Predictive Modelling of Mechanical Properties of Materials for Fusion Power Plants

Modelling Programme

1 Background and Overview

"Multi-scale modelling" of materials' properties has been seen as a desirable concept for over a decade, but actual successful instances of fully-integrated modelling have been rare (for example the finite-element / dislocation-dynamics (DD) models of the CNRS-ONERA group [1], the DD / kinetic Monte-Carlo (kMC) models of the UCLA group [2] and the "quasicontinuum method" of Shenoy, Phillips et al. [3], embedding molecular dynamics models within a continuum model). No models have been successfully formulated that cross a wide range of length-scales: e.g. from electronic via molecular dynamics (MD) and then dislocation dynamics to large-scale mechanical properties. The reasons for this are at least three-fold:

Technical: the timescale mis-matches involved in truly integrating methods of different types – for example embedding MD codes in DD models – restrain the timestep to that of the finest scale model. To a limited extent this issue can be addressed by hybrid models (e.g. [3]), but for investigations covering a wide range of length and time scales it remains a fundamental problem. The only realistic approach to multiscale modelling is by multi-layered modelling with parameter passing – each layer producing from "first principles" (at its own scale) parameters that are used by the layer above. This is the approach used in this proposal, which includes: ab-initio modelling producing potentials, MD modelling using those potentials to produce dislocation mobility laws and dislocation-defect interaction strengths, and DD models using the information from MD to predict flow and fracture behaviour. Recent advances in modelling methods and in computing power mean that such an approach is feasible over this range of length and time scales.

Organisational: Researchers modelling materials at the various length scales have tended to work in relative isolation; while they are aware in general terms of the methods used at other length scales, there has been relatively little collaborative work between groups specialising in the different levels. This of course is one of the reasons for the consortium-based approach of the "Modelling Initiative". The members of this consortium have been selected for their complementary and overlapping areas of expertise in the various scales and methods of modelling; the research programme proposed here provides an organisational framework for them to work collaboratively at multiscale modelling around a central theme.

Experimental verification: It is important that modelling effort is directed to problems where the predictions can be experimentally verified; this also allows experimentally-derived knowledge of the important factors controlling behaviour to influence how the modelling is done. Ultimately, one expects to use modelling to predict the behaviour of real engineering systems – but before this can be done reliably, models must be carefully cross-checked against specifically-designed experiments of simpler systems. This should preferably be done within the same research programme, allowing true two-way feedback between modelling and experiment. For this proposal, we have set up such a parallel experimental programme (~£750k), to be funded by UKAEA Culham.

1.1 Specific focus – materials for fusion power plants

Materials for fusion power plants provide one of the major structural materials challenges of the next 20 years. So far, relatively little demand has been made on the properties of the materials used for JET and other prototype reactors, since they had only to contain an operating plasma for very short times, to prove concepts and predictions of plasma physics. In the next stage of development of fusion reactors (ITER) and particularly in fusion power plants, materials issues will be crucial to success. The first wall will operate at temperatures up to 600ºC and will need to withstand stresses up to 300 MPa, and will accumulate over its lifetime radiation damage from fast neutrons amounting to ~100 dpa. It is essential that any material used here maintains adequate strength and toughness, while suffering minimal dimensional change through swelling and creep.

Materials currently proposed for this application are ferritic-martensitic steels based on iron ~9% chromium (RAFM steels) [4,5], vanadium alloys [5] and tungsten [6]. (SiC composites have also been proposed, but their stability in the high dose limit has not yet been proved.) These materials may offer adequate strength and toughness and minimal sensitivity to fast neutron / alpha particle irradiation, in terms of swelling and increase in brittle-ductile transition temperature. However, it has been noted that for RAFM steels, “Further reduction of brittle-ductile transition temperatures should be pursued.” [7]. It is difficult, expensive and time-consuming to perform experiments on irradiated materials. Moreover, a major facility for high-energy neutron irradiation, IFMIF, currently at the design stage, will not come on-line until at least 2013. To proceed with the development and testing programme for the first generation of fusion power plants, which starts with ITER test blanket modules, the principal structural materials must be selected in the near future. Modelling offers understanding of the limited amount of experimental data and the means to take this understanding forward so that these materials selection decisions can be made on a rational basis. At the most recent published International Conference on Fusion Reactor Materials (ICFRM) (2000), only12 out of ~300 papers concerned modelling, and these largely of radiation damage alone, rather than its effects on mechanical behaviour. However, modelling studies in this field are now becoming more frequent, especially from the UCLA group (e.g. [2, 8, 9])

The research proposed is aimed at thorough multi-scale modelling of the microstructure, flow and fracture behaviour of these types of material, both in their “normal” and post-irradiated states. We propose to study vanadium, tungsten, iron and iron-chromium binaries up to 12% Cr.

