2013 Computational Materials Design Workshop

June 20, 2013

Omni William Penn Hotel, Pittsburgh, PA

Breakout Sessions Considerations - Patricia Rawls – NETL, Crosscutting Research Division

- Time to conduct effort?
    - Near-term 2-4 years
    - Mid-term 5-7 years
    - Long-term 8+ years
- Information upon which to build future research?
- Who to do the research? (University, National Lab, Industry, Consortiums?)
- Is there any opportunity for collaboration outside of Fossil Energy (FE) office of DOE?
- Comments on current research efforts?

ALLOY DESIGN BREAKOUT GROUP

Facilitator – Patricia Rawls

Focus For Alloy Design

- What alloy/alloy systems?
  What material processing issues?
- What databases? (modeling roles?)
- What new experimental methods for alloy development?

Notes

Slide 1

- Iron and nickel (Fe+Ni) based
    - Thermo dynamics
    - Databases are well established
- Ni databases need to be more detailed, in terms of composition, and mechanical properties for tailoring properties
- Physical properties and kinetics are not good (metastable phases missing)
- Environmental elements need to be included (O_2, H_2, Cl, S)
- Start with Atomistic Properties database
- Big job with lots of experiments, need collaborations (National Energy Technology Laboratory [NETL], NETL's University Coal Research [UCR] Program and Historically Black Colleges and Universities [HBCU] Program). They could provide materials properties data development

Slide 2

- Start with lattice dynamics, which can lead to thermodynamics
- Kinetic databases are important (don't even have metal info)
- Atomic structure is lacking (Use Cluster Expansion [beginning at NETL] to predict thermodynamic properties combined with experiments)

- Property database → Long-term behavior
- Oxygen diffusivity databases built in the 1970s
- What about thru oxides?

Slide 3

- High Entropy Alloys (HEAs) (NETL, UCR) for structural and coatings- need to minimize thermal stress
- Define what the alloy will be specifically doing for each application
- Alloys that reduce cost/improve performance of 740 and 282
- Approach needs to have market pull
- Practical research is the key
- SBIR (Working with Paul [NETL Albany]) must be able to manufacture a new alloy.
- Need to understand properties of 740 and 282 to gain confidence that materials are ready for next level
- How to use existing data to design, build and test components; and then feed back into alloy design components

Slide 4

- Alloys for additive manufacturing:
    - Oxide-dispersion strengthened (ODS) (limitations)
    - Long-term
    - Small parts
    - Engineering study - potential for impact
    - Expensive materials
- Thermal Barrier Coatings (TBC) - best way to produce them?
- Alloys for fatigue:
    - Thermal creep fatigue
    - No data on current materials
    - Impacts scrubbers, water chemistry, complex problem
    - Reference –Aero Industry, what have they done to model /substitute material behavior
    - Understand weld properties
- Industry/Lab collaboration:
    - Steam fatigue testing (Oak Ridge National Lab)

Slide 5

- How do you approach alloy design for fatigue?
- Two multi-scale factors: Composition and Heat Treatment (thermal)
- Two other multi-scale analysis factors: Corrosion and Oxidation Behavior
- Fatigue resistant alloy design (understand deformation mechanisms first)
- Have to link material development to manufacturability (Paul)
- Replace rare earth elements, but retain properties (other critical elements, La, Co, Y)
- Critical Materials Institute (The Office of Energy Efficiency and Renewable Energy [EERE]) at Ames Lab.

Slide 6

- First principle calculations for kinetics/thermodynamics properties:
    - Many challenges
    - Multi-component systems needed
    - Grain boundary affect/interface affect (i.e., oxide/metal)
    - Challenge is to do calculations at relevant temperatures and to make it multi-component
- Two aspects of alloy design:
    - Accuracy (density functional theory [DFT])
    - Efficiency (thermocalc, simple parametric models)

Summary

Alloy designs are mainly based on Fe and Ni materials. The databases are well established, but some need to be more detailed in terms of composition and mechanical properties. Using cluster expansion to predict thermodynamic properties are best combined with experiments. HEAs need to have market pull and we must be able to manufacture them in order for it to be successful. The four multi-scale factors to approach alloy design for fatigue are composition/heat and corrosion/oxidation behavior. The two most important aspects of alloy design are accuracy (DFT) and efficiency (thermocalc, or simple parametric models).

