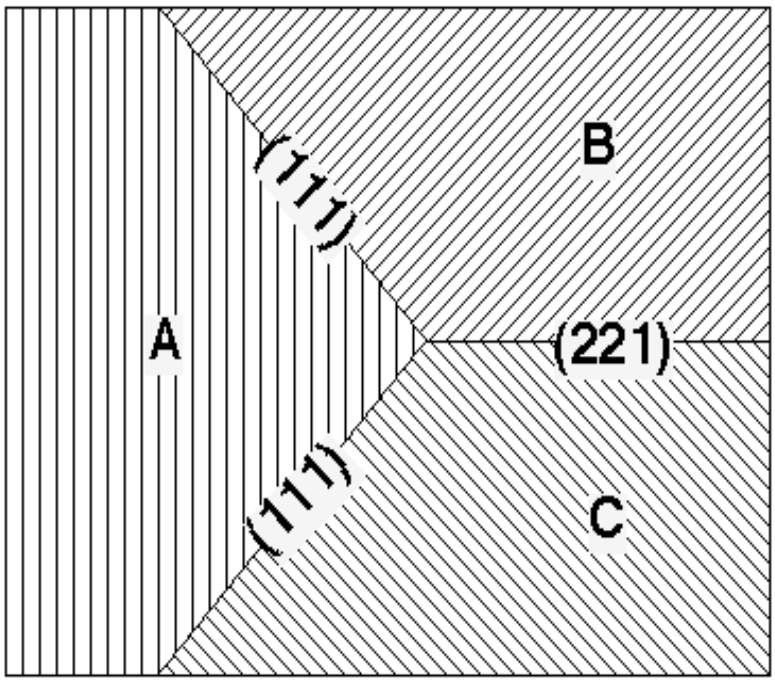


Figure 2

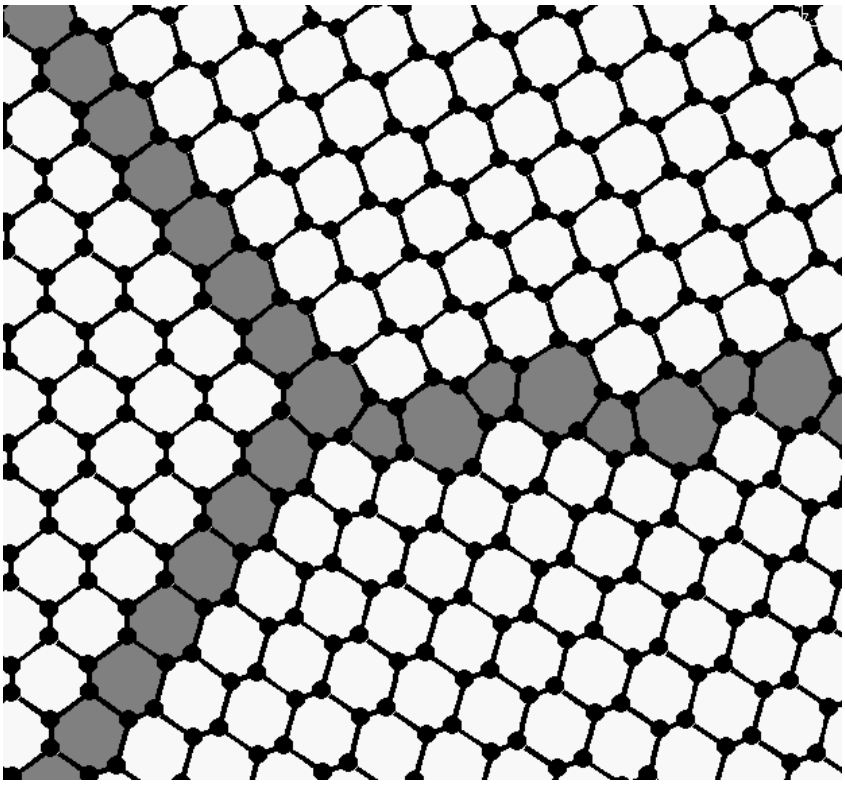


Figure 3

Figure 4

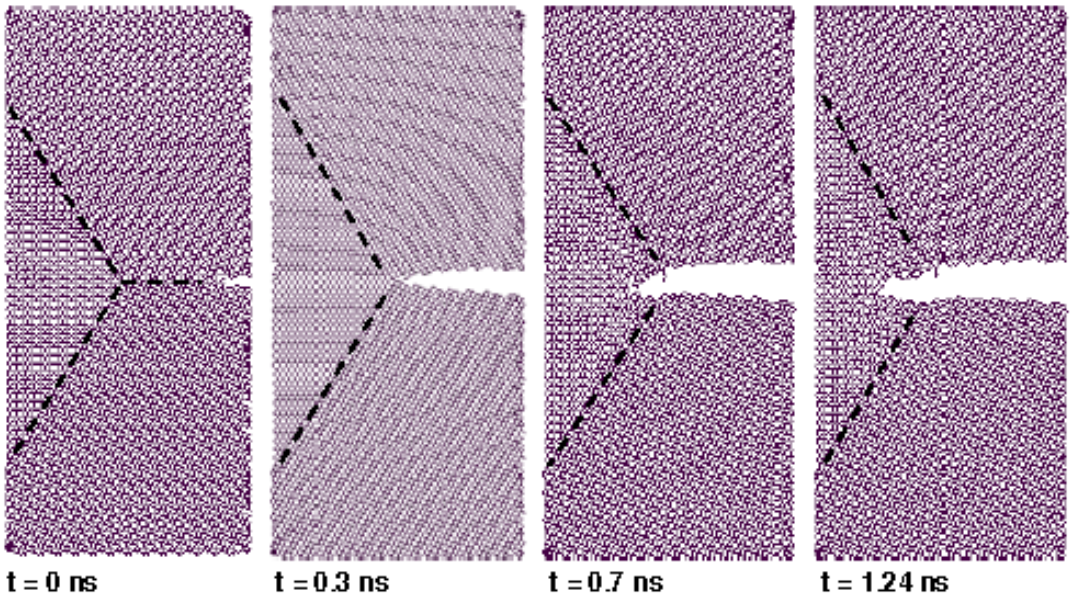
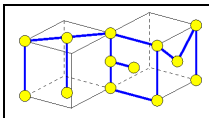


Figure 5



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D15: Comparison of results from atomistic simulations of defect-defect interaction

Author: F. Cleri
Date: 20/10/2004
Version 1

1. Introduction

The purpose of the present document is to give a summary of the status of atomistic simulations of defect-dectect interaction, with respect to the possibility of extracting fundamental information which would contribute to the modelling of microstructure evolution at a meso-macroscopic scale.