Vanadium and tungsten are included in the programme since, in addition to being proposed reactor materials, they offer a relatively straightforward route (since they are non-magnetic) for extending ab-initio methods into body-centred materials, so that MD and DD models can be built which are based on a fundamental understanding of the bonding in these materials. Modelling of iron will form the next step at the ab-initio level, dealing with the complexities introduced by ferromagnetism. Ab-initio modelling of the iron-rich end of the binary iron-chromium system will then follow. In each case, the potentials from the ab-initio modelling will be used in the MD and DD models of mechanical behaviour, developed in parallel strands of the overall project.

We recognise that the effects of radiation (including the effects of helium bubble formation) on the flow and fracture of the real engineering materials based on the Fe-Cr system will have complications that are not addressed in this research proposal. However, there are important systematic variations in behaviour with Cr content. The brittle-ductile transition temperature (BDTT) for a wide range of ferritic /martensitic steels varies over a ~100°C range with Cr content and follows the same pattern of variation with Cr content in all steels studied, with a minimum in BDTT at 5-10% Cr [4,10]. The upward shift in BDTT (ΔBDTT) after irradiation (7-36 dpa at 365-410°C) also follows a common pattern with Cr content across all steel studied, with a very small shift at 9% Cr [11], rising to a shift of 200-250°C at low (2%) or high (12%) Cr contents; Cr content has a stronger influence on ΔBDTT than other compositional or microstructural factors or irradiation dose (at least under conditions with little He production). Post-irradiation swelling also varies strongly with Cr content [12]. Oddly, the *maximum* swelling (up to 0.035 %/dpa) is found at 9%Cr [12,13] - the composition range with *minimum* ΔBDTT; this remains unexplained.

These systematic variations in behaviour with Cr content imply that modelling of the properties of simple Fe-Cr binaries should capture much of the core behaviour of more complex materials based on them. Hence the "fundamental science" approach of this study should find immediate applicability to these alloys.

1.2 Generic issues – modelling of mechanical properties

While this proposal has a specific focus on modelling of materials for fusion reactors (see §1.1), it is important to note that it will establish generic methods for developing usable, fundamentally-based potentials for body-centred cubic metals, alloys and magnetic materials, and will apply these to modelling their flow and fracture behaviour. As such, it addresses a wide range of fundamental issues in modelling mechanical properties of materials, especially those based on bcc metals. The programme will push forward the UK modelling capacity across a wide front of areas related to materials design: ab-initio modelling, development of potentials, molecular dynamics, kinetic Monte-Carlo and dislocation dynamics, and will promote communication and collaboration between leading UK research groups working at these different scales of modelling. The methods to be established in this programme have wide applicability. They will form the basis of future research programmes in modelling the flow and fracture behaviour of metals and alloys, especially steels. We expect to be submitting proposals for such programmes in the mid-to-late stages of this programme, so that model development and application can continue seamlessly beyond this project.

2 Project Methodology

A four-year programme is planned, employing three postdoctoral research assistants and at least six doctoral research students. Figure 1 illustrates the linking of the various aspects of the project. The key elements are given below. Figures in brackets after section headings indicate roughly the weighting of each section within the project, as the fraction of grant funding allocated.

2.1 Ab-initio modelling and interatomic potentials *(25% + staff contribution from UKAEA Culham)*

Current density-functional (*ab-initio*) calculations give reliable predictions of the properties of bulk metals, but are too costly to use on a routine basis for systems of more than 100-200 transition metal atoms, or for dynamic calculations in such systems. The aim here is to provide models that bridge the gap between the density-functional approach and the simpler but less reliable models. An interim approach will furnish potentials for use in MD calculations that, while not as universally applicable as those we are ultimately aiming for, will at least remedy the gross deficiencies in existing models.

