SAND2012-9322P

Theme, Scope, Objectives, and Evolution of PPM

(discussion)

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Predicting Performance Margins (PPM): Developing a stochastic framework to better quantify the effects of material variability on performance margins

- Materials are intrinsically inhomogeneous, but the relationship between microstructural variability and resulting properties is often unknown.

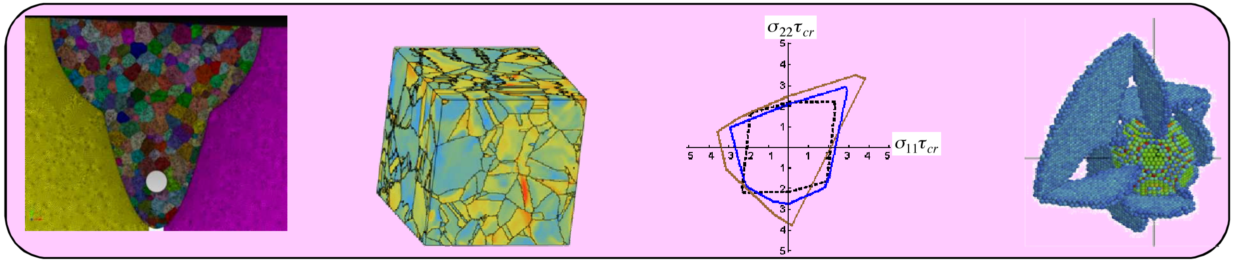
⇒Current design and analysis models are too often based on a few observations of material behavior rather than a statistical description.

PPM Project Goal: Provide a science-based, probabilistic underpinning for design and analysis capabilities that links microscopic differences to property variability.

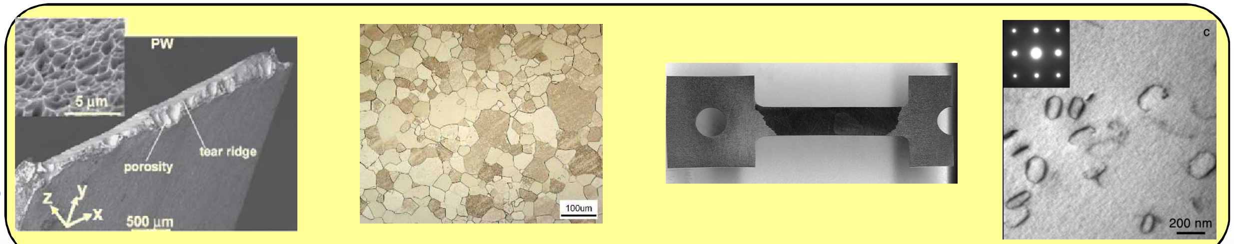
While PPM's technical focus centers around deformation and failure of welds, PPM is intended to be a *bellwether* program where the core theme of materials variability can expand into many other topics from glass/ceramic materials failure to polymer aging to electrical contact tribology.

PPM integrates models and experiments using parallel continuum-down and atoms-up approaches

Models



Experiments



Material performance	**Microstructural effects**	**Single crystal behavior**	**Atomic scale phenomena**
10^0 m 10^6 s	10^{-3} m 10^3 s	10^{-6} m 10^0 s	10^{-9} m 10^{-9} s

Atoms-up: Develop physics-based models to provide scientific insight

Continuum-down: Augment engineering-scale models to provide customer value

The large scale of PPM (>20 researchers) permits intentional unification of experiments and computational methods at all length scales bridging from atomistic up to component-level.

PPM provides the 'glue' that unites scientists with engineers. It fulfills our motto of 'science-based engineering'.

PPM strengthens bridges between the materials science, solid mechanics, and component engineering communities.