Multi-Scale Modeling Breakout Group

Facilitator – Vito Cedro

Focus For Multi-Scale Modeling

- What are the types of issues that need to be addressed?
- Who is doing the work in the community?

Notes

- Dislocation Dynamics Modeling coupled with ab initio first principles technique (to model the particle dislocation interface)
- Creep modeling (multi-scale) time and dimension:
    - Diffusion
    - Grain Boundaries
    - Microstructural complexity
    - Long-term predictive
- Use of non-destructive evaluation (NDE) tools and data coupled with models.
- Short-term data applied to long-term predictability
- Extrapolation of higher T data to lower T applications; use of models to define the relevant regimen and extension/extrapolate the data; (How?) → windows of applicability
- Communication and sharing of work, results, ideas
- Biggest issues are fatigue/creep (mechanical) and corrosion (environment)
- Multi-scale modeling of oxidation/corrosion behavior (long-term) lags the work on mechanical properties. Still rely mainly on experimental data
- Behavior of material during welding and how the welds behave long term
- Ease of use of multi-scale models (not easy now)
- Modeling and scale-up of alloy manufacturing process
- Effective validation of models (experiments)

- How would a large multi-scale modeling R&D effort be coordinated? How will it affect my work?
- Who would do this work?
    - Fundamental models – Universities?
    - Applied – Others?
- University of Michigan (John Allison)
    - Integrated Computational Materials Engineering (ICME) Initiative
    - Relevant efforts outside FE?
- Focus on one major problem to develop integrated multi-scale modeling tools that interact with each other.
- Common language to communicate across disciplines
- Gaps:
    - Coupled phenomena, creep understanding and modeling (creep/fatigue/oxidation)
    - Coupled dislocation dynamics and finite element method (FEM)
    - Coupled atomistic modeling and FEM:
        - Focus on what area – atomistic
    - Coupled FEM and crystal plasticity
- Particle Interaction – Particle/Particle Dislocation Dynamics
    - Very hard to simulate
- Need reliable input parameters and transferable
- Two levels of atomic level/ab initio
- Need > 1,000 atoms to compute realistic parameters
- Use experiments to refine the model and reduce need for large number of atoms
- Connectivity of mechanisms
    - That control behavior of the material across time and dimension scales
    - Mechanism maps
- Do not sell computing power short → rapid advances in computing power

Long-Term Behavior of Materials Breakout Group

Facilitator – Dave Alman

Focus For Long-Term Behavior of Materials

- What types of properties are we talking about?
- Data availability? Mechanical? Microstructural stability?
- What alloy systems?

Notes

What Types of Properties are we Talking About?

- Creep, fatigue and creep fatigue interactions, long-term oxidation, and microstructural stability are all parameters that need to be modeled
- Modeling To Reduce Safety Factors: The American Society of Mechanical Engineers (ASME) has models to use the data, but not to generate or predict the data
    - Modeling for guidance on testing (reduce the number of experimental tests needed for verification)
    - Modeling to reduce scatter in data

    - New lifeing methodologies
- Long-term, high-temperature oxidation/corrosion
    - Long-term is connected to multi-scale; to make it predictable, we need to look at small-scale and start from there
    - Oxidation/corrosion point of view, critical metal concentration for establishment and maintenance of protective scales
- Creep rupture time – strain vs. time; critical strain to failure
- Crack propagation with time – how to use data for predictions
- Microstructural chemical stability – critical composition
    - You need microstructural stability, a key for creep fatigue and that type of interaction and behavior
- Non Destructive Examination – can modeling be used to better understand the best way to interpret what is being measured? Is there a program to develop NDE? Maybe a technique could be developed. A modeling simulation could play a huge role.
- Generalized program for fatigue and creep (how to find funding for it?)