To this end, a specific set of atomistic (molecular dynamics) simulations have to be carried out, by properly selecting the type of elementary defects which will be represented in the meso-macro models, and by arranging the atomistic simulation model in such a way that it is indeed possible to extract the relevant information.

Within the ITEM project it was, at the beginning, planned to have a larger number of members performing atomic-scale simulation of extended defects (among these, the Swiss group of H. van Swygenhoven at PSI Villigen, and the Swedish group of P. Schiøtz at CAMP Lyngby). In the final set up of the network only the two Italian groups of L. Colombo, University of Cagliari, and F. Cleri, ENEA Roma, entered the project. This lack of groups performing concurrently atomistic simulations, while reflecting a European situation with respect to similar arguments in, e.g., the United States, gives this document an obvious limitation. In fact, the original title, "Comparison of atomistic methods..." loses a large part of its meaning since there is no comparison to be done, the two Italian groups sharing the same approach on this specific subject. Nevertheless, the two groups of Cagliari and Rome have a long-lasting collaboration on these subjects and the results which will be provided on this (and similar) specific topics should be substantial, albeit partial.

In the following we will describe a method to extract the non-linear part of the interaction (going beyond linear elasticity and superposition principle) between two kinds of defects, a microcrack and a rigid inclusion. This work is the recent result of the collaboration between

the two groups of Cagliari and Roma (see: A. Mattoni, L. Colombo and F. Cleri, Phys. Rev. B 70, 024124 (2004)).

When properly framed, this is a prototype example of derivation of a constitutive law for a microscopic model in which the atomistic degrees of freedom are integrated out, and only the mesoscopic objects (microcrack, inclusion) are described. The atomistically (molecular dynamics) derived interaction law provides the necessary microscopic information to the coarse-grained models, in a multiscale modelling strategy.

2. Interaction between a micro-crack and a hard inclusion in silicon carbide

The typical simulation cell adopted for molecular dynamics was a thin slab containing 60,480 atoms of a SiC monocrystal with zinc blend structure, so-called β-SiC. Atoms were arranged in a periodic supercell made of 84x30 unit cells (containing 12 atoms each) in the X-Z plane, and with a thickness of 2 cells in the Y direction. In the *x-y* plane the system was kept fixed at the equilibrium lattice parameter of β-SiC (4.318 Å) and periodically repeated. In the Z direction the crystal was elongated in steps up to a tensile strain of 8 % by means of the constant traction method (see F. Cleri, Phys. Rev. B vol.65 p.014107 (2002)). The typical loading condition adopted consists of fixed stress along Z, σ_{zz} =const, and fixed strain in the orthogonal plane, ε_{xx}= ε_{yy}=0. Therefore, this arrangement represents the plane-strain border condition of continuum mechanics.

In order to study the interaction between the atomic-scale microcrack and the inclusion, several molecular dynamics simulations were performed by varying the relative distance between the two defects. The distance was measured with respect to the defect centres (X_C , Z_C) and (X_I ,Z_I). The starting point for any run was a β-SiC monocrystal containing the inclusion relaxed at zero load. As a prototype of a hard inclusion it was considered the case of a cylindrical diamond fiber inserted into the β-SiC matrix as a pure chemical defect with no bond reconstruction or buckling at the interface (i.e. coherent with the crystalline matrix). In practice, a cylindrical region with axis parallel to the *y* coordinate and with radius *R*=1 nm was selected. The atoms of the cylindrical portion of the crystal were replaced by the same number of carbon atoms to represent the cross-section of an infinite fibre along the *y* direction. Since the C-C bond is 12 % smaller than the Si-C bond, the inclusion gives rise to a sizeable deformation field in the SiC matrix.

The system was then strained by the application of constant tractions (corresponding to 8 % of tensile strain in perfect β-SiC) and again fully relaxed. At this stage a microcrack was inserted into the system by a standard method [see e.g., F. Cleri et al., J. Amer. Cer. Soc. vol. 81, p. 501 (1998)]. The microcrack was always inserted in a (111) shuffle plane, at different distances *d* from the inclusion, along two different alignments: the case of horizontal alignment (H), and vertical alignment (V) , see Fig. 1 (top). The energy of a system containing both the inclusion and the microcrack is reported in the same Figure 1 for both H and V alignments. Being the inclusion an infinite fiber, the results are expressed as energy per unit length.

The relative map of the stress is represented in Fig. 2 for the case H. Here, the region corresponding to the highest tensile stress (delimited by the iso-stress contour σ_{zz}=0.27 eV Å^{-3}) at

the right crack tip is interacting strongly with the compressive lobe of the inclusion. At the same time, the iso-stress contour σ_{zz}=0.25 eV Å^{-3} (corresponding to a lower value of tensile stress) turns out to be extended all around the inclusion. The maximum depth of the attraction basin is reached when the crack tip and the inclusion are separated by just few Å and the defects are nearly in contact (ΔE ~ 0.12 eV Å^{-1}). In the case V a similar attraction basin is found, however the interaction is now stronger (although more short ranged) and the calculated energy basin has the depth ΔE ~ 0.18 eV Å^{-1}.

3. Non-linear analysis and derivation of constitutive equations

The present analysis does allow appreciating whether the interaction between the defects is purely additive, in a purely linear regime. The central objective is to investigate the possible "defect of linearity" of the overall (microcrack + inclusion) stress field, namely, the difference between the stress field when both defects are present and the sum of the stress fields of the two isolated defects.