The standard MD treatments of transition metals involves embedded atom models (EAM) or Finnis-Sinclair (FS) potentials fitted to crystal structures and elastic properties. However, magnetic materials are poorly described by such density-dependent potentials, because the stability of the bcc crystal structure arises from magnetic effects and details of the Fermi Surface, which in turn depend in a complex way on their local environments. We have previously constructed FS-type models for Fe and Fe-Cu bcc metals; these have been widely used, but lack transferability to configurations encountered with atoms in close proximity, as occurs in radiation damage and in dislocation motion.

We will perform first-principles calculations in supercells of 128 or more atoms for V, W, Fe and Fe-Cr binary alloys. Candidate interstitial configurations will be calculated, including mixed-dumbbells in the binary system. In addition, we will calculate the Kanzaki forces (the forces necessary to create the same displacements in a defect-free system). These can be used to calculate the formation volume [14,15] of each defect, and will also be useful data in the fitting procedure. Fitting and testing simple EAM or FS models in the first instance will establish a set of potentials for the initial large scale atomistic simulations. Models which reproduce the atomic configurations containing an interstitial, as well as the Kanzaki forces, will provide a good basis for simulation of all kinds of radiation damage.

These simplest fitted models will be useful in the early stages of the project for scoping the problem and suggesting qualitative mechanisms. Later stages of the project will focus on more sophisticated potentials, based on the idea of bond-order potentials [16], in order to deal with the non-central bond-angle dependent forces. We are currently extending such models to include terms due to magnetic moments. With such potentials we can be confident that the stability of the bcc lattice is due to the correct physical mechanism, and therefore the potentials are less likely to make poor predictions for configurations far removed from those used in the fitting. They should naturally give the correct ordering of energies for different interstitial configurations, and fit the energies of those configurations. In addition, the interstitial configurations mimic some of the atomic arrangements in a dislocation core, so our fitted potentials will be transferable to simulations of dislocation motion and interaction with defects.

Throughout the project, potentials developed will be passed forward for use in molecular dynamics simulations.

2.2 Molecular dynamics (30%)

2.2.1 Simulation of cascade damage

MD simulations will be used to obtain information not directly accessible from experiments on the number and disposition of the vacancy and interstitial defects produced in metals by cascades of primary-atom recoil energy up to ~50 - 100keV. It is now possible [17] to simulate many tens of cascades at any chosen condition, generating good statistics for use in Monte Carlo models and mean-field theories of damage evolution (§2.3). In this project, MD modelling will be extended to cascades in metals and alloys of relevance to the extreme conditions of fusion.

(i) Primary damage production. In the first part (months 1-18) of this project, existing interatomic potentials for V and W (and possibly Fe-Cr) based on the EAM or FS formalisms will be employed to generate a large data base of information on defect number, cluster fractions and cluster type (e.g. glissile, sessile, collapsed, etc.) as functions of irradiation temperature (up to 600K) and recoil energy (up to 50keV). In the second part of the project (months 19-36), the new interatomic potentials for these metals developed in §2.1 will be used to extend the data sets and test the sensitivity of cascade properties to interatomic potential and Fe-Cr alloy composition variations.

(ii) Interstitial cluster properties. The majority of interstitial clusters found by MD studies of cascades are sets of parallel glissile crowdions. In the later part of the project when the new potentials are developed, we will study: (a) the effects the highly elongated distortion fields of the crowdion on the bias dislocations are normally considered to have for the capture of single interstitials over vacancies; (b) the variation of the 1D/3D nature of clusters from metal to metal; (c) the dependence of the mobility of clusters in Fe-Cr on solute concentration.

2.2.2 Simulation of dislocation-obstacle interactions

Current models of hardening by point defects and clusters use simple approximations, such as critical breaking angle in the line-tension approximation. These neglect dislocation self-stress effects and changes in line and obstacle structure as the dislocation passes. Detailed information on obstacle strength, atomic structure change and defect absorption due to dislocation climb can be obtained by MD simulation, and the effects of temperature and strain-rate can be determined accurately [18]. In this project, dislocation-obstacle interactions in V, W, Fe and Fe-Cr will be investigated systematically; this will enable us to incorporate soundly-based interaction parameters in dislocation dynamics modelling (§2.5). In first phase of the project (months 1-18), we will use existing empirical potentials to investigate the effect on edge dislocations of interstitial and vacancy clusters. In parallel with this, a model for simulating behaviour of screw dislocations, which are rate-controlling in the deformation of bcc metals, will be developed. In the second phase, the research will be extended with the new potentials to study alloying effects on dislocation mobility, both in "clean" material and in the presence of distributions of damage defects.