Data (Experimental or Computational) Availability

- How do we use short-term data to make long-term predictions? A lot of short-term data exists, but how do we predict it out for 30 years?
- Experimental creep data for validation
- Diffusion data in oxide scales
- Accurate description of environmental species
    - Free energies of metals and compounds
        - *How do you calculate free energies? If you have three or four elements, how can you do that?*
- Need to be able to model multi-component – non-isotropic alloys
- You need information from three levels of modeling: (1) mechanical properties (involves physical, very complicated); (2) microstructural levels; and (3) thermodynamics
    - There are many tools available, but most of the time they were not sufficient, so models still need to be developed
    - Crystal plasticity models
- Corrosion testing is all over the map; there is no generally accepted format to generate corrosion/oxidation data. There needs to be one

Alloys

- Superalloys
- Steels
- ODS alloys.
- Nano-strengthened ferritic alloys

Computational Tools

- You need information from three levels of modeling: (1) mechanical properties (involves physical, very complicated); (2) microstructural levels; and (3) thermodynamics
    - There are many tools available, but most of the time they were not sufficient, so models still need to be developed
- Crystal plasticity models need improvement

- Long-term stability – what kind of tools are out there? Are there any generally accepted tools, or do we have to use an in-house code? Instead of spending a long time developing a new tool, we should see what already exists.
- Tools needed to reduce the number of tests/data needed
- Larson-Miller Parameter – If you can get a better model to predict fatigue, you can use less testing
- Tools for getting long-term data from short-term experimental or theoretical tests (creep fatigue, corrosion)
    - We want to simplify the number of experiments, but we need to capture details that may be relevant for specific application
- We use free energies to tell us what direction we should be going, but the challenge is in understanding kinetic pathways to the final product
    - With computational power, many pathways can be run to see which is the fastest. With computational speed, many scenarios can be run and probability codes can be generated.
    - Deterministic vs. probabilistic approaches
- Database format:
    - Standardized format?
    - Material genome
        - Genome is a large piece of data; the idea is not to throw away part of it, but to analyze all data
- Data analysis tools are important – The data has to be in its most pure form so that it can be used any way the person wants (two people may want to use it in separate ways).
- All data is eventually going to be available to the general public in an online database funded with taxpayers' money. "Crowd sourcing at its most powerful." Then the issue becomes the need for a standard way of collecting and reporting data, sorting the good data from the bad data.

Leveraging Other Agencies/Programs

- Nuclear energy
- Department of Defense/Air Force
- Medical applications
- EERE has standard test protocols and a way of predicting cost and performance, so they would be interested in databases in that point of view
    - Their thermal storage programs (concentrated solar power) – long-term behavior

What Type of Data Needed for Long-Term Efforts?

- What is the operating mechanism, data relevancy? Both critical when setting up a physical model.
- Qualitative predictions would be shorter-term projects
- Quantitative predictions would be longer-term projects

Software Development

- Example: a "thermal calc" for phase field modeling
    - The advantage for a unified software model is that it is more user-friendly; it would make verification of models easier

Who Should Do the Work?

- University and Industry
  - Generate data and databases
  - They need to be using the techniques at the same time. There is currently a gap of understanding in the passing of information. Industry labs do not have the resources necessary.
- National Labs
  - Repository of the data
  - Difficult to get long-term testing at universities – This is where the national labs and facilities come in, because they have the ability to generate long-term data with government money
  - If storing experimental data in a database, there has to exist some type of quality control, which is hard to do at the university level
  - Long-term experimental and validation tests in hazardous, hostile environments (industry also involved)

Information to Build On

- Existing databases for generation for nuclear power plants, an international forum.
- 1,400F Program – Common interest in 617 Program in the A-USC Program; data could be used for modeling; it is a good foundation

Comment on Current Research Effort

- There were some examples of stuff that is moving in the right direction. A lot of it is still in the material science realm, without a good connection to answering the long-term question that this specific program might want. It wouldn't take much effort to take exactly what is being done, and make it more focused. Many pieces that you would need for a good multi-scale method are already in the program, they are just not focused on the common problem.

Workshop Participants

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