The defect of linearity $\Delta_{nl}(x)$ of the *zz* component of the stress σ_{zz} is defined as:

$$\Delta_{\mathrm{nl}}(x) = [\sigma_{CI}(x) - \sigma_0] - [\sigma_I(x) - \sigma_0] - [\sigma_C(x) - \sigma_0] \qquad (1)$$

where I, C, and CI refer to configurations including an isolated inclusion, an isolated microcrack, and both inclusion and crack, respectively. The uniform stress background σ_0 is subtracted from each contribution. According to equation above, $\Delta_{nl}(x)$ should vanish if the interaction of the two defects I and C is purely additive. The result of this analysis clearly indicates that for an interacting pair of crack/inclusion under tensile loading, the mechanical response (stress field) falls beyond the linear regime.

$\Delta_{nl}(x)$ obviously depends on the relative distance *d* between the two defects. If one considers the $\Delta_{nl}(x)$ profiles corresponding to different relative distances d, scaled by some factor depending upon the relative distance, it is found (Fig. 3) that the behaviour of $\Delta_{nl}(x)$ is well represented by a function vanishing everywhere, but for two rather localized regions corresponding to the positions of the crack and the inclusion.

Accordingly, the defect of linearity $\Delta_{nl}(x)$ can be re-casted in the following form:

$$\Delta_{nl}(x) = s(d) \, [\, g_C(x - X_C) + g_I(x - X_I) \,] \qquad (2)$$

where *s* is a scaling function dependent only on the relative distance $d=|X_I - X_C|$, while the last factor is the sum of two suitable functions g_I and g_C localized at the defect positions. A plot of the scaling function $s(d)$ versus the distance *d* shows a power-law behaviour, $s(d) \sim d^{-2}$.

This leads to an important qualitative result, namely the total stress field can be formulated by means of the following constitutive formulation:

$$\sigma_{zz}(x) = \sigma_I(x) + \sigma_C(x) + [\, g_C(x - X_C) + g_I(x - X_I) \,] / d^2 \qquad (3)$$

This result is one step towards a continuous non-linear model for the stress of an interacting crack-inclusion couple that is inferred fully from atomistic analysis. A constitutive equation like the one above, can be directly used in a mesoscale model in which individual atoms are integrated out, and the only meaningful degrees of freedom are a network (for example, two interacting sub-lattices) of microcracks and of inclusions embedded in a linear-elasti c matrix, describing the composite material.

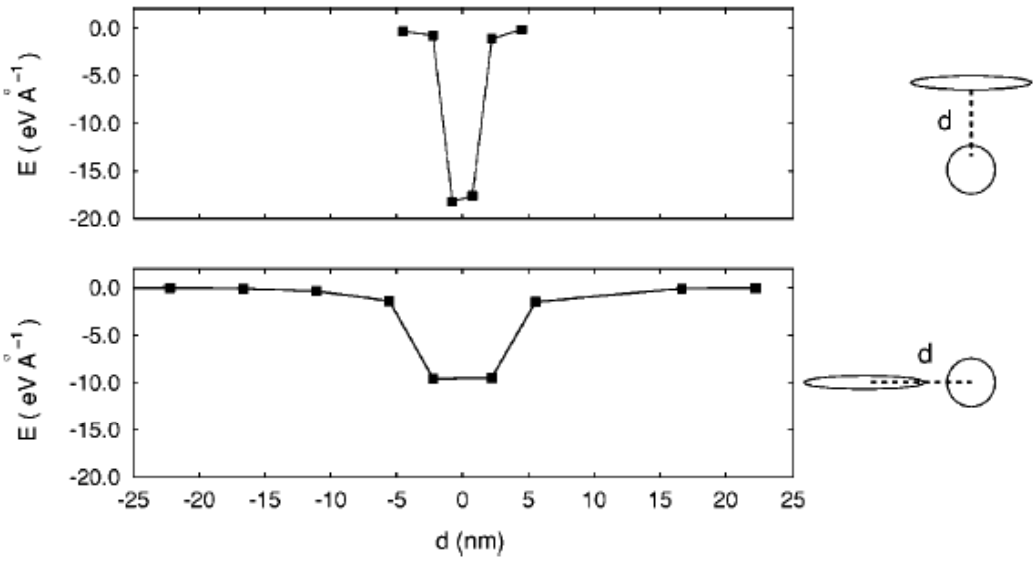


Figure 1. Top panel: energy of strained β-SiC (ε_{zz} = 8 %) containing a stable crack and a diamond inclusion as a function of the relative distance for a vertical (V) crack-inclusion alignment; bottom panel: the same for horizontal (H) alignment