2.3 Kinetic Monte-Carlo modelling (10% + staff contribution from UKAEA Culham)

Evolution of collision cascade structures beyond the MD timescale (a few tens of ps) will be modelled using kinetic Monte-Carlo methods already developed collaboratively at Oxford and Culham [19,20].These methods utilise defect structures and properties calculated in other sections of the project. KMC models will be used to describe long timescale evolution of populations of defects. These models will describe competition between random thermally activated motion of defects in the material and effects of elastic interactions between defects and elements of the microstructure of the material (impurity atoms [20], dislocations and grain boundaries) as well as interactions between defects themselves. This part of the project will provide information about densities of defects, as well as the dominant types of defects, at various stages of microstructural evolution. This information will be used in modelling plastic deformation and fracture (§2.5).

2.4 Microstructural modelling (5%)

This project focuses on simple elemental and binary materials, modelling from first-principles upwards; however, real steels contain a variety of precipitates and defects (such as martensite lath boundaries) other than those induced by irradiation. Recent advances in phase transformations theory [21] allow modelling of the evolution of these more complex systems. This part of the project will produce a detailed description of the nature, size and volume fractions of precipitates, as a function of long–term service. These data will be used as inputs to standard hardening theory, to give a check on the relative importance of effects modelled in the pure and binary materials. In the longer term, beyond this project, such data can be incorporated into extensions of the DD codes for brittle-ductile behaviour.

2.5 Dislocation dynamics, fracture and brittle-ductile transition modelling (30%)

Dislocation dynamics (DD) simulations will be used to model flow and fracture behaviour. The 2D models used so far at Oxford require arbitrary blending of the properties of screw and edge dislocations, and are not capable of being extended to take account of the interaction of dislocations with point and cluster defects. We will therefore import and adapt the 3D dislocation dynamics codes developed at LEM/ONERA in Paris [e.g. 1]. The ONERA group are enthusiastic about assisting us with the production of versions of the 3D DD codes for use in this project; a letter of support from them is attached.

Using 3D-DD codes, flow laws will be derived for defect-containing structures; these flow laws will be compared with those derived using analytical methods, based on standard hardening theory, for equivalent structures (similarly to [8]). These flow laws will then be used in 2D and 3D DD models of the brittle-ductile transitions. The evolution of the crack-tip plastic zone during a loading cycle will be simulated over a range of temperatures, calculating the influence of the dislocations on local crack tip stress intensity via back stresses ("shielding") and blunting. The simple 2D codes already developed at Oxford [22] will be used initially, at first with experimentally-derived or "best-guess" dislocation mobility laws, replacing these with MD-derived ones when these become available. An exploratory study has already shown how the 3D-DD codes can be used to model fracture behaviour of bcc metals [23]; 3D codes will be extended to include flow behaviour in defect-containing material, with the defects either being introduced as arrays of discrete obstacles (which will be computationally expensive), or via simple "broad brush" flow laws derived earlier in the project by DD and/or analytical methods. Comparison of the two methods will indicate the level of detail that is needed in the fracture modelling.

2.6 Task co-ordination

The overall aim of the project is to produce models of flow and fracture in bcc metals, firmly based on data from ab-initio studies, with each layer of modelling making use of information provided by a more fundamental layer. The programme has been designed so that each project partner can begin work on tasks aimed at the project goals even before potentials from the ab-initio modelling are available; data based on less precise models and from experiment will be used to develop the MD and DD methods. The timing of the stages of the project is indicated in Figure 2.