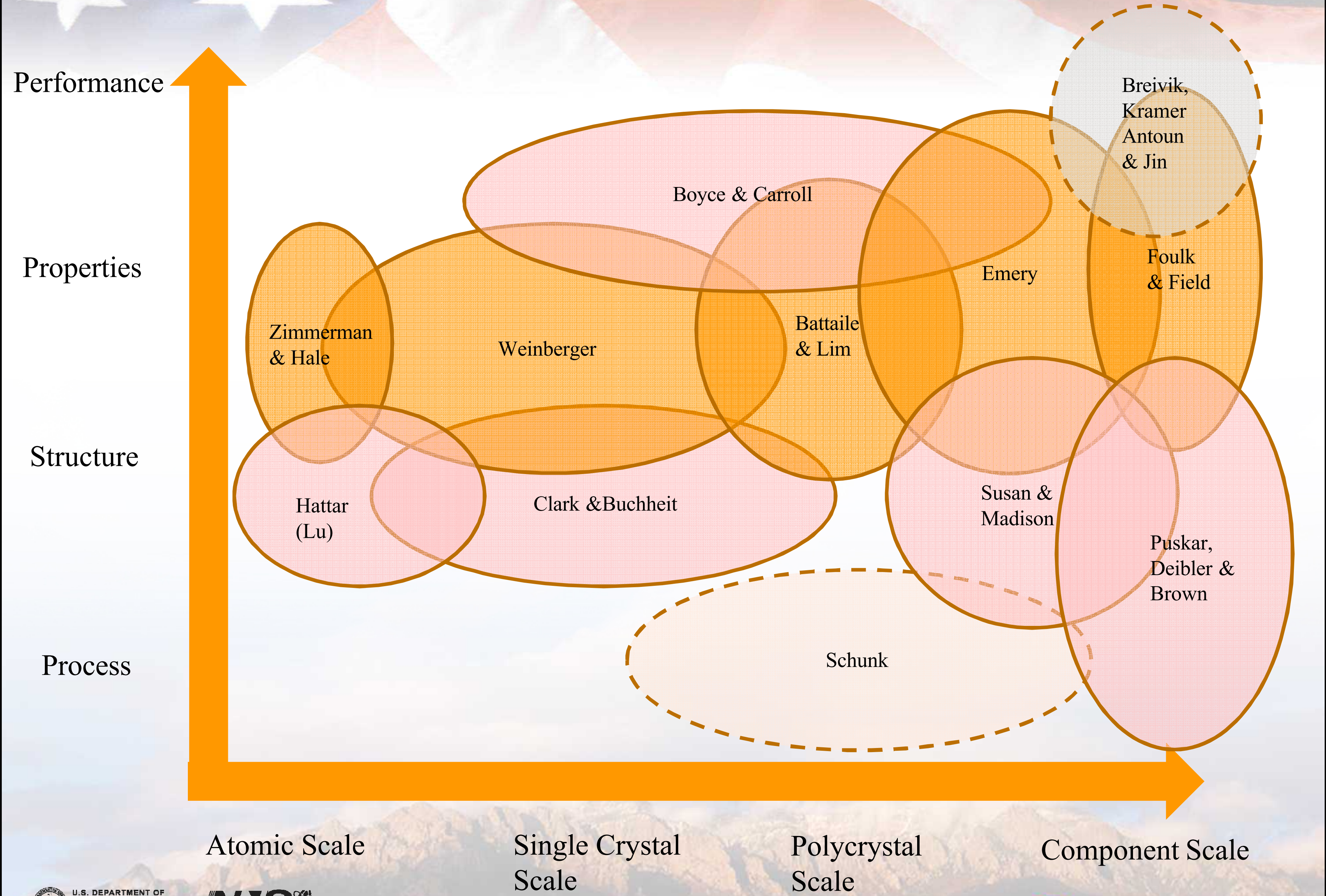
The PPM Program draws inspiration from Materials Genome and Integrated Computational Materials Engineering (ICME) Initiatives

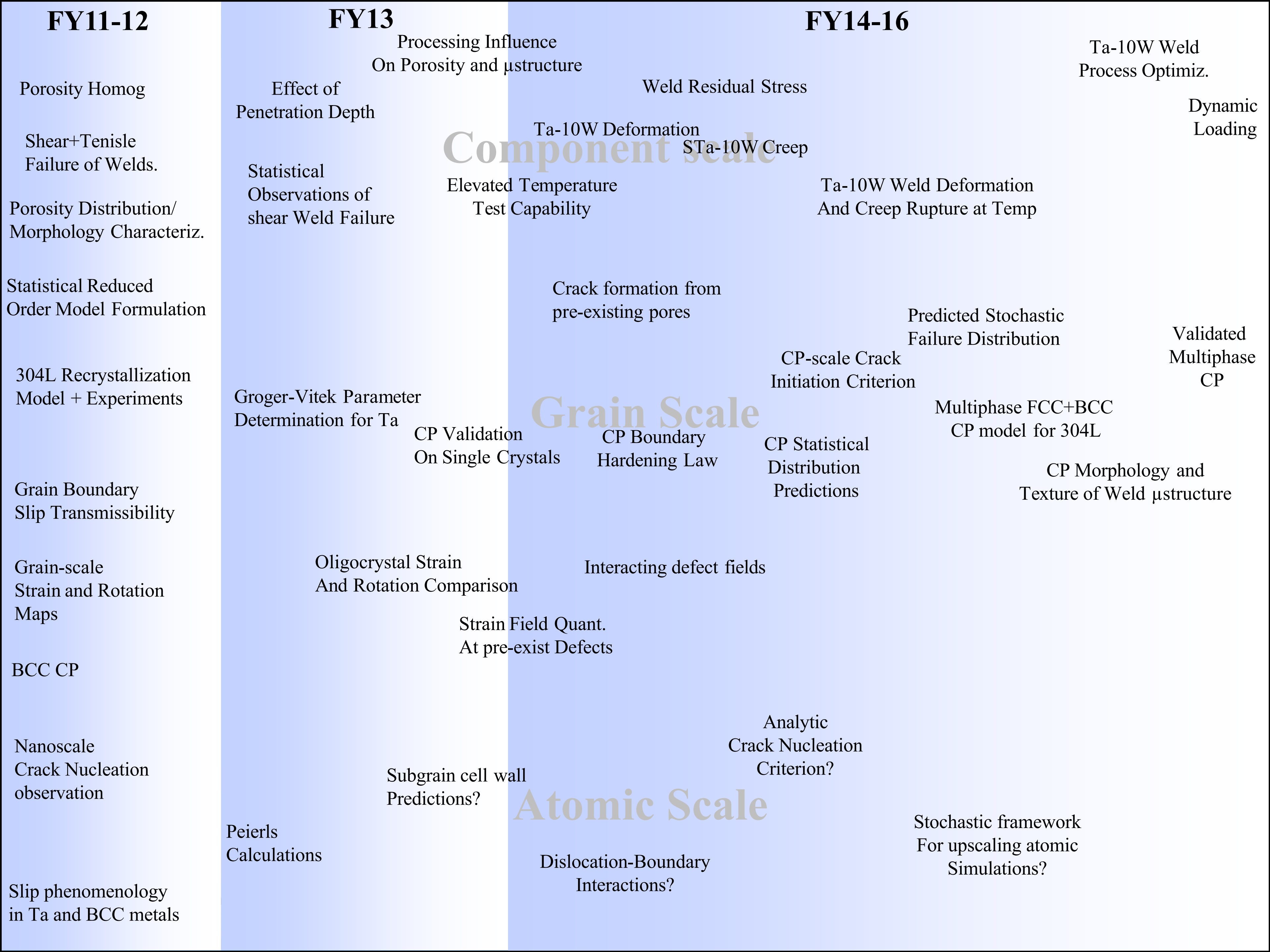
PPM builds a Materials-centric foundation to enhance agility and responsiveness for future mission needs