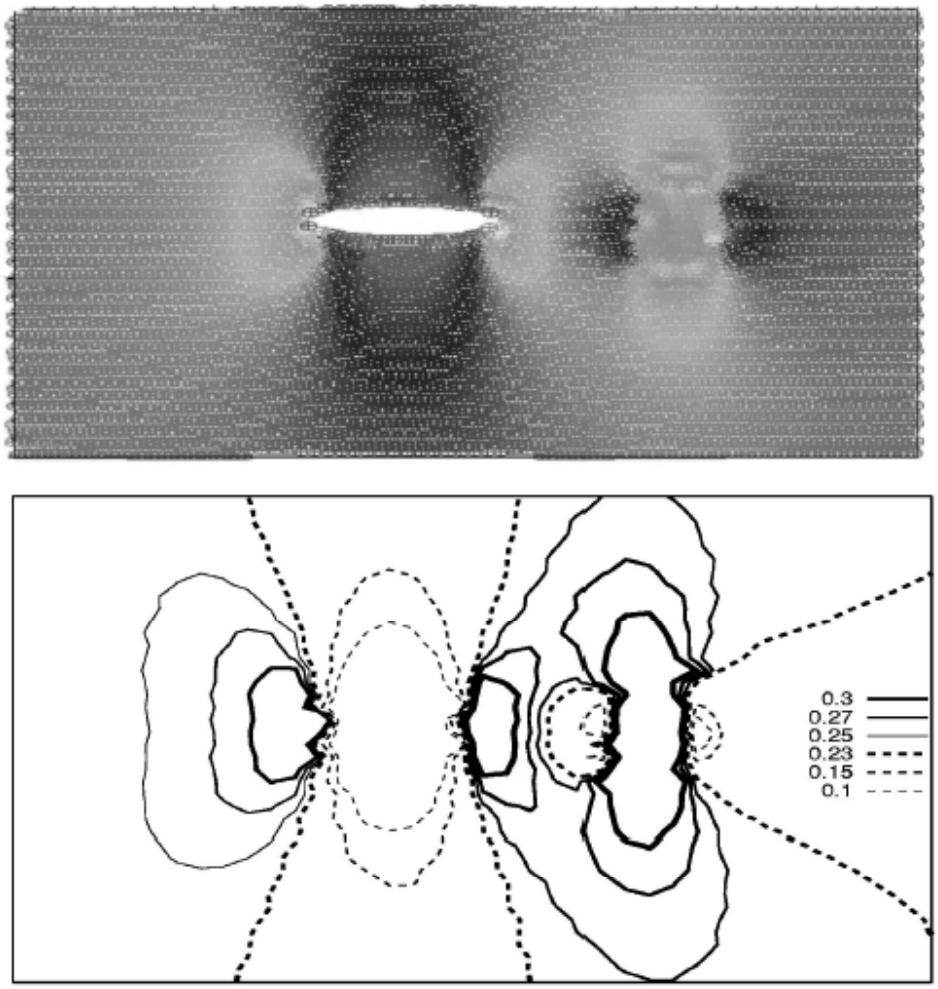


Figure 2. Top panel: *XY*-plane stress map $\sigma_{zz}(x, y)$ of β-SiC containing both a diamond inclusion (R = 10 Å) and a stable crack (of half-length a = 18 Å) at the distance of 5.5 nm. Bottom panel: iso-stress contour plot (units of eV $Å^{-3}$) for the same system. Only a small portion (18 x 10 nm^2) of the simulation cell is represented for the sake of clarity

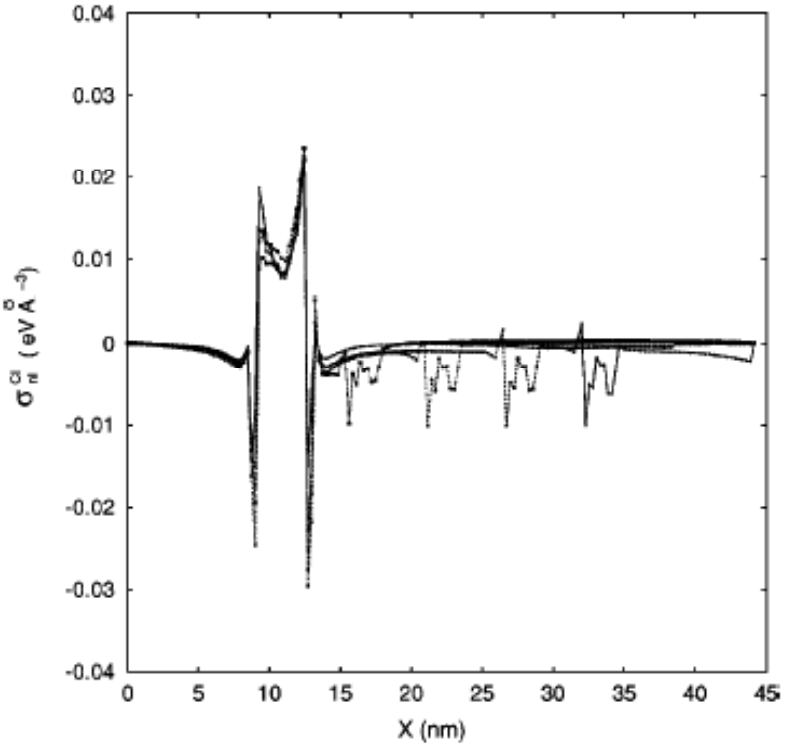
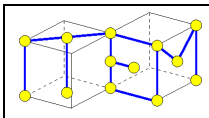


Figure 3. Defect of linearity $\Delta_{nl}(x)$ profiles corresponding to four relative distances d between the crack and the inclusion. Full line: d = 22.2 nm; long dashed line: d = 16.6 nm; short dashed line: d = 11.1 nm; dotted line: d = 5.5 nm (see text)



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D16: Definition of a reference atomistic simulation model for polycrystal plasticity

Author: F. Cleri
Date: 20/10/2004
Version 1

1. Introduction

The purpose of the present document is to give a summary of the status of atomistic simulations of polycrystal simulation methods at the atomic scale. The purpose of performing a full-scale polycrystal simulation is to find a comparison between coarse-grained mesoscale models of microstructure over a length scale at which the two descriptions overlap. This would provide a benchmarking of the mesoscopic scale model, which would include only extended defects as the degrees of freedom (grain boundaries, microcracks, inclusions, etc), with respect to the fully atomistic model, of which the former is a coarse grained representation.

Within the ITEM project it was, at the beginning, planned to have a larger number of members performing atomic-scale simulation of extended defects (among these, the Swiss group of H. van Swygenhoven at PSI Villigen, and the Swedish group of P. Schiøtz at CAMP Lyngby). Also in this case, as for the deliverable D15 ("Comparison of results from atomistic simulations of defect-defect interaction"), the fact that in the final set up of the network only the two Italian groups of L. Colombo, University of Cagliari, and F. Cleri, ENEA Roma, entered the project, weakens the conclusions that are reached on this specific point. Nevertheless, the ENEA Roma group has been working in international collaborations, notably with people at the Materials Science Division of the Argonne National Laboratory, Chicago, on the very subject of polycrystal simulations at the atomic scale, and we are thus in the position of providing a working atomistic model which, albeit with limitations, can be used as a reference for the purpose of the project.

In the following we will outline the basic ingredients of this model, and invite the interested readers to consult some already published papers for further reference.

2. Polycrystal simulation at the atomic scale

We illustrate the basic idea with a four-grain system to produce a textured polycrystalline substrate. To produce a microstructure of approximately hexagonal grains (Fig. 1), small cy-

lindrical, perfect-crystal seeds are placed in a bulk melt at the vertices of an imaginary lattice of equilateral triangles. When the temperature in the system is reduced below the melting point, the seeds act as nucleation centres for the growth of the grains to form a dense columnar microstructure.

