A facility for simulating the dynamic response of materials

Solid Dynamics

Michael Ortiz

Caltech

ASCI ASAP Site visit

Oct. 22-23, 2001

Personnel

- Faculty:
  - *Thomas J. Ahrens*
  - *Michael Ortiz*
  - *Robert Phillips*
  - *Alberto Cuitino (Rutgers)*
- Visiting faculty:
  - *Emily Carter (UCLA)*
  - *Patrizio Neff (Darmstadt)*
  - *Deborah Sulsky (UNM)*
  - *Anna Pandolfi (Milano)*
  - *Pierre Suquet (Marseille)*
  - *Kerstin Weinberg (Kiel)*
- Research staff:
  - *Jarek Knap*
  - *Raul Radovitzky*
- Post-doctoral students:
  - *Sylvie Aubry*
  - *David Olmsted (Brown)*
  - *Fehmi Cirak*
  - *Rena Yu*
- Graduate students
  - *Matt Fago*
  - *Bill Klug*
  - *Marisol Koslowski*
  - *Adrian Lew*
  - *Olga Schneider*
  - *Pururav Thouttireddy*
- Undergraduate (summer) students:
  - *Jay Carlton*
  - *Leslie Smith*

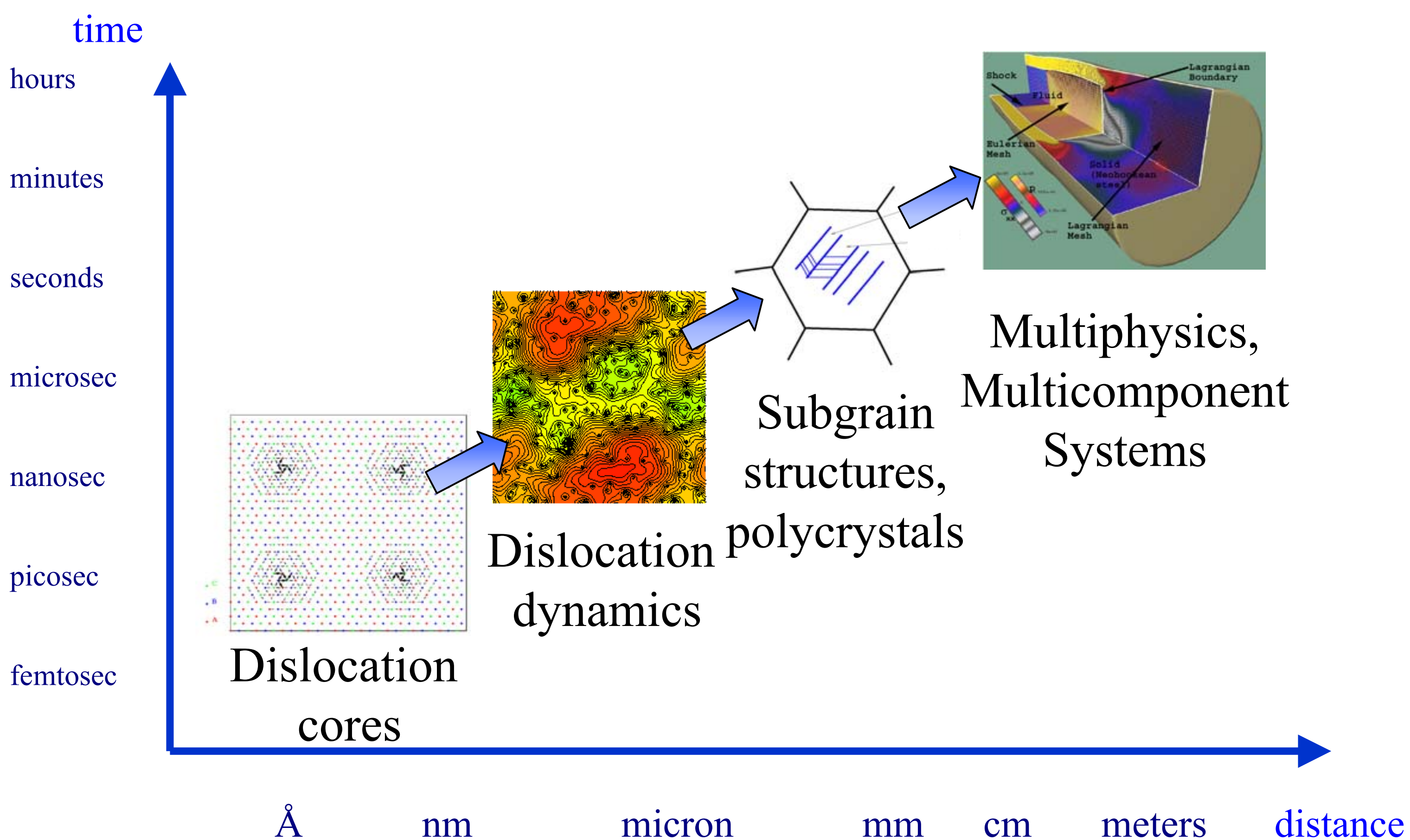
Description and goals of subproject

- The objectives of the solid dynamics group are:
  - *The development of effective theories of material behavior under extreme conditions of pressure, temperature and strain rate through a systematic bridging of scales (multiscale modeling paradigm).*