3 Management

The project leader will be Dr S.G. Roberts. The complex interlinking of research required by the project will be facilitated by frequent email contact, by informal visits between groups, and formally by quarterly meetings rotated around the project partners (researchers from the parallel experimental programme will also participate in these meetings). All partners will be required to submit a written report on progress to each meeting. Previous experience with LINK projects indicates that holding such formal "reportage" meetings at quarterly, rather than six-monthly, intervals acts well to keep large complex projects coherent. The project leader will prepare an overview report at each year end. Each year-end meeting will be followed by a low-cost one-day conference, consisting of talks by the project partners and discussion sessions, which we will promote to the wider academic and industrial community. These meetings will allow rapid dissemination of results and methods from the project to interested parties and will also allow identification of future research directions and partnerships. New research partnerships will be actively sought, so that the research methods established in this project can be taken forward beyond its end.

4 Beneficiaries

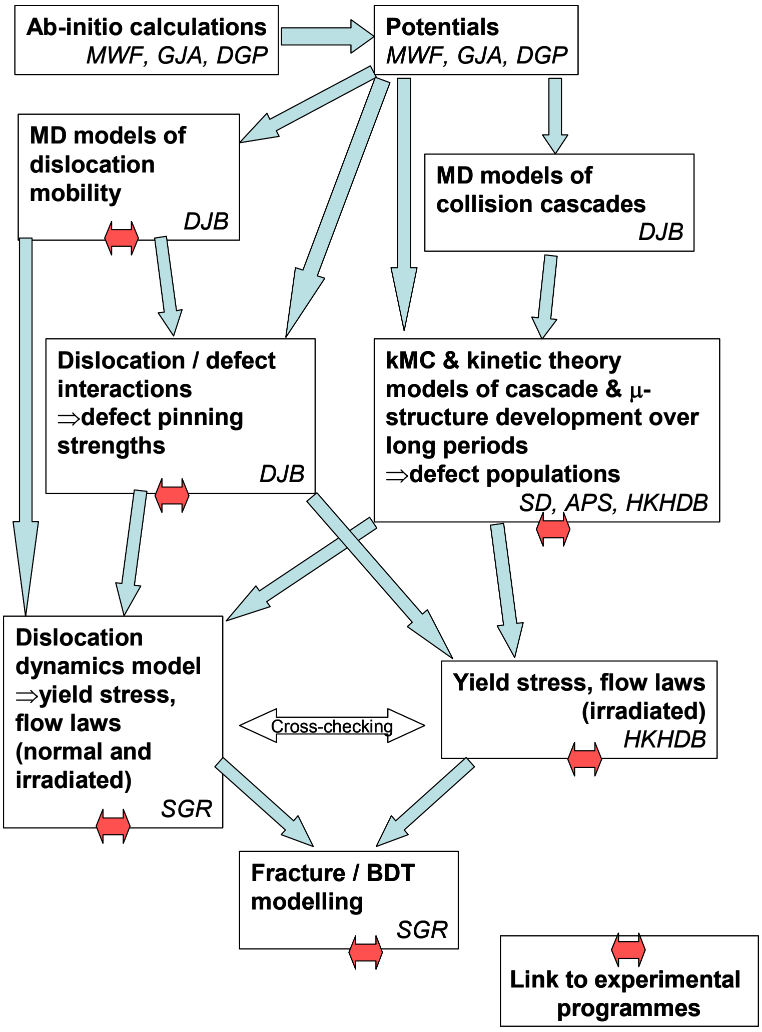
The project will offer significant benefits to the materials modelling community in the UK, bringing together expertise in different aspects of modelling to work together to produce a true multi-scale model of flow and fracture. The methods produced by the project will have wide applicability in modelling mechanical behaviour and radiation damage response in metals and alloys. The project will enhance the UK's reputation in this area. The UK research community will also benefit in that the project will produce 6-12 new researchers in this field, who will have worked in the context of an experimentally-linked multi-scale project with leading researchers. The project will benefit development of fusion power generally, and specifically via UKAEA Culham. The generic issues modelled are also relevant to fission power plant and ultimately to any safety-critical engineering components based on bcc alloys.

5 Dissemination and exploitation

Rapid dissemination of results will be provided by the yearly conferences (§3), and publication of project partners' reports on a website dedicated to the project. Results will also be made available to the general research community in the normal way through papers in the scientific literature and by presentations at UK and international conferences. The project's partnership with UKAEA Culham will provide routes for rapid dissemination of results into the fusion research community via regular publication of submitted papers as "Fusion Reports".

This is an "underlying science" type of research project; we do not anticipate immediate commercially exploitable output. To protect the interests of all parties, a general IPR agreement will be negotiated by the Research Services Office of the University of Oxford with all partners before the work starts.