We now describe a practical application of the method, in the case of the synthesis of a thin film of iron oxide. To describe the short-ranged interactions in FeO, the following Buckingham-like potential was used:

$V.(r) = A \exp.(-r/\sigma) - C/r^6$

with the interaction parameters derived by Sangster and Stoneham (Phil. Mag. B **43**, 597 (1981)), giving a_0=4:33 Å for the zero-temperature, perfect-crystal FeO rock-salt lattice parameter.

The starting configuration for the growth of a 16-grain polycrystalline FeO film, shown in Fig. 2, was prepared in the following manner. First a [100] oriented, 3D periodic, single crystal (with 8 ions/a_0^3) was constructed. Because the intent was merely to prepare a substrate layer, the simulation cell was chosen to be only $4a_0$ ~ 17 Å thick in the direction parallel to the substrate normal (the *z*-direction). To allow the straight growth of 16 grains of diameter ~$11a_0$ = 47 Å, the *x*-*y* dimensions of the simulation cell were chosen to be $44a_0$ x $38a_0$ = 186 Å x 160 Å, for which *x* : *y* is 1 : 0.86364, close to the ideal value of 1 : cos 60°/2 = 1 : 0:866025 required to periodically repeat the triangular arrangement of seeds. The total number of ions in the substrate simulation was 53,504.

The 16 seeds were chosen to be perfect-crystal cylinders of radius 7 °A with the [001] crystal direction parallel to [001] edge (the *z* direction) of the simulation cell (see Fig. 2). The seeds were rotated by random angles about an [001] axis located at the seed centre; the centres of each seed were offset slightly from the triangular lattice to introduce a small symmetry breaking.

This rotation about the [001] axis means that the *x*-*y* plane remains an (001) plane in all of the seeds and thus, that any GBs grown normal to [001] will be pure [001]-tilt GBs. The index numbers and randomly selected orientations of the seeds are given in Fig. 2 and Table 1 respectively.

To produce crystalline seeds embedded in a bulk liquid, the above system was then heated to 6000 K, with the ions in the seeds fixed, so that the rest of the system melted. Since melting involves a significant latent volume, the *x*-*y* dimensions of the simulation cell were allowed to equilibrate under a modified Parrinello-Rahman constant-stress scheme. The resulting initial structure is just the one shown in Fig. 2.

To produce the thin film, the system in Fig. 2 was cooled from 6000 to 3500 K. To account for the lattice expansion at 3500 K, the *z*-dimension of the 3D periodic simulation cell was increased from the zero temperature value by 3.74 % (the lattice expansion of the perfect crystal at 3500 K, previously determined from constant-pressure simulations). The ions in the seeds were allowed to move and the *x*-*y* dimensions of the simulation cell were allowed to change to maintain zero stress in the *x*-*y* plane. This growth of a dense microstructure from

the seeds took only 4,000 time steps (~ 9 ps) after which time the total energy remained essentially constant and the simulation-cell dimensions fluctuated by a only small amount about constant values. The system was then quenched to 1 K at zero stress in all three directions. As intended, the final microstructure (Fig. 3) is a columnar structured polycrystal of eight (001) planes: it is evident that quite dense grains have been formed joined by quite narrow GBs.

This 3D periodic microstructure can be further elaborated, for example by cutting it into 2D slices for promoting growth of columnar microstructures. This same simulation method has been up to now already tested and largely used for metal-like f.c.c. simple Lennard-Jones potentials, for true metallic-like embedded-atom Pd and Al polycrystals, and for pure Si polycrystals described by the Stillinger-Weber interatomic potential.

n	θ (°)	n	θ (°)
1	−39.2	9	8.1
2	31.1	10	19.9
3	23.6	11	−25.6
4	−20.9	12	−6.5
5	−1.2	13	−33.5
6	−38.4	14	30.3
7	−40.8	15	8.6
8	32.2	16	38.2

Table 1. Angle of rotation θ of each seed n about the [001] normal axis of the 16 cylindrical seeds. The angle $\theta = 0°$ corresponds to alignment of the [100] crystal directions parallel to the simulation-cell edges

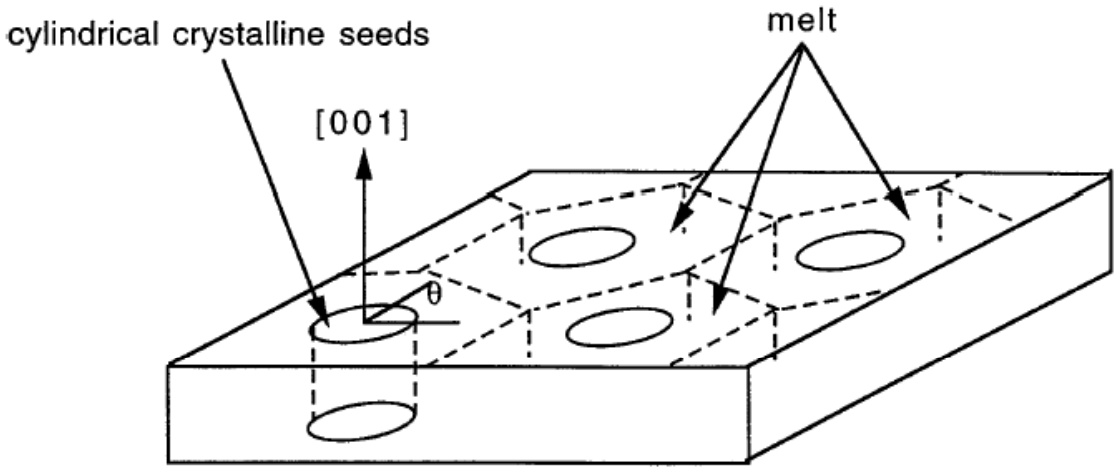


Figure 1. Schematic of the method for creating the polycrystalline substrate. The randomly oriented single crystalline cylindrical seeds act as nucleation sites to growth from the melt. The fully-grown substrate consists of approximately hexagonal grains separated by relatively narrow grain boundaries

