

Materials Data Centre – Report on User Requirements

Summer internship: 8th June – 28th August 2009

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1.0 Background:

The Materials Data Centre project aims to establish an OAI-compliant Materials Data Centre designed to promote data capture and systems interoperability in the engineering materials domain. The work will extend existing DDLs in the engineering sector to incorporate standards-compliant schemas and ontologies. The work will also enhance the fractography repository at <http://www.fract.ses.soton.ac.uk>.

The work will be undertaken as a 3 year PhD project (Mark Scott) starting 1st August 2009. A preliminary summer internship (Charlotte Rimer) has also been set up (8th June-28th August) to progress the work.

Why do we need such a facility?

The engineering sector (both research and industry) currently makes significant investments in generating materials test data. Although established testing standards specify what data needs to be recorded, this data is often not recorded, or may be incompletely recorded due to:

- (1) The data lifespan being longer than that of the storage facilities (computers, programmes etc.)
- (2) More “important” tasks taking precedence over data storage (or conservation), such as analyzing the results and writing reports or papers.
- (3) Concerns about security or IPR issues

Delays in storing the test data may also affect the quality of the information as the data become less accessible and their provenance (meaning records about origin, authenticity, and history of alterations) becomes less reliable or complete.

As surveys such as Material Information on the Internet (<http://www.brinell.kth.se/part1.html>) indicate, in the few cases where data are actually conserved, they are rarely made accessible to the wider community, often miss key information, and are not easy to aggregate with other complementary data sets or facilities. This all means we don't share data effectively, or aren't able to compare and contrast our findings in useful ways (e.g. data mining, or checking the accuracy of our own data, or finding interesting areas of new data space to explore)

The Materials Data Centre (www.materialsdatacentre.com) is one of a series of initiatives in which the University of Southampton aims to promote the capture and conservation of data in the engineering sciences. Similar data centres already exist in other domains. Such facilities allow the universal storage of data in a way that improves and simplifies access, while the application of

modern communication technologies improves data storage and data searching, shortening the processing time for both.

The primary objective of the Materials Data Centre is to allow an ever increasing body of materials data to be accumulated that is of high quality and reliable provenance, with appropriate levels of user access depending on the origin of the data.

2.0 Overview:

This report briefly reviews approaches taken by other projects to repository start-ups and associated e-Science issues and also introduces the key materials concepts that drive some of the suggested data capture requirements for the MDC. As part of the MDC project, an initial assessment of the user requirements has been made through a questionnaire distributed both with the University of Southampton (where the MDC is being developed) and across the wider materials community.

The questionnaire is now available at <http://www.materialsdatacentre.com/questionnaire.html> and we would welcome many more responses, as user requirements will be assessed as an ongoing process throughout the development of the MDC. Responses at this stage indicate that the user requirements are both wide-ranging and somewhat specific to the individual research questions being pursued by the respondents, which poses challenges to the structure of the MDC. There is a predominantly positive response to the concept of sharing authenticated and enriched data, which can be linked to material condition (e.g. including micrographs or even fractographs). However shared concerns include confidentiality of data (for both sponsors and clients) and storage space requirements (particularly for images). There is indication that the potential value of the MDC will be linked to how user friendly it is perceived to be. A number of internal and external users have agreed to test prototype versions of the MDC. The creation of this report by no means represents the end to the requirements gathering stage of this project, but is simply a starting point designed to ensure the initial formulation of the MDC is informed by user requirements. The initial survey aims to establish foremost the activities in which the user is engaged, then the ways in which they use collected data, and finally the individual's data management needs.

The final part of the report presents some user scenarios (based on research activities within the Engineering Materials research group at Southampton University) that span the range of activities revealed by the user requirements assessment, but that also work from established testing standards (where possible). More background on the Engineering Materials research group can be found at: <http://www.southampton.ac.uk/ses/research/engmats/index.shtml>

3.0 Aims:

The primary aim of this internship is to establish the needs of the data centre stakeholders. This will provide information both in terms of the major uses of the data centre, as well as the type and style of information it is required to provide. This is an important and effective step in creating a data centre since it should ensure that what is created is useful to the stakeholders, and therefore will generate further interest in the project.

The second aim is to set out the requirements for a data centre based on these needs. This is fundamental to the further progression of the project, since this will establish the criteria from which the data centre is created. Due to the fact it will be challenging to meet every requirement of every stakeholder from the start, this will take the form of a prioritised list of the major, or most popular, requirements.

4.0 Objectives:

As the project has such a large scope, first set out the problem via a background literature review and the establishment of a work plan.

Establish the stakeholders, their needs and their roles.

Then based on both of the above, establish the questions that would be most effective in finding out the information required, to establish the data centre criteria.

Once the correct questions are established, tailor to each stakeholder group, and question a variety of stakeholders (from research students to industry). This is facilitated since a variety of interested contacts have already been made via the link to the Engineering Materials.

Evaluate results, and create a list of most frequent uses, along with a structured idea of the data and metadata required to make the data centre useful.

Finally, establish some possible user scenarios in more detail to form a basis for the further definition of the MDC.

4.1 Work plan:

A Gantt Chart for the work plan can be found in the appendix of this report.

Week 1: (08 Jun 09 - 12 Jun 09)

- Settle into work.
- Familiarisation with documents on Huddle.
- Complete write-up on Brussels workshop.
- Write internship overview.

Week 2: (15 Jun 09 - 19 Jun 09)

- Develop qualitative description of alloys and failure mechanisms of interest to the project. There will be two exemplars for this; Al-alloys with strength/toughness criteria and Ni-alloys with high temperature property requirements.
- Set out the aims, objectives and work plan for the project.
- Establish who the stakeholders are (refer to stakeholder document).
- Literature review of the development of this approach in other research domains.

Week 3: (22 Jun 09 – 26 Jun 09)

- Research and write questions.
- Begin to interview research students.

Week 4: (29 Jun 09 – 03 Jul 09)

- Interview senior members of the research group.

Week 5: (06 Jul 09 – 10 Jul 09)

- Interview industry.
- Analyse results.

Two week break.

Week 6: (27 Jul 09 – 31 Jul 09)

- Create a use of most popular uses and most important requirements for that data centre.
- Submit interim Report.

Two week break.

Week 7: (17 Aug 09 – 21 Aug 09)

- Write-up user scenarios.
- Develop literature review.

Week 8: (24 Aug 09 – 28 Aug 09)

- Write up the report and finish correlating results.

5.0 Understanding the engineering materials problem:

5.1 Brief overview of alloys.

Materials performance assessment, selection and improvement requires both appropriate performance measurements (e.g. standardised mechanical test results) but also an understanding of microstructure-property relationships. The most enriched mechanical test data will incorporate appropriate microstructural information (including compositional and heat treatment information). A brief introduction to key microstructure/composition information in relevant engineering alloys follows.

5.1.1 Nickel Alloys

Nickel based alloys are developed for high temperature performance and environmental resistance. Nickel has the FCC crystal structure and is therefore both tough and ductile. A typical nickel base superalloy consists of the different following phases:

- A face centred cubic (FCC) continuous γ matrix, which contains α solid solution. Principally consisting of Ni, with Mo, W, Cr, Fe, Co, Re for solid solution strengthening. This is ductile at all temperatures and possesses moderate strength which decreases with an increase in temperature. [1][2]
- Coherent precipitates of which the main strengthening precipitate is γ' : $\text{Ni}_3(\text{Ti,Al})$. This is also FCC but ordered and usually coherent with the γ matrix. The γ' phase is brittle except at very high temperatures, and has very high strength which anomalously increases with temperature, due to thermally activated locking of cross slipping dislocations, up to $\sim 800^\circ\text{C}$. At small sizes it is spherical, but at larger/coarser sizes it adopts a diced cuboidal structure. If the volume fraction (V_f) of γ' is high, we expect a high yield strength, e.g. typically blade alloys have a high V_f of γ' .

Another precipitate strengthening system sometimes found is γ'' or γ^* : Ni_3Nb . This is a body centred tetragonal coherent precipitate, and forms as discs in the matrix. Nickel base alloys that contain this precipitate tend to be INCONELS (Fe containing). [1][2]

- Carbides and Borides. In cast and wrought forms of nickel based superalloys these also play a role in strengthening the material. They tend to be in either of the following forms. MC where Carbon is present in concentrations up to 0.2wt% and M is Ta, Ti, Hf, Nb, Zr. These carbides form initially from the melt, i.e. at temperatures above 1200°C . During processing or service, MC carbides can decompose to other species, such as M_{23}C_6 and M_6C , where M is

mostly Cr, with some Mo, W, Co. These carbides generally form in the solid alloy at temperatures in the range of 700 to 1000°C and prefer to reside on the γ -grain boundaries. In polycrystalline alloys this has an influence on creep. This can be important as they can act as grain boundary pinning. Boron can combine with elements such as Chromium or molybdenum to form borides which reside in the same place. [1][2]

Other phases, such as the topologically closed-packed (TCP) phase's σ , μ , and Laves, can be found in certain superalloys, particularly in the service aged condition i.e. after long thermal exposures. However, the composition of a superalloy is usually chosen to avoid the formation of these compounds. [2][3]

Alloy additions and their functions:

- Al, Ti, are used to form the γ' phase which leads to precipitate strengthening and therefore strongly reduce creep rates. The Al and Ti contents determine to a large extent the amount of γ' formed.
- Mo, W, Cr, Re are solid solution elements in the γ matrix and therefore lead to solid solution strengthening.
- W increases melting point.
- Co increases γ' solidus temperature making it possible to retain γ' to a higher temperature without dissolution.
- Cr increases corrosion resistance by forming a coherent Cr_2O_3 layer which is protective, however it limits Ti, Al additions.
- C is used to form carbides.
- Hf, Ta, Nb are used to form MC carbides. [1]

5.1.2 Aluminium Alloys:

Aluminium alloys cover a wide range of applications, but are often used in applications where light weight and relatively damage tolerant behaviour is required. The alloys also have a FCC crystal structure. There are three main classes of Al-alloys:

1. Casting alloys: based on Al-Si and Al-Mg alloy systems, not usually used in load bearing roles.
2. Wrought non-heat treatable: e.g. Al-Mn and Al-Mg, which have properties controlled by solid solution strengthening and by cold deformation casing work hardening.

3. Wrought heat treatable: e.g. Al-Cu, Al-Mg-Si and Al-Zn-Mg, which develop high strength through precipitation strengthening via heat treatment [4]

5.2 Brief overview of manufacturing processes.

The microstructure of Ni-alloys, in terms of grain size and the age hardening by γ' , are optimised using thermo mechanical and heat treatments.

- Directional solidification castings (DS) are made using controlled withdrawal of the mould from an electrically heated furnace. Where the mould is made by the investment casting (IC) process.
- Single crystal castings (SX) use a similar method, however a multiple turn constriction (or “pigtail”) is placed in the casting base. Only one grain orientation can therefore grow, and this is the $\langle 100 \rangle$ growth direction, which becomes the tensile axis.
- Wrought superalloys are processed by deformation (e.g. forging), solution treatment and subsequent aging process.