Figure 1:
Project information flow.



Flow chart of interlinking of scales of modelling within the overall project.

***GJA*:**	Dr Graeme Ackland (Edinburgh University)
***DJB*:**	Prof. David Bacon (Liverpool University)
***HKHDB*:**	Prof. Harry Bhadeshia (Cambridge University)
***SLD*:**	Dr Sergei Dudarev (UKAEA Culham / Oxford University)
***MWF*:**	Prof. Mike Finnis (Queen's University, Belfast)
***DGP*:**	Prof. David Pettifor (Oxford University)
***SGR*:**	Dr Steve Roberts (Oxford University)
***APS*:**	Prof. Adrian Sutton (Oxford University)

References

---

1. B. Devincre, L.P. Kubin, C. Lemarchand & R. Madec, *Mat. Sci. & Eng.* **309-310** 2001, 211.
2. N.M. Ghoniem, S.H. Tong, J. Huang, B.N. Singh & M. Wen, *J. Nucl. Matls.* **307-311**, 2002, 843.
3. V.B. Shenoy, R. Miller, E.B. Tadmor, D. Rodney, R. Phillips & M. Ortiz, *J. Mech. Phys. Solids* **47**, 1999, 611.
4. A. Kohyama, A. Hishinuma, D.S. Gelles,R.L. Klueh, W. Deitz & K. Erlich, *J. Nucl. Matls*. **233-237**, 1996, 138.
5. K. Erlich, *Fusion Eng. & Dsgn*., **56-7**, 2002, 71.
6. H. Bolt, V. Barabash, G. Federici, J. Linke, A. Loarte, I. Roth, & K. Sato, *J. Nucl. Matls*. **307**, 2002, 43.
7. B. van der Schaaf, D.S. Gelles, S. Jitsukawa, A. Kimura, R.L. Klueh, A. Möslang & G.R. Odette, *J. Nucl. Matls*. **283-287**, 2002, 52.
8. N.M Ghoniem, D. Walgraef & S.J. Zinkle , *J. Comp. Matls. Dsgn*., **8** , 2001, 1.
9. B.N. Singh, N.M. Ghoniem & H Trinkaus, *J. Nucl. Matls*. **307-311**, 2002, 159.
10. A. Hishinuma, A. Kohyama, R.L. Klueh, D.S. Gelles, W. Deitz & K. Erlich, *J. Nucl. Matls*. **258-263**, 1998, 193.
11. R.L. Klueh, M. A. Sokolov, K. Shiba, Y. Miwa & J.P. Robertson, *J. Nucl. Matls*. **258-263**, 1998, 478.
12. D.S. Gelles, *J. Nucl. Matls*. **225**, 1995, 163.
13. B.H. Sencer & F.A. Garner, *J. Nucl. Matls*. **283**, 2000, 164.
14. C. Domain & C.S. Becquart, *Phys Rev B* **65**, 2002, 024103.
15. S. Han, L.A. Zepeda-Ruiz, G.J. Ackland, R. Car & D.J. Srolovitz, *Phys Rev B* **66**, 2002, 220101.
16. D.G. Pettifor, I.I. Oleinik, D. Nguyen-Manh & V. Vitek, *Comp. Mat. Sci.* **23**, 2002, 33.
17. D.J. Bacon, F. Gao and Yu.N. Osetsky, *J. Nucl. Matls.* **276**, 2000.
18. Yu.N. Osetsky and D.J. Bacon, *Modell. Simul. Mater. Sci. Eng*. **11**, 2003, 247.
19. T.S. Hudson, S.L. Dudarev & A.P. Sutton, *J. Nucl. Matls.* **307**, 2002, 976.
20. S. L. Dudarev, A.A. Semenov & C.H. Woo, *Phys. Rev. B* **67**, 2003, 094103.
21. T. Kasuya, K. Ichikawa, M. Fuji & H. Bhadeshia, *Mat. Sci. & Techn.* **15**, 1999, 471.
22. S.G. Roberts, in *Multiscale Phenomena in Plasticity*, eds J. Lepinoux et al., (Kluwer, Netherlands) 2000, 349.
23. B. Devincre & S.G. Roberts, *Acta Metall. & Mater*. **44**, 1996, 2891.