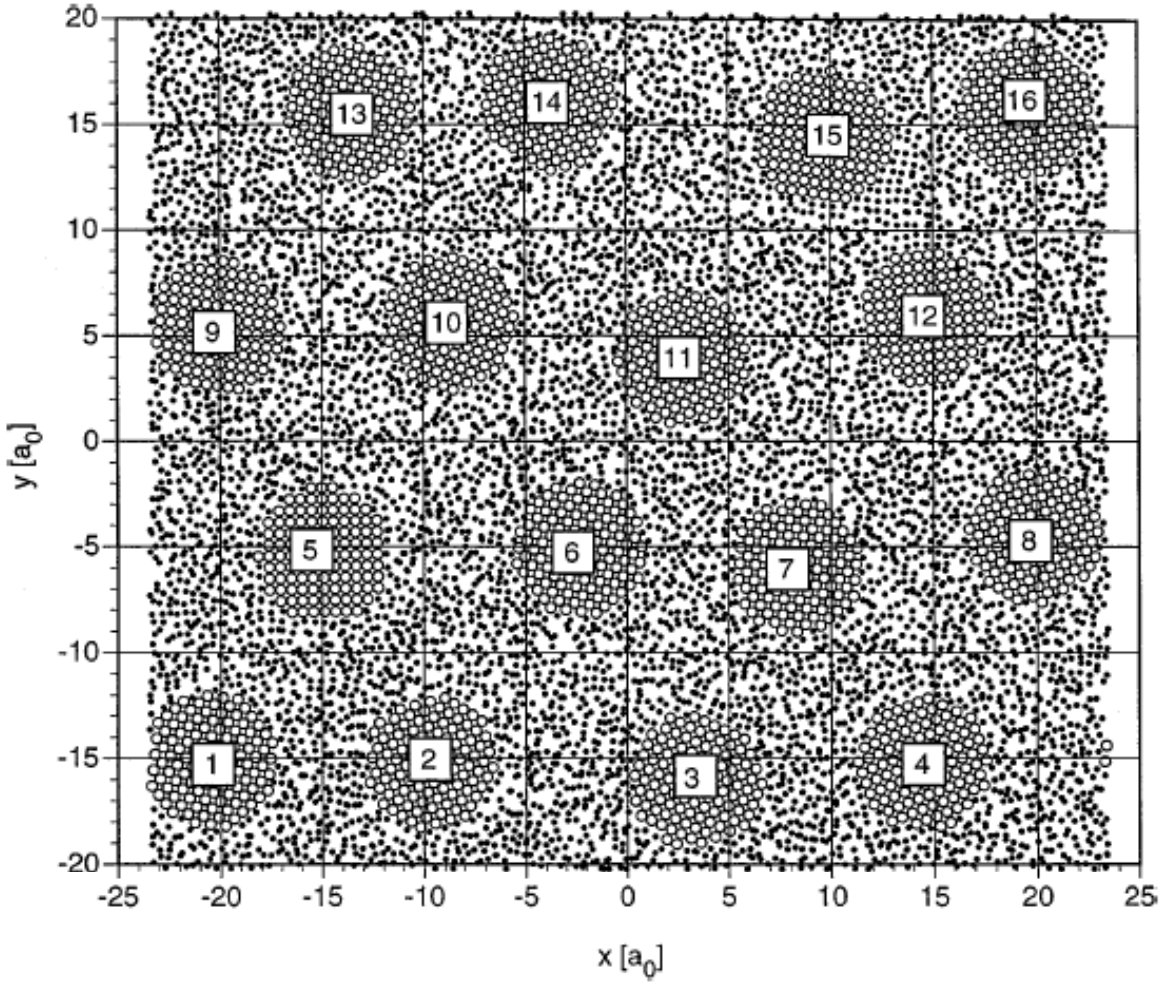


Figure 2. Plan view through the 16 cylindrical seeds embedded in liquid, showing 8471 of the 53,504 ions in the simulation cell.. The ions in the seeds are denoted by open circles; the initially liquid ions are denoted by small solid circles. Also shown is the numbering scheme for the grains in the substrate and thin film. For the relative disorientations of the grains, see Table 1

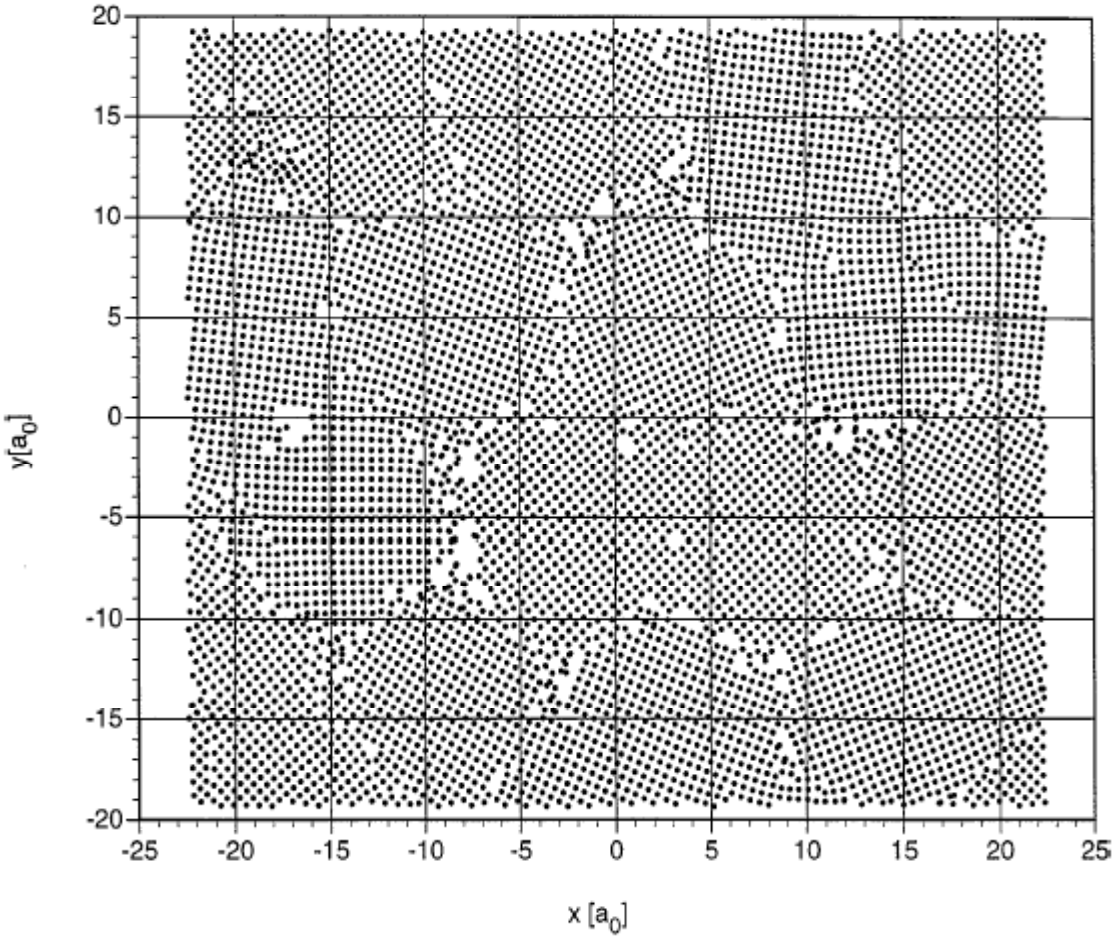
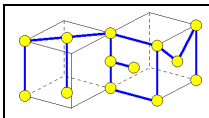