Wrought heat treatable Al-alloys are generally ingot cast via the direct chill (DC) process. The ingot is homogenised at high temperature. This removes soluble intermetallic phases (“eutectic phases”), and allows precipitation of small intermetallic particles (e.g. MnAl_6 and ZrAl_3) which control grain structure during any subsequent fabrication. [4]

5.3 Qualitative description of failure processes:

In understanding the performance of any alloys, we need to understand the mechanisms of deformation and failure, and then how these might be measured in standardised (or non standard) testing procedures, the following sections introduce mechanical property concepts and refer (where appropriate) to the relevant testing standards.

5.3.1 Yield Stress:

When a smooth metallic sample is loaded in tension (Fig. 1), initial deformation is elastic (recoverable) with a proportional relationship between stress and strain, defined by the stiffness, E . In this regime, atomic bonds are stretching, but the *relative* positions of the atoms do not change on loading, so on unloading the atoms return to their original positions. Beyond the elastic limit, the strain achieved on further loading suddenly increases, and plastic deformation is occurring. As the material starts to flow or yield, this point is known as the yield stress. The atoms are effectively slipping past each other, in most metals this is due to the movement of line defects (dislocations) in the crystal structure, which effectively cause overall atomic slip to occur once they have traversed the lattice structure. Dislocations can move at much lower stresses than those required to cause

whole planes of atoms to slip simultaneously. In metallic structures, plastic deformation is usually undesirable and the yield stress (or strength) is a primary mechanical property used in much structural design. Defining the onset of yield is therefore important, a usual engineering approach is to establish the stress at which 0.2% plastic strain has been achieved, this is more formally known as the 0.2% proof stress (or strength) but is often what is meant when people refer to the yield strength. The standardised testing approach for this measurement (and other related ones that can be taken from the test) is: BS EN 10002-1:2001. Other useful measures from this test can be the ultimate tensile strength (point M in Fig 1) the % elongation to failure (or ductility) and the stiffness, E . The heart of much materials development and optimisation relies upon predicting microstructure-strength relationships, whereby the microstructural features which affect dislocation motion (grain boundaries, solute atoms, other dislocations, precipitates) are all found to be important.

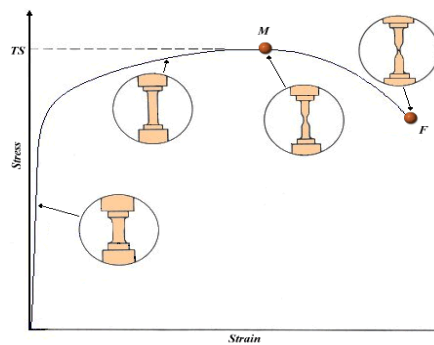


Figure 1: Schematic representation of stress-strain curve for a tensile specimen. After Callister [6]

5.3.2 Fracture toughness:

Fracture toughness is a measure of a material's resistance to fast failure processes in the presence of a notch, or stress concentration feature. In micromechanistic terms it represents the local crack-tip stress distribution required to cause an existing flaw (or notch), in the material, to propagate. It is clearly a useful design parameter in avoiding failure in structures.

The stress intensity, K_I , describes the local stress field at the tip of a crack under linear elastic continuum conditions and can be calculated from simple component geometry and crack length information. It is thus both measurable for a range of structures and physically representative of the local crack tip stress field that controls the fracture process under certain conditions. The fracture toughness, K_{IC} , is the highest value of stress intensity that a material under plane-strain conditions can withstand without fracture and linear elastic continuum assumptions must hold for this measurement to have validity. The worse case scenario for toughness is the highest constraint condition. [5]

K_{Ic} generally increases with decreasing strain rate and increasing temperature. General strengthening methods, such as solid-solution hardening and strain hardening, tend to increase the material's yield stress, but these procedures commonly lead to a decrease in K_{Ic} . Additionally, K_{Ic} typically increases with decreasing grain size as composition and other microstructural variables are held constant [6,7,8]. The standard testing approach to determine fracture toughness in notched and pre-cracked test coupons is detailed in: BS ISO 12108:2002, but the use of K is also important in determining fatigue behaviour of materials. There is a great deal of theoretical background in the use of fracture mechanics to justify this measurement approach, a key requirement is similitude, i.e. that the test coupon result can be used to predict failure processes in a much more complex notched structure or component.

5.3.3 Fatigue:

Fatigue is caused by repeating load cycles often below the yield stress, these fluctuating stresses (and/or strains) produce localised progressive damage. Fatigue cracks will initiate and propagate in areas where the strain is most severe. The process of fatigue has three stages:

- Crack initiation
- Crack propagation
- Sudden fracture across the section. [9]

Fatigue evaluation can take the form of:

1. Total life evaluations, where smooth samples are tested at a range of stress or strain ranges and the no. of cycles to failure recorded (S-N) curves, this combines the process of initiation and growth of the defect. Whilst useful in producing materials ranking, this is not always directly mappable to a component or structure lifing, as these are rarely smooth samples! Additional observations may be made by interrupting the test to image the surface and try to map initiation and crack growth (but this is typically a research approach, rather than a standardised testing procedure)
2. Damage tolerant approaches: these assume a pre-existing defect and attempt to measure the rate of crack growth as a function of some appropriate parameter (usually K).

Fatigue behaviour can be highly dependent on the loading cycle (load range, mean load, waveform, frequency) and testing conditions (environment, temperature) as well as initial defect size and shape. Standardised testing procedures do exist: BS ISO 12108:2002 and ASTM E 647-95a. An understanding of fatigue micromechanisms is required to both improve and select appropriate materials, and these mechanisms are linked to the underlying microstructure. Some regimes of

fatigue behaviour are relatively microstructurally insensitive and generalised design curves can be produced, but other regimes are extremely microstructurally sensitive. Fatigue is essentially a highly localised process (especially when considering initiation or early stages of crack growth) and this throws up challenges in characterising the relevant microstructural information.

5.3.4 Creep:

Creep is defined as deformation (or strain) with respect to time, under stress and at high temperature. Creep is essentially a diffusion controlled deformation mechanism. Mechanisms include bulk diffusion of atoms to relieve stresses, diffusion to assist dislocation motion and grain boundary diffusion allowing grain boundary sliding. Essentially then, creep is the movement of dislocations through the lattice over time. Creep is a time dependent, inelastic and irrecoverable deformation. There are three stages to creep; primary, secondary and tertiary. [10] Standardised testing approaches to creep behaviour also exist.

5.3.5 Fracture mechanism assessment: fractography

All of these failure processes have standardised testing procedures identified, but further evaluation of the failure process at a micromechanistic level is often required. Fractography can be identified as the interpretation of features observed on materials fracture surfaces using a range of analytical techniques. For more background detail see: <http://www.fract.ses.soton.ac.uk/>

Typical assessment approaches include low magnification observations of overall fracture surfaces, sectioning and optical microscopy assessments, scanning electron microscopy observations at a range of magnifications, characterisation using EDX, backscattered electron imaging etc. Typically 2D sections or surface observations are only possible, but a growing body of work is advancing the use of 3D tomography approaches to characterise failure processes in a wide range of materials in-situ. Many of these techniques produce large numbers of images, showing how deformation or local failure processes are interacting with the materials microstructure. For these images to be really useful, they require very careful matching, not only to the specific test conditions, material etc, but also to their specific location on a particular test sample, the conditions under which they were captured (imaging machine settings) any post image processing etc. The sheer volume of data as well as the level of metadata required is challenging, but potentially a highly worthwhile possible extension of the MDC data capture requirements.

5.4 Overview of stakeholders.

Materials Science researcher: a central location to store and manage project data. This group are expected to be the primary users.

Materials Research Groups: data sharing provides a mechanism to promote their work and interact with other groups.

Materials Science Data Reuser: easy access to data of predefined quality.

Data Manager: ability to manage and preserve data in a structured standards-compliant format.

Funder: preservation of the research investment and a guaranteed auditing trail.

Systems developers: data made available in a structured standard-compliant format.

Looking at the role of each stakeholder, in terms of the database, allows the tailoring of questions to be more relevant to each group. The project aims to consider ideas from all of these stakeholder groups. The solution found should aim to satisfy as many of these groups as possible. It is therefore important that we have a candidate from each group in our overall user requirements analysis.

6.0 Literature review:

As previously stated the area of research and development this project covers is highly relevant to current data curation concerns. The concept of storing and sharing data is certainly not new; therefore this is a brief review of existing concepts and data centres from other research areas which will form a basis to the technical background of this project.

The University of Southampton have already been involved in the creation of a data centre for the school of chemistry, and therefore collaboration with the leaders of this project is ongoing. The following is therefore a very brief overview of the findings of the existing project in Chemistry which are considered relevant to the MDC approach.

eCrystals (<http://ecrystals.chem.soton.ac.uk/>) is closest project to the MDC and R4L is also very similar.

eCrystals divided their users into the following groups:

1. Institutions: The federation partners were selected on the basis of their significance in crystallography, but also because they represent a truly global multi-platform data network.
2. Scientists: the individual crystallographers in the laboratory and practising chemists who create the crystal structures as part of their routine workflow.
3. Data centres: The primary data harvesters of eCrystals.
4. Publishers: The RSC is a key publisher in the field and Chemistry Central is an emerging Open Access publisher who will operate a repository to store and link data relating to publications in their journals.
5. Users: scientists in related disciplines, students and other third parties who have a requirement to use crystallographic data as part of their research.

Two additional groups who are associated with the Federation are advisory and third party services. [11]

“R4L (Repository for the laboratory) is a research project investigating and developing digital data and document repositories for laboratory-based science.” [12]

The CombeChem project was developed to test e-Science and integrates existing structure and property data sources within a grid-based information-and knowledge-sharing environment. “[e-](#)

[Science](#) is about global collaboration in key areas of science and the next generation of infrastructure that will enable it.”[13].

The Scientific metadata schema by RAL attempts to outline all the information of interest relating to measuring as part of experiments.

To provide a single method of browsing and searching the contents of all the CCLRC data resources a web based data portal is being developed. The central philosophy is that each facility/data centre is responsible for its own data and metadata and that ownership and residence are untouched by the Portal.

In this context, metadata is considered to be “all the information, additional to the raw data itself, which a potential user of the data would need to know to be able to make full and accurate use of the data in a subsequent scientific analysis.” [14]

Another case study of relevance is the Research Information Centre (RIC) a “virtual research environment” currently being developed by the British Library and the Technical Computing Group at Microsoft. Its purpose is to support researchers in managing the complex range of tasks involved in researching. This involves providing structure to the research process, simplifying resource access, guidance and tools to manage information assets, and integrated collaboration services. It is a response to researcher’s needs and should make the research process more efficient. RIC supports but it does not restrict. [15]

There is a challenge for Computer Science community and the IT industry to deliver powerful and easy-to-use tools and technologies to support Data-Intensive research, and from this comes the development of eScience. World Wide Telescope; a “Seamless Rich Social Media Virtual SkyWeb application for science and education”.