    - *Understanding and modeling the unit mechanisms which underlie the effective behavior of materials at all relevant length scales, atomistic to continuum (in close collaboration with the MP group).*
    - *The development of numerical and analytical tools for bridging length scales and determining scaling laws and effective behavior.*
  - *The development of scalable solution procedures enabling high-fidelity integrated simulations of multi-component systems within the Virtual Testing Facility (in close collaboration with HE, CS groups).*

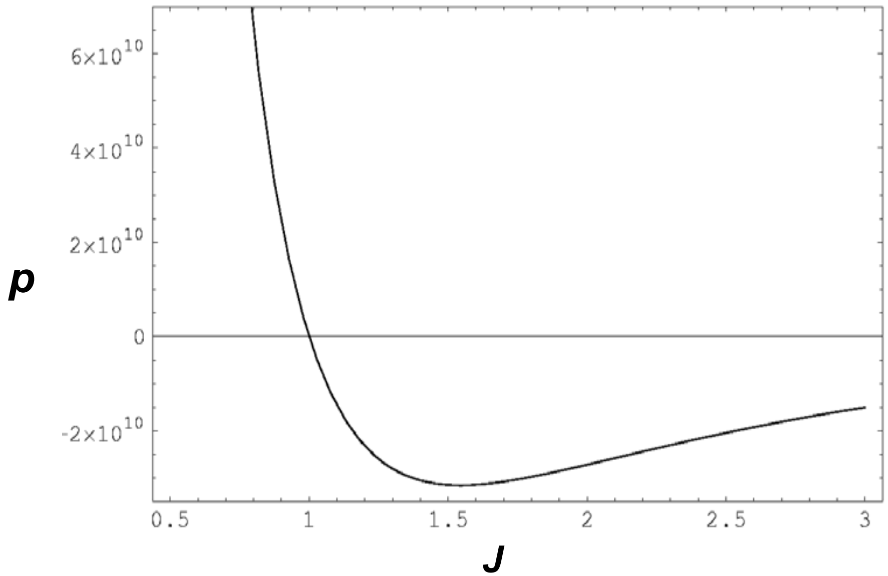
Research activities in FY’01

- Multiscale Ta model:
  - *Integration of ab initio EoS, elastic moduli (R. Cohen)*
  - *Atomistic calibration (with MP group)*
  - *Experimental validation*
  - *Phase field model of dislocation dynamics*
  - *Subgrain structures, validation*
- Fracture and fragmentation:
  - *Nanovoid nucleation by vacancy aggregation*
  - *Nanovoid expansion, porous plasticity model*
  - *`Spall elements’ for simulating ductile rupture*
  - *Validation of cohesive elements*
- Integration into the VTF:
  - *Multiscale Ta model running in the VTF*
  - *Artificial viscosity model implemented, verified*
  - *Parallel meshing*
  - *Parallel fragmentation*