Figure 3. Plan view of a slice of thickness dz = 0.5 a_0 through the grown substrate showing highly crystalline grain interiors separated by relatively narrow grain boundary regions



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D30: Elaboration of experimental programme to validate selected results obtained using simulation tools (month 24 and 36)

D31: Complete set of experimental results validating computational results produced by the network (month 48)

Author: L. Malerba
Date: 20/10/2004
Version 1

The performance of experimental activities within ITEM must necessarily rely on the availability of funds from other projects. Since the beginning it was therefore recognised (see summary of outcome of TA-VI meeting at the kick-off meeting in November 2001 and presentation given at 2nd plenary meeting in Brussels in January 2003) that the network's experimental programme for the validation of the results of the simulation (Deliverables D30 and D31) could only coincide with the sum of already ongoing experimental activities in the different laboratories.

At the time, the only ongoing experimental programme that could be close to be a common programme was that related to the REVE project, in which many of the participants in TA VI were involved. In this framework, not yet involved partners, such as CRPP-EPFL and CUP, could have contributed, in selected cases, with their expertise in, respectively, TEM image simulation and positron response calculations.

That situation was eventually overcome by the events with the setup of the PERFECT IP. D30 (elaboration of the experimental programme for the validation of computer simulation results) became the obvious and necessary pre-requisite for PERFECT and right now the execution of such an experimental programme, coincident with D31, corresponds to work packages II-WP3 and II-WP6 of PERFECT. These work packages consist of the following:

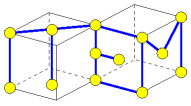
– perform quantitative micro-structural characterisations of irradiated RPV steels to get a precise description of the irradiation-induced hardening defects and segregation by merging complementary advanced characterization methods : Transmission Electron Microscopy (TEM), with image simulation, Energy Dispersion Spectroscopy (EDS) associated to field Emission Gun Scanning Transmission Electron Microscopy (FEG-STEM), Atom Probe Field Ion Microscopy (APFIM), Small Angle Neutron Scattering (SANS) and Positron Annihilation Spectroscopy (PAS). These techniques will be ap-

plied on a selected set of model alloys with increasing complexity and steels, western and VVER type, irradiated by neutrons or charged particles

– perform quantitative micro-structural characterizations of the austenitic steels, examined by FEGSTEM for intra-granular characterization of microstructure and grain boundary segregation.

For more details, see Annex I to the description of work of IP PERFECT (FI6O-CT2003-508840).

Thus, it can be concluded that D30 was accomplished during the preparation of PERFECT and the accomplishment of D31 has been now transferred to PERFECT.



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D32: Recommendation on improvements of computer techniques to compare experiment and simulation (month 24)

D33: Development of a new computational technique for experiment/simulation comparison or high optimisation of an existing one (month 48)

Author: L. Malerba
Date: 20/10/2004
Version 1

One of the sessions of the ITEM workshop organised on 23-24 October 2003 in Mol (Belgium) in the framework of TA-VI was explicitly devoted to the issue of computer techniques for the comparison between experiment and simulations. For details about the outcome of the meeting in this regard reference is made to the proceedings of the meeting (in preparation, corresponding to D34).

In short, three are the messages:

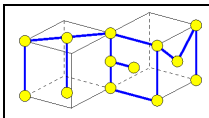
1. TEM image simulation techniques, based on the reproduction in the computer of diffraction contrasts resulting from determined (e.g. MD-simulated) defect configurations, given as atomic positions, are being constantly improved and provide the possibility of exploiting diffraction-based experimental techniques, down to their intrinsic resolution limit, such as not only TEM, but also – and this is relatively new – SANS.

2. Positron response calculation techniques are the only means of extracting quantitative information from PAS studies. These techniques are particularly important because they are the only ones sensitive to defects of size below diffraction technique (TEM, SANS) resolution and provide information on the presence of vacancies, which cannot be detected even by extremely sensitive techniques such as the TAP

3. Very recently a computational tool for the simulation of the reconstruction that the atom probe provides of a given defect (e.g. precipitate or vacancy-solute complex) has been developed and applied at the University of Rouen (member of TA-VI). This tool enables artefacts related to the aberrations of the instruments to be detected and removed, thereby greatly increasing both the wealth of information that can be deduced from TAP studies and the possibility of comparing TAP results with simulation results.

The conclusion is that these techniques are absolutely necessary for a correct validation of simulation results and their development and use should therefore be a priority for any experimental validation programme.

The development of the technique mentioned in (3), by the way, fulfils the requirement implicit in D33, long before the due date. Optimistically it seems that we can therefore still expect even further improvements in this field before the end of ITEM and within PERFECT.



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D36: Recommendation on methods to simulate the long-term evolution of radiation damage in multi-component alloys

Author: F. Soisson
Date: 20/10/2004
Version 1

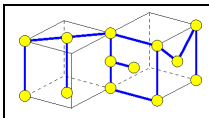
Classical methods to study the long-term evolution of radiation damage in pure metals are Rate Theory (RT) or Cluster Dynamics (CD) and Object/Events KMC (see deliverable D6). A comparison between these methods and their application to dilute alloys can be found in ref. [1].