The research pipeline was defined in this project as follows:

- Data Acquisition and Modelling

–Data capture from source, cleaning, storage, etc.

–SQL Server, SSIS, Windows WF

- Support Collaboration

–Allow researchers to work together, share context, and facilitate interactions

–SharePoint Server, One Note 2007 (shared)

- Data Analysis, Modelling, and Visualization

–Mining techniques (OLAP, cubes) and visual analytics

–SQL Analysis Services, BI, Excel, Optima, SILK (MSR-A)

- Disseminate and Share Research Outputs

–Publish, Present, Blog, Review and Rate

–Word, PowerPoint

- Archiving

–Published literature, reference data, curate data, etc.

–SQL Server [16]

Why capture data? Data driven approaches can be broadly classified as follows; regression approaches where the input data set produces a continuous output or outputs, and classification where input data is used to define the class to which it correlates. “An adaptive numerical model effectively searches parameter and function space in finding a solution, which can also be considered to be an optimising problem” [17]. In searching across a broader range of materials data, drawing together authenticated, quality data from many users, new knowledge discovery should be a possibility, but data driven approaches are only as good as the data upon which they are based.

Metadata is data about data; it can be syntactic or semantic [18]. This is a huge area of research for the PhD student to explore.

Another existing case study for this type of data centre is the Health Care and Life Sciences interest group who used linked data principles whereby;

1. Use URIs as names for things.
2. Use HTTP URIs so that people can look up those names.
3. When someone looks up a URI, provide useful RDF information.
4. Include RDF statements that link to other URIs so that they can discover related things.

They found that terminology varied across users and therefore there was a requirement to define set terminology in order to create a universally usable data centre. [19]

The following reasons as to why sharing data is difficult have been defined:

- Unusual file formats mean that finding a method of sharing and storing these files is considered more effort than the end result is worth.
- Experimental conditions are highly variable and therefore data is rarely comparable or useful beyond its original purpose.
- A lack of motivation for researchers to share data. [20]

Therefore any data centre created must aim to combat these difficulties.

Whilst this information can be used to ensure this project avoids the difficulties of previous projects it remains unique to the area of research on which it is focused, thus creating the need for user scenarios and research into user requirements.

6.1.1 Semantic Web:

“The semantic web is an extension of the current Web that enables navigation and meaningful use of digital resources by automatic process. It is based on common formats that support aggregation and integration of data drawn from diverse sources.”

It establishes connects between data sets using statements known as “triples” which are a subject, predicate and object.

A Resource Description Framework (RDF) is fundamental to the semantic web creation, as it gives a formal specification for the syntax and semantics of triples. Other requirements are:

- The specification of a query language which will retrieve related statements from the data centre.
- Languages which define the controlled vocabularies and ontologies which aid interoperability.

- Tools and strategies to manipulate data into the required format.

Semantic coupling of the database to an ontology offers a solution to interoperability. [21]

6.1.2 Glossary of terms:

ISO = International Standards Organisation

Ontology = “explicit (formal) computer stored specification of an agreed and shared conceptualisation” Gruber TR (1993).

Schema = describes the structure of the document.

URI = Uniform Resource Identifier = a string of characters used to identify a resource on the internet.

XML = Extensible Mark-up Language – designed to carry not display data. [22]

RDF = Resource Description Framework – an initiative of the World Wide Web consortium (W3C) and is about metadata for web resources. Essentially it is a means of developing tools and applications using a common syntax for describing these resources. [23]

Metadata = structured information that describes the characteristics of a resource. [24]

MatML=an extensible language developed specifically for the exchange of materials data. [25]

UML = Unified Modelling Language = a modelling syntax aimed primarily at creating models of software based systems. [26]

GUI = Graphical User Interface = a graphical rather than purely textual user interface to a computer. [27]

OWL = a web ontology language designed for use by applications that need to process the content of information rather than just presenting it. [28]

6.1.3 Software development requirements gathering methodologies:

This is essentially researching different approaches to forming a specification that can be used to design the software.

In software and systems engineering a use case is a description of a system’s behaviour as it responds to a request originating outside the system. The technique is to capture a system’s behavioural requirements by detailing scenario-driven threads through the functional requirements.

The important part of Use Case is writing not the diagrams and relationships. Use case diagrams can be considered as context diagrams.

A key motivation of the use case idea is the consideration and organisation of requirements in the context of the goals and scenarios of using a system. This improves cohesion and comprehension. Non-functional requirements can be placed in a Supplementary Specification. [29] However the requirement to pin down possible materials researcher's use of the future MDC requires an initially less formal detailing of the research process, which we term a user scenario.

7.0 User Scenarios:

A user scenario should capture the process a researcher (and potential data centre user) goes through in performing the type of standardised test the centre hopes to gather data from. These user scenarios will therefore form examples from which the data centre can be built. In other words user scenarios aim to bridge the gap between what the user does and the capabilities of the data centre. It is important to establish that these are business style user scenarios not software use cases and are therefore less technically defined. There was originally some difficulty in the materials users understanding why the use case/user scenario approach would be of benefit, as they seemed very focused/specific and therefore didn't allow room for originality or modifications as is desirable from a materials research perspective. However they should help the MDC software designer to understand the process undertaken by a materials researcher, and therefore allow the data centre to be tailored towards the users. As the user scenarios themselves will reveal, their style is highly dependent on the person who provided them. In other words people who have more of a teaching background explain a process in one style, whereas a fourth year EngD student looks at it much more from the prospective of what he'd like the database to provide with respect to a particular use. Another researcher has provided a very detailed "how to" procedure in using the testing equipment.

User Scenario 1: Long Crack Threshold Fatigue Testing:

User: K.A.Soady@soton.ac.uk

1. Measure sample dimensions accurately: 2D large scale foil analogue of specific specimen geometry – incremental extension (by cutting) and monitor voltage (potential difference) change, V/V_0 as a function of a/W (standard geometry definitions).
2. Overall experimental procedure, three point bend follow (BS12108.2002)
3. Define likely range of ΔK and then work out the load levels required for a midpoint in the ΔK -range as per the British Standard.
4. Set up specimen carefully ensuring alignment, sharpen notch root with razor blade to ensure uniform crack initiation. Use displacement control and "load protect" safety feature. With specimen under low load, apply constant current contacts and spot weld P.D. wires at diagonal points across crack mouth. Check p.d. amplifier gains and constant current settings, leave specimen to stabilise for at least an hour to ensure no current drift when no crack growth occurring.

5. Using load control on test machine, complete constant ΔK level growth for four monotonic plastic zone sizes at each ΔK level, and apply successive ΔK step decreases (known as “major” turndowns, of no greater than 10%) to threshold.
6. Calculations completed before the experiment (typically in a spreadsheet format) are used to monitor how “constant” ΔK is within each step, so p.d. used to define crack length, which defines ΔK in terms of constant load range applied by the test machine, as crack length increases, for a constant load range, ΔK will also increase. Once ΔK has risen by 2% loads adjusted to maintain desired ΔK level. So constant ΔK achieved to within $\pm 2\%$ via “minor” turndowns.
7. P.D. monitored continuously to ensure load turn downs occur at correct p.d. (crack length) readings
8. $< 1 \times 10^{-8} \text{m}$ per cycle means the threshold has been reached.
9. Phase 2: turn loads back up to a defined ΔK point to get some overlap in crack growth rate data between load shedding and this subsequent constant load, growth out regime. Then apply constant load range, monitoring P.D. changes until failure.
10. In setting test machine must calculate mean load and load amplitude for all required load ranges.
11. When a/W is equal to 0.75 calibration no longer applies and K no longer valid (probably, although this needs checked post-test and is also dependent on yield strength). So test terminated (may get fast failure before this point)
12. Then measure the crack from the fracture surface at three representative points (as per testing standard) and re-calibrate V/V_0 versus a/W calibration for this particular test. This calibration to be used in subsequent data analysis.
13. The data logger records potential difference as a function of time, therefore need to convert V/V_0 to a/w and time to N (no. of cycles) then plot a against N . This is for both grow down to threshold, where a vs N should be constant for constant ΔK steps and for growth out where load range is constant so ΔK is increasing and a versus N will be an accelerating curve. This is a possible raw data upload point, but LOTS of metadata and experimental method would need to be captured.
14. For threshold, we recalculate constant ΔK levels (using post-test calibration and known loads etc) therefore determine da/dN (should be a constant gradient for a given ΔK) for each ΔK step and plot finite da/dN versus ΔK points.
15. To obtain growth out accelerating a versus N curve is non trivial. Original V/V_0 versus time curve has lots of noise (dependent on many factors in p.d. system, which are not captured

for paper reporting purposes), therefore need to data smooth to produce a useable a versus N . The data for grow-out is more continuously varying, hand measurements from the old charts in Philippa's time (!) used to produce an "expert" smoothing, which is actually much more difficult to produce from the vast amount of data logger data. Curve fit approaches can be applied, or digitising of the experimental curve and taking representative values via human intervention – this is typically not discussed in journal experimental write-ups

16. Once you have a useable a versus N curve Use the secant method to obtain the average gradient (defined in standard).
17. The final output is the curve of da/dN against $\log \Delta K$, with all relevant test and materials conditions attached. (A user should want to know how someone had analysed their data i.e. the reduction method).

User Scenario 2: Tensile Testing: User: K.A.Soady@soton.ac.uk

1. Measure sample dimensions accurately.
2. Place the strain gauges or extensometer on the sample gauge length. Three lead wire connection to Vishay Strain Smart.
3. The loading conditions/rate for the tensile test is defined by BS 10002-1:2001.
4. Control test using displacement control on machine and set rate of extension on testing machine.
5. End test at defined maximum load for predefined stress, to avoid damaging strain measuring devices (or can continue until sample failure, it depends).
6. Vishay connected to Instron testing machine which records load (and strain) data and is calibrated with control software.
7. The outputs (data point number, time, strain, and load) give everything required.
8. Data analysis is in terms of engineering stress/strain; convert the load using equation for nominal stress, requires specimen dimensions, other metadata also required on material, test conditions (temperature) etc.

User Scenario 3: Fractography: User: stewart@soton.ac.uk

Fractography is essentially the imaging and analysis of a fracture surface.