- **Develop people with the right expertise to solve non-nuclear material problems.**
  - **Build staff relationships and foster growth at every career-stage**
    - Sustained, focused research opportunity, support individual initiative, expand NW contacts, provide project leadership opportunities, intentional mentorship.
  - **Pass on knowledge to the new generation**
    - Familiarize new staff with common NW problems and materials, foster new capabilities, propagate corporate knowledge, provide foundation for science-based requirements and future NW customer support
- **Ready experimental and computational infrastructure for future needs.**
  - **Advanced characterization and testing capabilities are honed:**
    - 3D microscopy, FIB, tomography, digital image correlation quantitative nano/microstructural scale deformation, multi-axial weld test capabilities
  - **Modeling and simulation capabilities are brought online and 'put to the test':**
    - Physical mechanistic models, constitutive relationships, homogenization / reduced-order models, integration within existing SIERRA solid mechanics and structural dynamics
- **Own the vision to address recurring non-nuclear materials concerns.**
  - **Materials community takes ownership to champion NW material problems which *transcend* tail-numbers and production schedules.**
    - Other potential *transcendental* topics beyond weld reliability: microelectronic packaging reliability, glass-to-metal seal failure, electrical contact tribology, aging degradation of foams and polymers, long-term material compatibility…

Five ways in which you can contribute to PPM:

1. Show connections where your PPM work provides a foundation for NW efforts
2. Find useful ways to bridge length scales (homogenize, reduce order, etc)
3. Connect experiments & models (phenomenology, validation, etc)
4. Develop statistical insight and framework for material variability.
5. Publish high quality journal articles


Performance
Properties
Structure
Process
Boyce & Carroll
Breivik,
Kramer
Antoun
& Jin
Emery
Foulk
& Field
Zimmerman
& Hale
Weinberger
Battaile
& Lim
Hattar
(Lu)
Clark &Buchheit
Susan &
Madison
Puskar,
Deibler &
Brown
Schunk
Atomic Scale
Single Crystal
Scale
Polycrystal
Scale
Component Scale



FY11-12
FY13
FY14-16
Component scale
Grain Scale
Atomic Scale
Porosity Homog
Shear+Tenisle Failure of Welds.
Porosity Distribution/ Morphology Characteriz.
Statistical Reduced Order Model Formulation
304L Recrystallization Model + Experiments
Grain Boundary Slip Transmissibility
Grain-scale Strain and Rotation Maps
BCC CP
Nanoscale Crack Nucleation observation
Slip phenomenology in Ta and BCC metals
Processing Influence On Porosity and µstructure
Effect of Penetration Depth
Statistical Observations of shear Weld Failure
Groger-Vitek Parameter Determination for Ta
CP Validation On Single Crystals
Oligocrystal Strain And Rotation Comparison
Strain Field Quant. At pre-exist Defects
Subgrain cell wall Predictions?
Peierls Calculations
Weld Residual Stress
Ta-10W Deformation
STa-10W Creep
Elevated Temperature Test Capability
Ta-10W Weld Process Optimiz.
Dynamic Loading
Ta-10W Weld Deformation And Creep Rupture at Temp
Crack formation from pre-existing pores
Predicted Stochastic Failure Distribution
Validated Multiphase CP
CP-scale Crack Initiation Criterion
Multiphase FCC+BCC CP model for 304L
CP Boundary Hardening Law
CP Statistical Distribution Predictions
CP Morphology and Texture of Weld µstructure
Interacting defect fields
Analytic Crack Nucleation Criterion?
Stochastic framework For upscaling atomic Simulations?
Dislocation-Boundary Interactions?