Point defects, solute atoms, or clusters are considered as simple objects defined by their size (in RT/CD) and position (in OKMC and EKMC). Reactions between these objects depend on parameters such as migration and binding energies, capture radius, etc [2-4]. Alloying effects can only be included through a modification of these parameters. This method has been successively applied to simple cases, i.e. mainly to dilute solid solutions. A CD model for point defect clustering in ferritic alloys under electron irradiation is described in ref. [2]: the only effect alloy composition is to modify the di-interstitial binding energy. OKMC simulations of iron-copper dilute alloys have been performed to study cascade annealing and long-term damage accumulation [4]. Formation of Cu-vacancy clusters is observed. It is controlled by the Cu migration mechanism (direct migration of Cu-V pairs) and by binding energies, which have been computed in detail using molecular statics and an EAM potential. Moreover, OKMC and EKMC methods can easily take into account the 1D glide of small interstitial clusters observed in MD simulations.

For the time being, previous methods seem difficult to extend to concentrated and multi-component alloys, because they cannot take into account the complex microstructure of the objects and the detailed atomic diffusion properties which control the coupling between point-defect and solute fluxes. Atomic KMC on rigid lattice do not suffer from these drawbacks. They have been applied to the kinetics radiation-induced segregation and precipitation [5]. However point-defect clustering and, above all, the collective glide of self-interstitial clusters is more difficult to include in AKMC simulations.

[1] F. Soisson, A. V. Barashev, C. Becquart, M. J. Caturla, J. Dalla Torre, C. Domain and L. Malerba, *Proc. of the 2nd International Conference on Multiscale Materials Modelling*, Los Angeles, (2004)
[2] A. Hardouin-Duparc, C. Moingeon, N. Smetniansky-de-Grande and A. Barbu, J. Nucl. Mater 302, 143 (2002)

[3] J. Dalla-Torre, J.-L. Bocquet, N.-V. Doan and E. Adam, *Proc. Int. Symp. on Microstructural Processes in Irradiated Materials*, TMS Annual Meeting, San Diego 2003, to appear in Philos. Mag.
[4] C. Domain, C. Becquart and L. Malerba, J. Nucl. Mater. 335, 121 (2004).
[5] F. Soisson, *Proc. Int. Symp. on Microstructural Processes in Irradiated Materials*, TMS Annual Meeting, San Diego 2003, to appear in Philos. Mag.



ITEM network

IMPROVEMENT OF TECHNIQUES FOR MULTISCALE MODELLING OF IRRADIATED MATERIALS

FIR1-CT-2001-20136

D37: Method to study alloying effects on the interaction between dislocations

Author: F. Soisson
Date: 20/10/2004
Version 1

While the elastic theory is well suited for most problems related to dislocations, atomic scale modelling (mainly molecular dynamics, for the time being) is unique for describing the core of dislocations, the effect of chemistry on the latter and ultimately on the selection of the glide systems.

Glide of edges dislocations in concentrated NiAl solid solutions (1 to 8 %) have been studied by molecular dynamics (MD), using an embedded atom potential which has been optimised to reproduce the relevant properties of the solid solution and of the $L1_2$-Ni_3Al ordered phase [1,2]. The main conclusion of the study is that chemical hardening is not simply the result of a direct dislocation-solute interaction, but the result of close Al-Al repulsion. When the passage of the dislocation forces them one against the other, the repulsion opposes the glide of one half crystal with respect to the other.

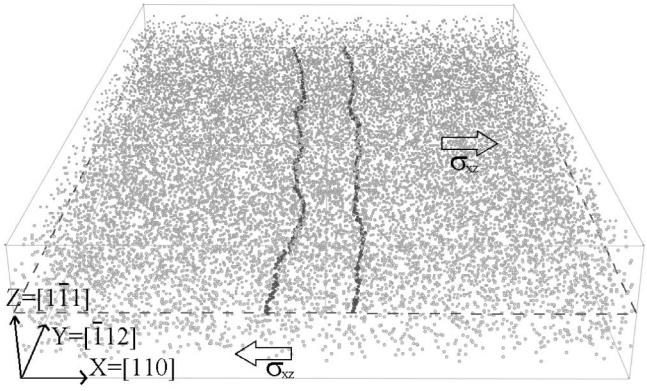


Figure 1: MD simulations of dislocation glide in a Ni(Al) solid solution (ref. [1]). The dislocation is split into two Shockley partials in its glide plane

The MD results have been used as input parameters for a micro-mechanical approach in order to predict macroscopic stress strain curves [3]. These studies are still in development in Saclay and Grenoble and other ones are planned in the framework of the PERFECT programme, for example on Fe-Ni alloys (as a model for austenitic steels). Alloying effects can

also be integrated in dislocations dynamics (DD) codes (see deliverable D12): the friction stress in solid solutions, for example, has been taken into account by a modification of elastic interactions between dislocations and of the strength of their junctions [4].

Ab initio calculations are of course much more time consuming, nevertheless some studies on solute segregation in dislocation core (segregation of S on dislocation in Zr [5]) are now possible which could provide reliable data to less time consuming simulation techniques.

[1] E. Rodary, D. Rodney, L. Proville, Y. Bréchet and G. Martin, Phys. Rev. B 70, 054111 (2004)
[2] L. Proville, D. Rodney, Y. Bréchet, G. Martin, proceedings of *Dislocations 2004*, La Colle-sur-Loup, September 2004 (to appear in Mater. Sci. Eng. A)
[3] T. Noguaret, D. Rodney, proceedings of *Dislocations 2004*, La Colle-sur-Loup, September 2004 (to appear in Mater. Sci. Eng. A)
[4] R. Monnet, proceedings of *Dislocations 2004*, La Colle-sur-Loup, September 2004 (to appear in Mater. Sci. Eng. A)
[5] F. Ferrer, A. Barbu, T. Bretheau, J. Crépin, F. Willaime and D. Charquet, Zirconium in the Nuclear Industry: 13th International Symposium, ASTM STP 1423, 863-887 (2003)