1. Specimen Identification: Material (specification – composition/reference), heat treatment/processing history, test conditions (loading conditions – fatigue, creep, tensile, LCF, temperature, environment – air, vacuum, fluids, lubricants, and associated parameters), date and relevant calibration certificates.
2. Specimen Preparation:

- a. As tested
 - b. Polished and mounted – technique used (need to know grinding stages, polishing stages, cloths/lubricants/polishing pastes used)
 - c. Plated – material and application method/process
 - d. Etched – etch used (exact composition and function), time, temperature etc.
 - e. Any further cleaning
3. Microscope/imaging technique – camera, optical microscope, optical microscope, electron microscope (SEM, FEGSEM. TEM)
 4. Microscope details – magnification, scale bar/graticule comparator, microscope/camera combination (define camera type, image sizes, grey-scale/monochrome), SEM – working distance, power of beam.
 5. Type of image
 6. Identify image – generation/input
 7. Annotated overview – location on fracture surface, attributes e.g. ΔK , what was being looked at (general surface condition, striations, features of note and why the shot was taken e.g. investigation of feature/general overview).
 8. EDX – x-rays within SEM – relevant INCA files.

Would also like to know if and where the original specimen is held and where, and possibly identify the academic involved for vetting purposes. Avoiding mandatory fields for data upload is ideal and an option for inputting general remarks would also be appreciated.

User Scenario 4a: Plain bend bar testing for SN curves: User: tom2g08@soton.ac.uk

(the full instructions for the machine set-up can be found in the appendix of this report)

1. Polish the surface of interest to OPS standard.
2. Turn on machine
3. Turn on agitator
4. Leave for 20 minutes
5. Apply pressure (high or low), normally high
6. Warm-up machine
7. Make sure of position control
8. Chose waveform (cyclic/static) – cyclic for fatigue. Type of curve is square, sinusoidal or trapezoidal.
9. Set to 15mm and low frequency (approximately 2)

10. Press Start (leave for 20minutes to warm up)
11. Start test by:
12. Place appropriate reaction block – check alignment!
13. Load cell – reads the load applied.
14. Place dowels – these allow movement – corrects misalignment. (point contact would allow full adjustment)
15. This is a four point bend.
16. Beam theory calculations are only accurate to the point of yield stress. Therefore to measure the actual stress across the specimen use of a strain gauge is required.
17. Set up the amplitude and type of loading to achieve required top surface stress.
18. Position control – can use auto tune but this process ensures the machine knows where it is.
19. To load sample – raise the actuator so that the specimen just touches the rollers. Set the machine so that if a mistake is made it stops, in other words set limits. 0.2kN will hold the specimen without bending it.
20. Start test – switch from load protect to load control.
21. Maximum stress = maximum load (apply load not stress) – add and subtract amplitude – set points.
22. Set cyclic waveform, setting amplitude and frequency (normally 15-20).
23. Load auto-tuning – for this the specimen must be loaded before the yield point.
24. To tare load balance the machine.
25. Go to minimum load and set up loading parameters.
26. Set up adaptive.
27. Set up amplitude control.
28. Set up reading i.e. what you want to measure, using the counter. Interested in cycles to failure in this case.
29. Set limits 10% above maximum and below minimum to ensure the machine stops the test at the correct point.
30. Put safety screens in place.
31. Start and supervise machine, record number of cycles to failure.
32. Supervisor note, this is what all the other users also have to do, but they didn't give this level of detail!

User Scenario 4b: Plain bend bar testing for short crack initiation and growth with replication: User: tom2g08@soton.ac.uk

1. Short crack test has the same set-up as SN.

2. Interested in how the specimen is failing not just the cycles to failure (short and long cracks don't form or behave in the same way!). Want to know at what stage the crack forms and what influences its formation.
3. Need acetate replicas every 5000 cycles, set machine to halt cycling every 5000 cycles.
4. Apply acetone to the acetate block surface (by dipping) to make it melt, then place the acetate on the specimen surface until it dries (approximately 1minute), then remove acetate replica and place under the microscope for examination.
5. A series of acetate replicas can then be used to plot number of cycles against observed surface crack length (note issues raised in fractography about scale measurement requirements) and from this the a versus N curve is found. This also provides a record with which to trace the movement from the origin and observe the microstructure interactions.
6. a versus N curve can be converted to da/dN versus ΔK using secant method and appropriate K – calculation from literature (NOT a standard)

8.0 Questionnaire Methodology:

The primary aim of this project is to establish the user requirements of a materials data centre. To that end several methods of questioning users have been developed to achieve this. For each method a common set of questions was created using an iterative process. The primary stage in establishing user requirements was to establish the potential user groups themselves. This allowed questions to be created from the perspective of a user.

The questions created, finally totalling twelve, each consisted of two parts; a leading introductory part with a yes/no answer, and then a follow up part which allows the user to impart further explanation or comment. The topics for questioning flow throughout the questionnaire, and can be considered to be in three parts; data, standardisation and storage.

There were three methods of distributing the questionnaire; paper copies filled out by individuals but in a group environment, one on one interviews with academics and a web-based questionnaire.

8.1 Sample:

The sample taken is as wide ranging as possible and varied from undergraduate users to academics and some members of industry. Contacts used ranged from within the Southampton University engineering materials research group to other universities, and contacts met at conferences. To date (28th August) there are 54 user responses. As it stands currently the sample group consists of the following; 17 PhD students, 22 academics, 3 people from industry, 3 undergraduates and 9 postdoctoral researchers. The responses from the web-based questionnaire have been incorporated into this report, but this ongoing user-requirements assessment will be updated on a monthly basis (Action on Mark Scott).

9.0 The questions:

1. Does your research focus on specific materials? Yes/No

74% of users answered yes.

Which ones and with what objectives?

Most common alloys named here were Aluminium (20%), Titanium (20%), Nickel (15%), Steel (20%) and CFRP (25%). Less specific answers were given in the website responses.

2. Do you already use standardised testing techniques? Yes/No

77% of users answered yes

If so which ones and would you want to specify new testing methodologies?

BSI and ASTM were the most common sources for standardisation. These predominantly included fatigue, tensile, hardness, surface roughness, three point bending, four point bending, long and short crack tests and Charpy impact. Users also reported use of ISOs.

3. Does your research depend on working with experimental data? Yes/No

80% of users answered yes.

Measured (observational, experimental) or derived and for what purpose e.g. FEA, modelling, data mining?

The most common answer by far here, with 54% of users citing it as a purpose, was FEA. Most users were interested in measured data, but there were also a proportion (18%) interested in derived data.

4. Do you ever use data from other sources? Yes/No

74% of users answered yes

What is your experience of the availability, quality, and usefulness of this sort of data?

Essentially the outcome of this question showed that the availability, quality and usefulness of this data were highly variable. It is fair to say that for the most part that simple data (common values) was much easier to find than more difficult data (see appendix of comments), such as high quality images.

5. Is there ever a requirement to augment your data from other sources, such as literature and web-enabled databases? Yes/No

71% of users answered yes

What are the circumstances?

The most common answers here were that data augmentation is used either in the literature review, or as a comparison for results achieved by the user.

6. Would you find it useful to have a universal method of storing data? Yes/No

75% of users answered yes

What type of data would you find it useful to store and to whom would you like to make it available?

It is fair to say users were unsure of the possibilities and viability here. To get a clear list of deliverables a much larger sample size is required, as there is currently little commonality of requirements established.

7. Have you ever needed to use experimental data from earlier years and/or previous projects? Yes/No

76% of users answered yes

What are your experiences locating and using such data?

Overwhelming response (57%) reporting finding this data was difficult and time consuming.

8. Have you ever shared your data either on request or in the context of collaboration? Yes/No

67% of users answered yes

What have been your experiences and did/would you have any reservations about sharing your data?

The major concerns here were confidentiality and acknowledgement, although there were also concerns over the commercial value of data. Mutually beneficial relationship required.

9. Do you have security concerns for the data you would be adding to the data centre?

Yes/No

46% of users answered yes

What are the major issues?

Out of all the questions this was the question with the lowest percentage of users answering yes. Commercial sensitivity was a major concern in this area, however sharing published data was not considered an issue.

10. Do you consider conservation of experimental data worthwhile? Yes/No

87% of users answered yes

What do you think would be the advantages and disadvantages?

The question had the most positive response of all the questions. Here users wanted the facility in order to back-up their work, but also believed it would prevent the repetition of work and therefore create greater continuity. Concerns were related to the cost and space requirements.

11. Would you be prepared to trial the data centre? Yes/No

66% of users answered yes

If you supplied data to the centre how do you envisage it being used and what constraints would you need to apply?

Most users agreed there would need to be some sort of restriction on data access, however to get a clearer view of the uses envisaged again a greater sample size is required.

12. In general would you like to see the engineering materials sector moving towards a more consistent/standardised data layout? Yes/No

83% of users answered yes

If this is the case what would you ideally like to find in a data centre and what are your major concerns as a user?

Once again for this question there were lots of concerns over feasibility, with the majority of users agreeing it's a good idea in an ideal world. There were also concerns that standardisation would inhibit progression. (Fuller listings can be found in the appendix).

9.1 Website information:

The full results from the website to date are displayed in the appendix to the report. However it is important to note that the comments from the website survey matched well with the paper copies of the questionnaire.

9.2 Comparison of Website and Paper Questionnaire Results:

Question number	Percentage answered yes		
	Web results	Paper results	Average
1	81	66	74
2	68	86	77
3	84	76	80
4	76	72	74
5	80	62	71
6	80	69	75
7	76	76	76
8	72	62	67
9	44	45	44
10	84	90	87
11	56	76	66
12	80	86	83

Table 1 : table comparing the percentage "yes" responses between the two types of questionnaire. (Highlighted figures show marked variation in results from the website and the paper questionnaire).

As shown by the table above the level of response to the questions is not always comparable between the website results and the paper questionnaires. This may have something to do with the unintended influence which occurs during a face to face interview. The significant differences in results show users from the website answers are more likely to focus on a specific material, are less likely to use standardised testing techniques, are more likely to augment their data and are less

prepared to trial the data centre. However overall the feedback for the questions was very positive, showing this area of development is welcomed by users.

10.0 Conclusions:

This report briefly reviews approaches taken by other projects to repository start-ups and associated e-Science issues and also introduces the key materials concepts that drive some of the suggested data capture requirements for the MDC. As part of the MDC project, an initial assessment of the user requirements has been made through a questionnaire distributed both with the University of Southampton (where the MDC is being developed) and across the wider materials community.

The questionnaire is now available at <http://www.materialsdatacentre.com/questionnaire.html> and we would welcome many more responses, as user requirements will be assessed as an ongoing process throughout the development of the MDC. Responses at this stage indicate that the user requirements are both wide-ranging and somewhat specific to the individual research questions being pursued by the respondents, which poses challenges to the structure of the MDC. There is a predominantly positive response to the concept of sharing authenticated and enriched data, which can be linked to material condition (e.g. including micrographs or even fractographs). However shared concerns include confidentiality of data (for both sponsors and clients) and storage space requirements (particularly for images). There is indication that the potential value of the MDC will be linked to how user friendly it is perceived to be. A number of internal and external users have agreed to test prototype versions of the MDC. The creation of this report is a starting point designed to ensure the initial formulation of the MDC is informed by user requirements. The initial survey aimed to establish foremost the activities in which the user is engaged, then the ways in which they use collected data, and finally the individual's data management needs.