Figure 2: Project timing

			Year 1 (10/04 - 9/05)				**Year 2** (10/05 - 9/06)				**Year 3** (10/06 - 9/07)				**Year 4** (10/07 - 9/08)			
			Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
2.1	Ab-initio, potentials: V, W		▓	▓	▓	▓ 2												
	Ab-initio, potentials: Fe, Cr				▓	▓	▓	▓ 5										
	Ab-initio, potentials: Fe-Cr binaries						▓	▓	▓	▓	▓ 7	▓	▓	▓ 9				
	PDRA (B'fast), RS (Edin), RS (Ox)		░	░	░	░	░	░	░	░	░	░	░	░				
2.2	MD: Collision cascades,	(generic)	▓ 1	▓	▓	▓	▓ 4											
	Screw disln. dynamics,	(V,W)				▓ 2a	▓	▓	▓ 6									
	Disln / defect interactions.	(Fe, Cr, binaries)						▓ 5a	▓	▓	▓ 8,7a	▓	▓	▓ 9a,10	▓	▓ 12	▓	▓ 13b
	PDRA (L'pool)		░	░	░	░	░	░	░	░	░	░	░	░	░	░	░	░
	RS (L'pool)						░	░	░	░	░	░	░	░	░	░	░	░
2.3	kMC - Evolution of cascades		▓ 1a	▓	▓	▓	▓ 4a	▓	▓ 6a	▓	▓ 8a	▓	▓	▓ 10a	▓	▓ 12a		
	kMC RS (Ox)		░	░	░	░	░	░	░	░	░	░	░	░				
2.4	Microstructural modelling						▓ 4b	▓	▓ 6b	▓	▓ 8b	▓	▓	▓ 10b	▓	▓	▓	▓ 13a
	Hardening theory						▓ 4c	▓	▓ 6c	▓	▓ 8c	▓	▓	▓ 10c,11	▓	▓ 12b	▓	▓ 13b
	Microstructure, hardening RS (Cam)						░	░	░	░	░	░	░	░	░	░	░	░
2.5	3D-DD - learning and code importing		▓	▓	▓	▓ 3												
	3D-DD - flow and BDT in "clean" matls					▓ 3a	▓ 4d	▓	▓ 7d	▓	▓ 8d	▓						
	3D-DD - flow and BDT in defect distrns.								▓ 6e	▓	▓ 8e	▓	▓	▓ 10d, 11a	▓	▓ 12c	▓	▓ 13b
	2D-DD - BDT in "clean" matls		▓	▓	▓	▓	▓	▓										
	2D-DD- BDT in defect distrns.						▓ 4e	▓	▓ 6f	▓	▓ 8f	▓	▓	▓ 10e	▓	▓		
	PDRA (Ox)		░	░	░	░	░	░	░	░	░	░	░	░	░	░	░	░
	RS (Ox)						░	░	░	░	░	░	░	░	░	░	░	░

1. Begin work on MD using simple FS- based potentials; pass initial results on radiation damage on to kMC studies as "starter data" (1a). Potentials for V,W derived; pass to MD modelling (1a).
2. Potentials for V & W; pass to MD modelling (2a).
3. 3D-DD code imported from ONERA: adaptation for this project begins (3a).
4. Finish generic MD work, results passed to kMC, and as "starter data" to microstructural modelling and hardening theory, 3D-DD (screw and edge mobilities) and 2D-DD (defects) (4a-e).
5. Potentials for Fe, Cr derived; pass to MD modelling (5a).
6. Finish MD based on new V,W potentials, results passed down as in (4) and to 3D-DD with defects (6a-f).
7. Potentials for Fe/Cr binaries - initial useable potentials; pass to MD modelling (7a).
8. Initial MD results based on new Fe, Cr potentials, results passed down (8a-f).
9. Potentials for Fe-Cr binaries - final potentials; pass to MD modelling (9a).
10. Initial MD results based on new Fe-Cr binary potentials, results passed down (10a-e); results continue to be passed down as MD results acquired.
11. Comparison of results from hardening theory and DD models of flow in defect distributions (11a, 11b).
12. Final stages. Full multi-scale model of flow and BDT functioning.
13. Project finishes. Predictions from (13a) microstructural modelling and (13b) multi-scale model of flow and BDT.