The final part of the report presents some user scenarios (based on research activities within the Engineering Materials research group at Southampton University) that span the range of activities revealed by the user requirements assessment, but that also work from established testing standards (where possible). More background on the Engineering Materials research group can be found at: <http://www.southampton.ac.uk/ses/research/engmats/index.shtml>

11.0 Future Work:

The User Scenarios and user requirements developed in this report create a starting point for the development of a Materials Data Centre (MDC). However the User Scenarios are only a simplified/standardised case and will require further development as the project progresses. Also

the current user requirements are by no means an exhaustive list. The website continues to run, and there is definite potential to get further, more detailed input from parties interested in the project. The website should be continually checked monthly throughout the duration of the MDC project.

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Appendix 1: Gantt Chart

Task Description	Week Starting	08-Jun	15-Jun	22-Jun	29-Jun	06-Jul
	Week no.	1	2	3	4	5
Workshop Overview						
Internship Overview						
Background Research						
Literature Review						
Project Aims, Objective and Workplan						
Establish Stakeholders						
Research Interview Questions						
Write Interview Questions						
Develop case studies						
Interview Stakeholder Groups						
Analyse Results						
Create Database Requirements						
Develop Use Cases						
Write-up report						

Appendix 2: Instron One - Setting up for high temperature fatigue testing

1. Emergencies

The Instron 8500 Series can be stopped quickly in an emergency by taking the following action:

IN EMERGENCY

Press large red button on front of Instron

2. Safety Limits

Safety limits can be set in terms of load and position. They are set for several reasons:

- a. As a back up to protect you during setting up – BUT NOTE they should not be relied upon, and the onus is on you to keep any part of your body outside of the loading path of the machine. (Load protect limit)
- b. To stop the experiment when the specimen fails (Max and Min limits)
- c. To prevent a specimen being overloaded (Max and Min limits)

Always apply appropriate safety limits and think before setting them what they are trying to prevent.

3. Sign Convention

Think about what inputs you are making as normally compressive loads are required. These should be preceded by a “-“(minus) sign, otherwise unloading can occur with obvious loss of set up etc.

4. Switching on

- a. At wall switch on Box A and Box B. (Both boxes are required for cooling fans to operate).
 - i. By turning knob to 1 and pressing start.
- b. Wait until hydraulics are ready (about 3 minutes wait)

5. Warming up

- a. Turn hydraulics on.
 - i. Press actuator standby button
 - ii. Press low button
 - iii. Press high button (possibly faulty light)
- b. Raise lower grip (as actuator ram settles on lower internal stop, lower stop is about -60 on position display)
 - i. Use actuator jog buttons to move
 - ii. Ensure sufficient clearance for warm up wave form **suggest position of 25mm**

- c. Choose a display for load information
 - i. By selecting display 1 or 2 from load panel
 - ii. **Select track**

- d. Choose a display for position information
 - i. By selecting other display (2 or 1) from **position** panel
 - ii. **Select track**

- e. Define waveform to warm up machine
 - i. Press position
 - ii. Select immediate (lower panel) – position light should now be lit
 - iii. Press waveform
 - iv. Select parameters on lower panel by using keying in pad (Suggest 10mm amplitude, 2 Hz frequency, Sine wave)
 - v. Press start on lower panel (left side)
 - vi. Allow Instron 20-30 minutes to warm up
 - vii. Press finish on lower panel (left side) to stop waveform.

6. Installing test sample

- a. Ensure appropriate reaction block fitted

- b. Balance load train (to account for any mass added or taken away, if this is not done load protect value may be lower than mass difference and therefore cause a nuisance disconnection of the Instron)
 - i. Press load pad
 - ii. Press set up
 - iii. Press Cal
 - iv. Press Cal
 - v. Press Balance
 - vi. Calibrate light flashes until calibration complete
 - vii. Done only once for the same set up.

- c. Position autotune. Ensure actuator is at the mid point of its stroke.
 - i. While in the position channel, press set up
 - ii. Press loop
 - iii. Change autotune settings if necessary
 - iv. Press auto
 - v. Calibrate light flashes until calibration complete
 - vi. Done only once for the same set up. The values can be saved & recalled during subsequent tests.

- d. Apply load protection (Minimise damage to user – 0.2kN is around 20 kg)

- i. Press load protect button
 - ii. Define load on keypad (Suggest 0.2kN)
 - iii. Select on (lower control panel)
 - iv. Check warning light comes on

- e. **THIS STEP IS ONLY REQUIRED IF THE LOWER RAM IS OBVIOUSLY STICKING I.E. WHEN YOU MAKE A SMALL ADJUSTMENT TO THE POSITION IT DOESN'T MOVE OTHERWISE THIS SHOULD BE SET BETWEEN 1-2%** Set up Dither during sample positioning, as fine movements are required – helps overcome seal sticking in hydraulic ram.
 - i. Press set up **IN POSITION PAD**
 - ii. Press more
 - iii. Press Dither
 - iv. **Set to around 7% OR UNTIL YOU HEAR IT KICK IN**

- f. Check Instron is still set to position control
 - i. Light by position on top control panel is lit, if not
 - ii. Press position pad
 - iii. Press immed
 - iv. Position light should now be lit

- g. Lightly clamp test sample to hold it steady
 - i. Check load protect light still on
 - ii. Position rollers etc required for test
 - iii. Raise lower grip slowly using hydraulic ram “jog” buttons on front of Instron (two buttons, one fast, one slow!)
 - iv. Aim to “pinch” specimen so that final set up can be carried out
 - v. Raise lower grip until approximately 0.1kN is indicated on load screen.
 - vi. Carry out final set up

7. **REFINE** position limits to protect machine

- a. Maximum position
 - i. Press max (On position control panel)
 - ii. Set position limit to 1mm more than actual current displayed position
 - iii. Choose action (Systop)
 - iv. Press on
 - v. Check light by max

- b. Minimum position
 - i. Press min (On position control panel)
 - ii. Set position limit to 1mm less than actual current displayed position
 - iii. Choose action (Systop)
 - iv. Press on
 - v. Check light by min (both lights now lit)

8. **REFINE** load limits to prevent specimen being unloaded

- a. **Minimum load**

- i. Press **max** (On load control panel)
- ii. Set load limit to -0.1kN (compressive loading situations)
- iii. Choose action (Systop)
- iv. Press on
- v. Check light by min
- vi. Check the min value is correct and still lit

From this point onwards load protection has been removed and anything in the way of the loading path of the machine will be subjected to the requested and any error load – This includes you or any part of you!

- b. Remove load protection
 - i. Press load protect
 - ii. Press off
 - iii. Check load protect light now off

- c. Still in position control increase load to desired level.
 - i. Press set point
 - ii. Use thumb wheel control on lower panel to change set point?
 - iii. Stop when the desired load is registered on load display
 - iv. Remember to precede any load entry with a -ve sign (**otherwise unloading with occur!**)

9. Loading specimen (Trapezoidal waveform - load)

- a. Put Instron in Load control
 - i. Press load button
 - ii. Press immed
 - iii. Check light next to load button now lit

- b. Load autotune. Ensure specimen is loaded below its yield point
 - i. While in the load channel, press set up
 - ii. Press loop
 - iii. Change autotune settings so that specimen remains elastic during autotune
 - iv. Press auto
 - v. Calibrate light flashes until calibration complete
 - vi. Done only once for the same type of specimen & set up. The values can be saved & recalled during subsequent tests.

- c. Apply mean load
 - i. Calculate mean load required (remember sign)

- ii. Press set point
- iii. Increase / decrease load with thumbwheel until mean value reached (when near the load you can just type it in)

d. Set Waveform – sets each half of waveform separately (check set up is either side of mean)

- i. Press waveform (on load control panel)
- ii. Press load
- iii. Press Trapz
- iv. Press kN, input required amplitude, press enter
- v. Press kN/sec, set required loading rate
- vi. Press more – to set up other side of waveform
- vii. Press kN, input required amplitude, press enter
- viii. Press kN/sec, set required loading rate
- ix. For sinusoidal wave form, press load, sine, press kN & input amplitude. Set the required frequency and you are ready to go!

e. Reset counters

- i. Press counter timer
- ii. Press reset
- iii. Press current cycles
- iv. Press total cycles
- v. Press elapsed time
- vi. Press return

f. Change Maximum position limit

- i. Press max (On position control panel)
- ii. Set position limit to 1mm more than actual current displayed position
- iii. Choose action (Systop)
- iv. Press on
- v. Check light by max

g. Change Minimum position limit

- i. Press min (On position control panel)
- ii. Set position limit to 1mm less than actual current displayed position
- iii. Choose action (Systop)
- iv. Press on
- v. Check light by min (both lights now lit)

h. Set Maximum load limit

- i. Press max (On load control panel)
- ii. Set load limit, max load + 5-10%
- iii. Choose action (Systop)
- iv. Press on
- v. Check light by max

- i. Reduce dither to between 1-2%?

START WAVEFORM

- a. Set adaptive control
 - i. Press function
 - ii. Press more
 - iii. Press adaptive
 - iv. Press on

b. Check amplitude prior to applying amplitude control

- v. Amplitude on display should be 95% of selected, if not gain should be changed
- vi. Press set up
- vii. Press loop
- viii. Press prop
- ix. Increase or decrease gain to obtain required amplitude
- x. This is done if load autotune failed.

- c. Start loading
 - xi. Start with low waveform (i.e., low frequency) – No mandatory!
 - xii. Press start
 - xiii. Press amplitude control
 - xiv. Check amplitude correct on load display

10. Run test

- a. Complete unattended experiment card if required
- b. Check on test periodically
- c. If high temperature test, check water supply and thermocouple
- d. Test will auto stop when complete

11. Record information

- a. Record
 - i. Current cycles
 - ii. Total cycles
 - iii. Elapsed time

12. Completion

- a. Remove limits to allow hydraulics to be applied
 - i. Select each limit in turn
 - ii. Press off

- b. Turn off adaptive & amplitude control

- c. Lower sample
 - i. Select position
 - ii. Press immed
 - iii. Use "jog" buttons to lower sample

- d. Switch off hydraulics
 - i. Press off on hydraulic control panel

- e. Remove sample etc.

- f. Switch off Inston at wall

Appendix 3: Full listing of question responses.

Specific materials:

- (phd) WC-Co
- (phd) Al-alloys
- (phd) Hydroxyapatite titanium alloy
- (undergraduate) Acrylic bone cement
- (phd) 12 Cr ferric heat resistant steels
- (PostDoc) Ni-superalloys
- (phd) CFRP
- (phd) Carbon Fibre Composites
- (Academic) Ti alloy, Ni superalloy, Al, Carbon Fibre, pressure vessel steels
- (academic) Al, steel alloys, single crystals DS (creep fatigue, fracture)
- (academic) Mostly metallics in engine applications (Ni based – aero engines, steels – power generation, Al-Si – pistons)
- (academic) Al alloy – micro structural properties, plastic deformation, expected failure mechanisms
- (phd) Bone/lung tissue
- (academic) hard coatings, shape-alloys (based on properties/cost)
- (PostDoc) dyes, silicon solar cells
- (PostDoc) Ti and CoCr alloys
- (Phd) Inert bio ceramic
- (undergraduate) ceramic with CFR-PEEK
- (industry) aluminium, steel, CFRP.
- (phd) Ti, CoCr, UHMWPE, PMMA.
- (academic) austenitic stainless steel, nuclear graphite, magnesium alloys, understanding the mechanisms of stress corrosion, fracture, fatigue.
- polymethylmethacrylate, stainless steel, titanium alloy, cobalt chromium alloy)
- mechanical performance prediction of biomaterials (e.g. alumina, zirconia,
- Martensitically Transforming Materials
- 304 austenitic stainless steel in relation to residual stress and surface treatments
- cool ones
- Nuclear Graphite Decommissioning
- Ceramics. Nuclear.
- Aerospace and automotive materials with an emphasis on damage tolerance

- Mechanical properties of Polymers and of Functional Materials (optical fibres and flexible flat-panel displays); Polymer tribology.
- Microstructural analysis
- Tribology
- Rare-earth metals/alloys/intermetallics-crystal growth and characterisation PLD thin films of functional materials for device manufacture
- Steels - microstructure-property links
- Several alloys
- Structural materials like Steels, sometimes coated steels e.g. Galvanised and colour coated materials.
- Cast aluminium Al-Si alloys for pistons in light vehicles. The objective is to characterise their microstructure and the micromechanisms of fatigue failure.
- Aerospace aluminium alloys
- steels - understanding phase transformations, resulting microstructures and the effect on properties; improving the properties of welds
- crystalline and amorphous metals. Measurement of residual stresses at micron and sub-micron scale.
- My research focus on ferritic steels for pressure vessels and pipelines, and my objective is to analyze the correlation between fatigue crack propagation and redistribution/relaxation of welding residual stresses.
- ductile materials to determine component life

Standardised tests:

- ISO ones
- Fatigue, tensile testing, occasionally fracture toughness. Several variants on the fatigue methodologies, often have non-standard specimens due to materials supply constraints
- nanoindentation, testing ok for my use currently. optical and SEM microscope, testing ok for my use currently. surface roughness, via laser scanner, standard technique not found (or not easy to find) for surfaces in general in AISI standard volumes, need protocol set out. xray diffraction to measure residual stress at surface, protocol ok, but could do with what each time of machine is capable of and how and also how to use data acquired. tensile testing, standard good.
- I use both standard and non-standard test techniques - mainly for research purposes, e.g. residual stress effects on fracture, miniaturised testing, etc.
- ISO 7206 mainly - represents a worst case scenario in terms of implant fixation and could be improved
- ASTM Standard E111 ASTM Standard 1820

- Standardized mechanical testing methods
- In the future I will use standardised fatigue testing techniques based on BS ISO 12108.
- We are developing residual stress measurement techniques based on SEM-FIB mechanical relaxation, Digital Image Correlation Analysis of displacement/strains and Finite-Element Analysis
- Tensile and ETMT for temperature affects.
- (1) ASTM E8M for tensile testing, (2)BS EN ISO 6507-1 1998 for vickers hardness tests and (3) BS ISO 12108:2002 for long crack growth.
- We use electrochemical techniques like ac impedance measurements, dc polarisation to generate Evans diagrams and microscopic characterisation by optical microscopy and SEM.
- Mechanical testing Microstructure characterisation NDT for cracks
- Critical current,AC susceptibility,resistance ratio etc
- computational and theoretical analysis
- Depends what you call a "test".
- Tribology of polymers and of plastics gears
- (phd) British standards: fatigue, tensile, hardness, surface roughness.
- (phd) High temp testing methodologies
- (phd) British standards; implant testing
- 3 point bending, force spectroscopy, nano indentation
- (PostDoc) BS and ASTM: long-crack tests, Bespoke (comparable in-house): short-crack tests
- (academic) Many ASTM and BSi mechanical testing methods
- (phd) Implementing new standards in a field governed by commercialism is difficult
- (Academic) UKAS accredited x-ray stress measurement unit. Developing composites test and evaluation facility, certifying carbon fibre properties. New methods of certifying composite test pieces and structures required.
- (academic) Astm, BSI
- (academic) mostly fatigue and tensile and toughness and hardness, variants on testing approaches and develop methodologies.
- (academic) would use standardised testing if given standard samples – adapting to situation.
- (academic) tensile, static, 3 point, 4 point, flexural, fatigue, tensile tension-tension.
- (academic) ASTM
- (phd) 3 point bending, force spectroscopy, nano indentation
- (academic) standard tensile test, sharpey impact, composition, wear test have no European standard but are common.

- (PostDoc) Many spectra (absorption, fluorescence, time fluorescence, ellipsometry, transmittance)
- (Phd) 4 point bend, light/semicroscopy → FEA
- (undergraduate) British Standard materials testing
- (industry) ASTM, British Standards, coefficient of linear thermal expansion (Non standard)
- (phd) 4 point bend, tensile test, compression test.
- (academic) tensile testing, fatigue (S-N), fracture toughness, DL-EPR testing (corrosion test), as for new test perhaps a standard test on reporting/acquiring EBSD data.

Data:

- (PostDoc) Measured for data analysis
- Flying
- Measured, and derived, and it is used in models, including FEA and in data mining
- residual stress, looking at depth and magnitude of RS in relation to surface treatment surface finish, work hardening, microstructures all evaluate of surface treatment as an overall evaluation as to what treatment is applicable to what material is applied in.
- To help understand geometry and loading effects on properties, e.g. fracture toughness, and for input to FEA including the calibration of fracture models.
- Experimental.
- mostly measured, and used to verify FE models or NDE observations
- I need to measure the residual stresses and the length/depth of the crack propagation with the purpose of modeling in ABAQUS FEA.
- Engineering
- FEA
- Both, measured and inferred from FEA
- measured (experimental) for simple models
- We often test supplied material in different corrosive environments, e.g. seawater or rainwater.
- I need property data with temperature for FEA of welding.
- The research depends on measuring experimental data such as load versus deformation or number of loading cycles required for the material to fail under various loading conditions. It also involves observing microstructures before, during and after testing using optical microscopy, scanning electron microscopy and X-ray microtomography.
- Modelling
- Corrosion research (not that much leading to standardised data)
- Measured

- Not much
- measured data ,some used to test modelling,other for publication
- modelling and simulations
- (phd) Experimental data image analysis with the potential for FEA
- (phd) FE-measured (experimental) and derived from observations
- (academic) Wide ranging purposes including 3D visualisation, FEA, modelling and data mining
- (phd) Measured/derived crack length
- (undergraduate) Measured (TEM, SEM...)
- Measured data from experiments
- (phd) Measured data from experiments and FEA
- (phd) Measure and compare with modelling results
- (phd) Using Matlab, ANSYS, maple and solidworks
- (academic) FEA and modelling
- (PostDoc) Measured and derived
- (academic) Measured and derived for FEA, modelling and data mining.
- (academic) experimental and derived for FEA and modelling.
- (academic) Measured experimental data for FEA models.
- (academic) Measured and derived for data mining.
- (academic) Mechanical properties/ testing and hardness properties for image data e.g. SEM
- (phd) measured data from experiments
- (academic) measured – wouldn't trust models. Would be useful for FEA, massive lack of data for this and FEA limited by data input.
- (PostDoc) Experimental (e.g. spectroscopic measurements, IV measurements) and modelling (ellipsometry, time fluorescence decays)
- (PostDoc) Muscle forces derived from patient data to drive FEA models.
- (PostDoc) Measured for FEA
- (phd) Measured – statistically derived – FEA
- (undergraduate) experimental
- (phd) Gait analysis data for the purpose of FEA.
- (industry) Experimentally measured, FEA used to interpret results.
- (academic) All types especially input into FEA.
- (phd) FEA and other computational techniques.
- (academic) measured data mostly, used for simple modelling.

Other data sources:

- (phd) Quality dependent on information given to provider
- Inadequate
- Wikipedia
- Limited, experimental background often not detailed in an open honest way. Very difficult to rely on other literature results.
- BSSA stainless steel website, information of physical properties of steels i treat, very useful
NPL website and contacts for guidance criteria, very useful and informative
- Variable - it depends how close you can get to the original test data.
- Modeling.
- literature data on clinical investigations help to support the tests i conduct (use of similar test set ups, comparison of lab data with clinical data)
- No at this moment, but I am sure that later I will do it.
- Mechanical properties of materials
- I mine data from papers, so the quality of the data depends on the paper. It can be hard to find the correct data.
- Very very poor availability. Even the material suppliers don't have it and I have had to even supply data to Corus.
- The data is useful but I have to request the owner to send it to me every time I need the information. It sometimes takes time. Some of the information was however made available from the start.
- We often compare results to published data. This is normally quite useful as although experiments may vary, it is usually clear to see how an experiment has been performed.
- Limited, questionable, variable
- We have tried to use literature data for neural network modelling of corrosion performance, and have found this generally to be difficult due to missing information and incompatible measurement methods.
- Mixed - generally we obtain data direct from known sources (industry collaborators / partners within projects) or data handbooks.
- variable, and can be expensive
- sometimes it become difficult to reach a specific data, but generally they are useful
- (phd) From a specific proposal quality is excellent
- (academic) Quality highly variable
- (PostDoc) Not easily available, some proprietary issues, quality variable, usefulness depends on quality
- Databases are available for academic papers but not well categorised

- (phd) Published papers used
- (phd) Older sources difficult to find and often incomplete
- (academic) Rolls Royce COMMIT database is high integrity.
- (phd) Very difficult to locate data in the literature that is relevant to material type and type of test under consideration
- (academic) Invalidated and usually not trustworthy.
- (academic) Variable – some tracing issues. Need quality assurance, the more background data on the material the better. All the information required is not always present in the paper.
- (academic) there are too many different alloy possibilities so it's better to repeat tests.
- (academic) Good experience because needs are simple – numbers can be approximate because of the sensitivity analysis.
- (academic) Standard materials properties – readily available and self contained.
- (academic) try to get whatever is available on the internet, published papers etc – especially true for fatigue data under specific conditions. Would be useful to have lost data back. The data exists but can't be found. Poor funding for publishing a paper about data. Data is in commercial hands.
- (PostDoc) Spectra from dye databases available in html format. Optical constants available from commercial software.
- (PostDoc) Good availability, quality and usefulness.
- (phd) quality is unknown or from peer review journals.
- (industry) nit much is available, the quality is questionable and usefulness can be low due to the large ranges quoted.
- (academic) things which can't be measured easily e.g. coefficient of thermal expansion.
- (phd) Tediously rawl literature for useful figures.
- (academic) generally use for basic properties or simple comparison. Do not require high quality data.

Augmentation:

- (phd) Determine baseline characteristics and compare expected results.
- Often
- web of science, science direct journal papers and also books for literature support to findings and also as to why experiments have been carried out.
- Cast-to-cast variation can be an issue in my experience.

- as above - clinical trials reported in the literature are useful
- Variability of operating conditions
- Yes, there is. I am aware that there is not much data related to my work, and to count on more data it will be useful for my research.
- As a reference
- If one paper has only some of the data I will look for others. I will look on the web for basic values, well understood parameters but I wouldn't trust it for recently developed parameters, unless I knew the original source well.
- Poor availability. If someone else has it, I use it if the source is reliable. It isn't always.
- My research is an extension of previous work and comparing my results with those of previous researcher is a major objective of the research.
- We would often like to do this, if we knew of such a database.
- As previous question
- Use of new techniques - for example recently started acoustic emission for crack detection, wanted AE data for cracks in steels etc.
- Confirmation of phase diagram accuracy, publication of new materials data
- scientific database
- Lack of knowledge of physical data such as dielectric constants ...
- To improve sample sizes
- (PostDoc) Compare and contrast results
- (academic) Research always involves some cross-checking
- (PostDoc) For a literature review
- (academic) From literature for FE modelling
- (academic) Augment when there is unavailability of good data.
- (academic) Uses literature, might need to interpolate data or make assumptions on material without having to do the test.
- (academic) Only as comparison/discussion.
- (academic) potentially. If data was readily available would be more inclined to use it. Ease and availability.
- (academic) Not a strong requirement currently but can see that changing.
- (phd) database would be useful in providing large sample sizes
- (academic) especially on consultancy activities and if you want to be more quantitative – growing trend towards this due to guarantee period.
- (PostDoc) mainly dye databases with spectra or solar cell efficiencies, or optical constants.
- (PostDoc) Gathering data (loading, implant positioning, material properties, friction). For FEA inputting strengths of materials, failure mechanisms.

- (industry) to sanity check experimental values.

Universal method:

- (PostDoc) Not sure
- World
- standards for testing standards for measurement techniques using certain types of equipment as not all equipment is the same standards for physical properties of materials. encyclopedia of knowledge like wikipedia but academic and industry based search engine for definitions make it available to universities and also to industry at a fee, but the fee be respective of how many people in that company will have access to it.
- Yield, flow and fracture toughness.
- Mechanical properties.
- a 'superdatabase' of relevant bibliography is something we've tried using end note but that didn't seem to take off. also, as much data as possible is necessary to feed our probabilistic modelling. access to that can be hard to come by.
- Mechanical properties, crack propagation properties
- I don't understand the question
- Material properties data (mechanical, electrical, etc.) as a MATLAB compatible files. I would like to make it available to other scientist and students.
- Material properties at different temperatures, composition dependent properties. Available to researchers who understand the importance of proper recognition for those who obtained the data.
- Property data for all use.
- Micrographs, tensile data, crack growth data. The data should be made available to researchers within the engineering materials group in SES.
- Polarisation curves, along with values for key features such as the open circuit potential and current densities, passivation potential/current density, pitting potential.
- All kinds
- Any/all - a properly managed open repository would be preferable
- Possibly, not sure how useful it will be - possibly for getting full data that is referred to in a journal paper so from a known source.
- physical properties data of all types, available for other research groups
- tribology of polymers
- As much as possible, available free to all at the point of use.
- (academic) The possibilities are complex to understand. Data handling is an important topic. Can't personally see a good solution.
- Depends on data

- (phd) Storing raw data from CT scans (4 TB), available with in group and external applicants
- (academic) Property measurements, images, model formulations, model outputs
- (PostDoc) Would depend how much extra information would have to be recorded to make it useful to others. Post processed information. Access controlled by request or perhaps output e.g. graphs rather than full data access (cost of production, could charge for access)
- Make data available to in house researchers
- Sample information, raw data and processed experimental data
- (phd) Shared set-up
- (phd) Processed data with relationships. Also share data between individuals working on the same or similar projects.
- (academic) mechanical property and thermal data. There is a composite database in the US.
- (academic) yes-validated data with known pedigree.
- (academic) hesitant. “Universal” may be too general to be useful – requirement for tailoring!
- (academic) yes. Good to have data to compare but won’t be exact as there are too many different alloys.
- (academic) Basic mechanical property data. Dynamic and static.
- (phd) sample information, raw and processed experimental data.
- (academic) don’t want to store data only for the software to change. Any sort of data related to service performance (properties) or fatigue and wear data. The more data the better, helps designers to design things that don’t fail – reduce safety factor, save money.
- (PostDoc) Spectropic data, IV curves – make them available to academic staff and other researchers.
- (postDoc) Good for results and inputs for FE but not for patient data.
- (undergraduate) material strength data, probabilistic data.
- (phd) gait analysis data for users
- (industry) any measured data. Available to the UoS research community. If made externally available would need to charge and ensure data quality.
- (phd) As a repository of computed tomography data would be useful. Also catalogued store of previous model results
- (academic) standard fatigue data would be useful, as well as standard tensile data, would make freely available.

Past projects:

- (phd) Difficult to find the correct, useful data.
- Complicated.
- A challenge to find the original test data - which is what is needed, i.e. raw experimental data such as load versus displacement data from tensile and fracture toughness tests.
- It is always difficult to find results you filed long time ago. Specially to remember what you did.
- 50/50...they are in my office somewhere - i tend to hoard!
- Only data relevant to the old project is found, guesstimating was required
- Sometimes I have spent time in locating data of several sources, and the time -in a research- is a valuable element.
- Mixed. We have quite a problem here with trying to use data taken by experimenters who have since left the group.
- Depends on how well it was stored. Some are in spreadsheets and have been sent to me. Other data was promised and never materialised.
- I have to request the owner to send it to me every time I need the information. It sometimes takes time. Some of the information was however made available from the start.
- We have had projects working with materials not used outside our area, so projects often have to rely on previous students work, as there are not other sources in the literature.
- Difficult
- Generally good if I generated the data (I have a good filing system), less good if a student / post-doc generated the data as labelling is sometimes inconsistent.
- change in storage formats and staff moving on cause the biggest problems
- Hard
- This is an odd question. Surely the point of previous projects would be to provide data and/or insights for future use. Else why did you do it?
- Would be easier if deposited in a database together with accompanying information-sample description and test parameters
- (undergraduate) Time consuming, depends on quality, difficult if there are contradictions within teams of researchers.
- (PostDoc) Data, not too bad. Images, poor, photographic images often degraded or lost.
- (academic) Variable if outside own research
- (phd) Very difficult if author is not known personally
- (phd) Good if data format is the same as currently used
- (PostDoc) Make sure data is transferable within one person's research area, but difficult to access other's data

- (academic) Haphazard experiences in this area.
- (academic) difficult.
- (academic) Variable. Can be hard- everyone uses different filing systems, data formats change.
- (academic) Problems locating it.
- (academic) data easily available in lab books.
- (phd) would be much easier if deposited in a database together with accompanying information- sample description and test parameters.
- (academic) struggle – not searchable, sometimes destroyed.
- (PostDoc) Accessing own data is a lengthy process, accessing other people's data is impossible.
- (PostDoc) Located using literature search, not always reliable.
- (phd) difficult sometimes
- (industry) usually in previous log book and papers but finding it is time consuming.
- (academic) near impossible, especially with raw data.
- (phd) Lucky if you receive information.
- (academic) generally ok, but can be problems if researcher has moved on and has not left a full copy of files and explanatory notes! Publication of data in paper is usually sufficient to archive key data for specific type of research. Having the raw data without explanatory notes is rarely useful.

Collaboration:

- (PostDoc) Fine if properly acknowledged
- Overall good, have to be very careful who you discuss scientific finds with.
- everything seems to take a long time to get collaboration achieved and papers take a long time to be processed as well.
- No problems
- Reservations are always placed to the sensitivity of our work.
- not a problem in most instances but there are some commercial in confidence investigations that I would be reluctant to share data on.
- No at the moment, but I am available to share any kind of information useful for other researchers. I think the collaboration is necessary in our work.
- I would like to be included as a co-author of a future publications (or at least acknowledged) if my shared data is utilized by others.
- I would have reservations about sharing my data if I wasn't confident I would get credit.

- Don't mind. There isn't enough to go around so we need to share what we have.
- My project is in its early stage and I am likely to share my results later on but to selected researchers.
- Benefits are variable
- No problems other than locating the data.
- sometimes the data is sensitive and has commercial use so have to get third party agreement
- Data shared within collaborative projects. Happy to share relevant data.
- All information should be shared, in a civilized society.
- (phd) Size is the main issue (typical scan 7GB)
- (phd) Only processed images
- (academic) Depends on novelty, commercial value and competitiveness
- (PostDoc) Sharing data on precondition of receiving material
- Good experiences, no reservations on sharing of published data
- (phd) There is potential to share between a relevant company and the university
- (academic) share with industrial collaborators.
- (academic) difficulty in different formats.
- (academic) worry that data is “expensive” or that industry won’t give credit appropriately.
- (academic) with other universities no reservations in collaboration since each party tends to only be interested in their section of the project.
- (academic) No real reservations. Important issue is how the data is used.
- (academic) no reservations. Straight forward data – easy to transfer
- (phd) good experiences, no reservations on sharing if published data.
- (academic) if on a project together. Share as long as it doesn’t conflict with confidentiality.
- (PostDoc) if published and acknowledged no problems.
- (PostDoc) No reservations – only shared with established contacts/collaborators or with people on the same project.
- (PostDoc) Get useful feedback from others, no reservations(phd) working with industrial partners causes a problem, require data protection.
- (academic) have shared EBSB data and 3D microstructural data with modelling groups .
Good experience, no reservations.

Security concerns:

- (phd) Yes due to external funding
- ownership

- annoying my industrial sponsors, not getting cited for my data
- Steal data without at least referencing us.
- no for the most part.
- How the people that provides greater amounts of info will be rewarded in comparison to the ones that do not contribute to the centre
- I would want to be sure I would get credit for measuring the data if others were to use them in a publication, or to lead them to a publication.
- You may have to restrict it for specialised materials, but generally it should be okay for everyone.
- I have no security concerns as long as appropriate levels of access via password protection is put in place.
- Where our projects are sponsored, we would need to get clearance to make some data public.
- My main concern would be liability arising from use of the data
- How the data would be used and how referenced.
- No if published
- (PostDoc) Possible proprietary issues from sponsor. Cost of production and time. Others could publish data before the author
- (academic) Commercial sensitivity of sponsors in particular
- (phd) Only available to external parties through application and direct permission
- (phd) Plagiarism
- (PostDoc) Risk of inappropriate use of data without author's knowledge. Also some data has potential commercial sensitivity.
- (academic) liability.
- (academic) Funder issues
- (academic) Not for published data.
- (academic) Issues with sponsors, ownership of data.
- (academic) Other's would as it is other people's data.
- (phd) not if published
- (academic) confidentiality (ok if informed), security (changing values without authority), ok if everyone gains
- (PostDoc) Patient confidentiality, external back ups.
- (phd) commercial confidentiality.

Conservation:

- On the whole - - of not too trivial.
- some
- avoid reinventing the wheel
- No loss of data overall advantage. Method used must also be described effectively.
- data should not be made available until published in a paper. after that you could be seen as a contact for that technique and e-forums could be carried out within expertise groups
- Access to data by other workers
- Data by its own without describing how it was obtained or what parameters were used to obtain it would reduce its usefulness.
- main advantage would be to gain as large a database as possible to feed models. also good for verification or to highlight deficiencies in past/current test methods. possible disadvantage of having work plagiarised - but unlikely.
- The archive needs to be very well organised to be useful and that will take time. The rewards will be significant, though.
- I consider that the conservation of experimental data has advantages only, and any disadvantage, because the researcher can save time or compare their experimental results more easily.
- It will reduce the number of unnecessary repetition of standard experiments. However the experimental setup and condition must be very precisely presented.
- Useful for future. Takes up space, need to be sure users recognise how old the data are and if they become obsolete because new techniques have made better measurements possible.
- It saves time and helps to be able to reproduce and confirm other people's work.
- It is good for future reference and protects against data loss in case of accidents or other unexpected events such as computer virus attack. The disadvantage is a possible misuse of the data by authorised persons.
- It would be a good demonstration that we are making our results available, and I imagine the public funding bodies would welcome this.
- Not wasting experimental effort
- Need to understand how data is generated and potential sources of error. Ability to trust data held centrally in terms of quality - especially if limited information (e.g. full processing histories etc) available. However, having data available to help verify models would be very beneficial.
- to broaden data access available, very useful for comparative use
- (PostDoc) Useful only to a certain extent. Advantage of shared research activities, discussions, collaboration etc. Disadvantage of breach of data security etc.
- (phd) Advantage – back up and security. Disadvantage – lack of speed depending on access type.

- (phd) May prevent unnecessary repetition of work. Space/cost. Easy access to previous/relevant work.
- (PostDoc) Advantage – easier access (especially micrographs), other data may be available. Disadvantage – security, pre-publishing
- (undergraduate) Can see others finding. Avoids the loss of data.
- Repository of interest to community, especially researchers waiting to use experimental data for modelling or for reproducing experiments.
- (phd) Advantage – check data any time. Disadvantage – accessibility, storage space.
- (phd) It will save time in getting useful data. Researchers can do fewer experiments individually.
- (phd) Continuity of previous work. Creating additional information rather than dealing with the necessity of possibly repeating already known information.
- (phd) Follow on projects can then easily find a start point to define the work that needs to be done
- (academic) Yes for data that is expensive to get. No for simple data (personal experience). Long-term data is a big issue so yes. May be cheaper to re-do test than conserve data.
- (academic) Disadvantage – pollutes database if data is not sufficiently accurate or well characterised.
- (academic) good for future use.
- (academic) Avoids re-inventing the wheel. Checks and balances. Reveal wider ranging relationships.
- (academic) Advantage for similar alloy comparison, reference only, could create relationships that weren't exactly truthful, caution required.
- (academic) very useful as past data is often lost.
- (phd) repository of interest to community, especially researchers wanting to use experimental data for modelling or reproducing experiments.
- (academic) All experimental data is useful – shouldn't be buried in thesis.
- (PostDoc) advantage - easy access. Disadvantage – large disk space and resources.
- (PostDoc) Future generation can use it. Avoids duplicating work. In the spirit of “research community”.
- (PostDoc) Advantages: access for people interested in using the data, comparison purposes. Disadvantage – storage.
- (phd) Linking postgrad research, not just discrete projects.
- (undergraduate) Advantage of future reference.

- (phd) it can be compared to new studies but it might have large space requirements. People may have varying techniques.
- (industry) for future use.
- (phd) advantage-no repetition of experiments, disadvantage-only useful if properly catalogued.
- (academic) Ok for standardised tests, where it is clear what data needs to be recorded. For general research data, it does not make sense (except as short term back-up) as key integrating factors and details may not be readily recorded.

Trial:

- I'm retiring in 2 days' time, so will probably not generate any more data - ideas perhaps, but not data.
- as i am funded by a sponser i would have to have all my data ok'd by them, which may prove difficult
- No constraints. I would wish to include the raw tests data.
- not at this time
- The data should be used giving credit to the source
- You can contact to me via e-mail: Carlos.JimenezAcosta@postgrad.manchester.ac.uk
- We are developing stress measurement methods at micron and sub-micron scale based on mechanical relaxation methods, namely incremental slitting and incremental hole-drilling. These new methods require integration of three different measurement techniques: SEM-FIB, Digital Image Correlation Analysis and Finite-Element Analysis. Ultimately we are going to applied these methods to infer stress profiles in materials with pronounced microstructure, such as micro-electronics, MEMS, thin films, coatings, grain boudaries, etc. These methods require, so called, stress relaxation coeffients usually obtained from FEA predictions. Tabulated sets of coefficients for various materials and microstructures will allow broader access to these techniques. Besides that we are developing 'tool boxes' that will allow for automated calculation procedures. Contact Details: Dr Bartlomiej Winiarski PDRA Stress Damage Characterisation Group (SDC) Materials Science Centre, E13 School of Materials, University of Manchester, Grosvenor Street, M1 7HS Manchester, U.K. b.winiarski@manchester.ac.uk Line manager: Professor Philip Withers FEng FRAes FIMMM Professor of Materials Science Director of the University of Manchester Aerospace Research Institute The University of Manchester Room D41 Sackville Street Manchester M1 3NJ +44 (0) 161 306 8872
- I have property data for steels under various conditions. I think people might use them for comparison with their measurements. They might be of some interest for simple models.
- Don't mind how it is used. david.g.richards@postgrad.manchester.ac.uk

- The data could be useful and should be used within the research group. Any other person
- wishing to use such data should request for it from the head of the group who will decide whether to grant access or not.
- I would be happy to add results to a database for other academics and students to access, subject to the agreement of sponsoring bodies.
- dependant on the data collected we would probably have an interest
- (phd) Used in follow on projects (if sponsor is constant), outside this sponsors permission required.
- Storage facility for extra work
- No reservations for published data
- (phd) Access for measurement of progressive damage growth from direct observation. Copy right concerns and acknowledgements.
- (academic) Consider against resource levels – CT data!
- (phd) Only as a backup facility. Access restricted to selectable users
- (PostDoc) Interested parties have discussion with author first
- (academic) depends on agreement.
- (academic) might need to restrict access of some users. Should be used in every way possible.
- (academic) probably, only use as a reference, general property. No restraints required.
- (academic) supply of data is difficult as it is not usually produced as a formalised data sheet in a thesis. Data provided may be a trustworthy, common form.
- (academic) Need to do something with data generated, data is diverse, would be useful in-group
- (phd) at first only published data, no reservations
- (academic) data should be used in design context, provides more information from which to select alloys, avoids repeating experiment.
- (PostDoc) Used for demonstrations, and not shared without permission.
- (industry) for anyone who would find it useful, can't envisage any constraints.
- (academic) improving info on scatter and variability. Standard tests and data such as tension, fatigue, microstructural data (e.g. EBSD)

Standardised layout:

- (PostDoc) Lots of potential cautions

- standards is good, but placing your data online would be difficult as it would be a slow acquisition. maybe have the data to be placed on AFTER the standardisation has been peer
- reviewed, the the paper can be linked to it and then contact details and e-forum details can be added
- Where possible
- The definition of that standardised data layout.
- I don't really understand the question. All the appropriate standards for materials property measurement specify reporting methods and formats. So why not use them? It seems to me that this is based on a lack of understanding of what engineering standards already exist, what they are for and what they contain. It's also not possible to separate out materials properties from process route...
- Data that are easy to search; units, methods clearly identified; a clear way for the provider to indicate to the user his or her preferences for use/collaboration/restrictions.
- Specific heat capacity, density, thermal conductivity, yield stress, elasticity, all as a function of temperature. They have to be material based and from recorded experiments and tests that can be accessed with the data. It all needs to be referenced data for future publications.
- Well structured data with details of experimental methods used to obtain the data. Both raw data and analysed data would be useful.
- In corrosion measurements, the purity of chemicals used can be a major factor. The difference between a corrosion test in a solution using DI water and one made with tap water can be quite significant.
- I coordinated an EC-funded Thematic Network (OCEAN - Open Corrosion Expertise Access Network) that was concerned with the representation of corrosion metadata, and I am also associated with a NACE proposal to regenerate an existing standard for the representation of corrosion information using XML linked to MatML - I would hope that the data centre would build on such developments.
- Would need full data sets of all relevant information - often difficult to collect.
- Physical property data,crystallographic data,would want to know data comes from a reputable source
- Ease of access
- (phd) Ideal world
- (academic) Provenance
- (phd) Access to relevant data/easy to find specific data among vast quantities.
- (PostDoc) Utopia = full data for all materials. Optimum = mandate fields for different types of data rather than all fields
- (undergraduate) Simple to use. Results dated, short loading time, history of previous searches.
- Description of sample, experiment, date. Raw experimental data and processed data.

- (phd) Test set-up (equipment used), standard used, outputs
- (phd) Concerned with data reliability.
- (phd) Concerned with data management. Key word specific search. Security, author's permission
- (phd) Processed data for comparison. Graphical data and data used to generate it. Micro structural and fracture surface images.
- (academic) Major concern is that the data isn't sufficiently well characterised or reliable e.g. heat treatment condition of alloy etc.
- (academic) standard format and ease of access.
- (academic) not sure this allows for new knowledge. Searchable in a flexible way. Provenance.
- (academic) Yes for traditional alloys only because the nature of the sector is developing and fast moving.
- (academic) Timescale is massive. Unpopulated resources are frustrating.
- (academic) Not convinced it's feasible. Researcher and designer use data differently.
- (academic) easy comparison, lots of applications aren't standardised. Ideal world – any data anyone has done – find it easily – great help.
- (phd) description of sample, experiment, date. Raw experimental data, and processed data.
- (PostDoc) major concerns will be IP publications
- (PostDoc) easy to use layout i.e. advanced search functions. Either actual data or links to where data can be found.
- (PostDoc) major concern is reliability.
- (Phd) enjoyed the “logs, blogs and pods talk”. Most work is commercially confidential.
- (phd) material properties, standard gait analysis tests from a range of people, CT scans.
- (industry) useful material, the validity of it.
- (academic) standardisation is a barrier to progression.
- (phd) ease of access uploading and downloading information.
- (academic) In limited areas, in others we don't know which factors to standardise. Basic material data, correlated with microstructure characteristics, details of standard test used. No data not collected using standards. Main concern would be poor quality data.