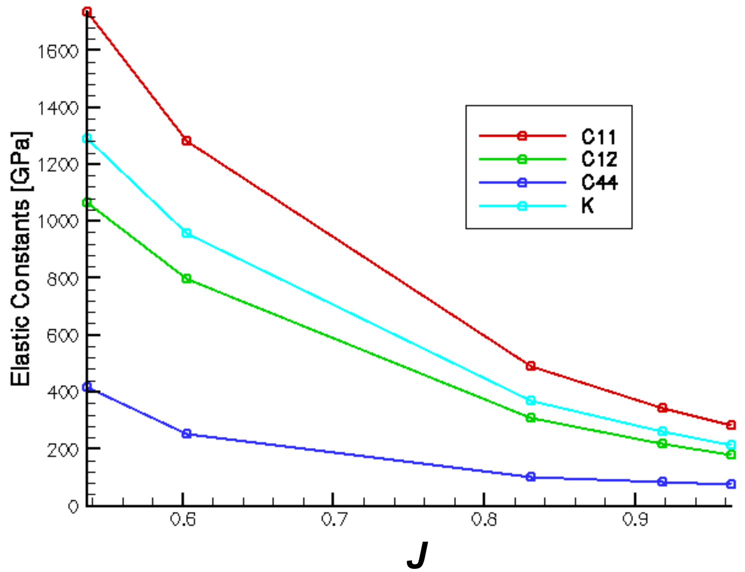
Achievements - Multiscale modeling



Multiscale Ta model – *Ab initio* input

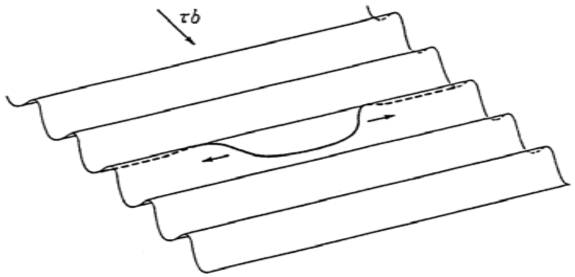


Ta EoS isothermal (R. Cohen)

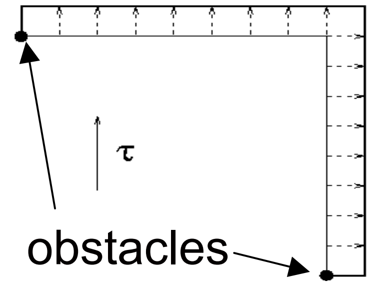


Ta elastic constants (R. Cohen)

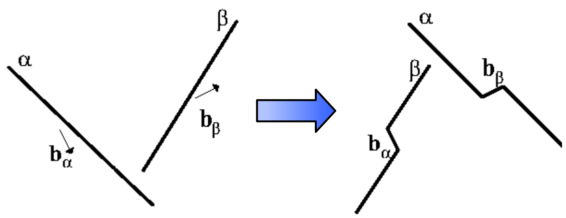
Ta single-crystal plasticity



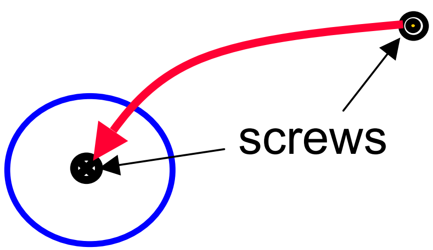
Double-kink mechanism



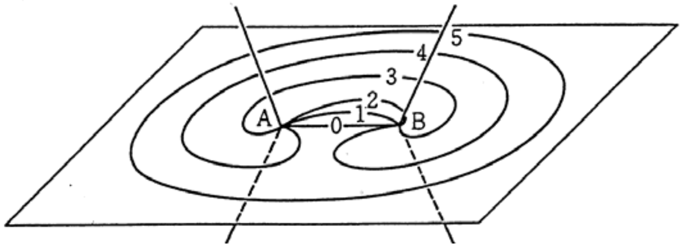
Bow-out mechanism



Jog formation



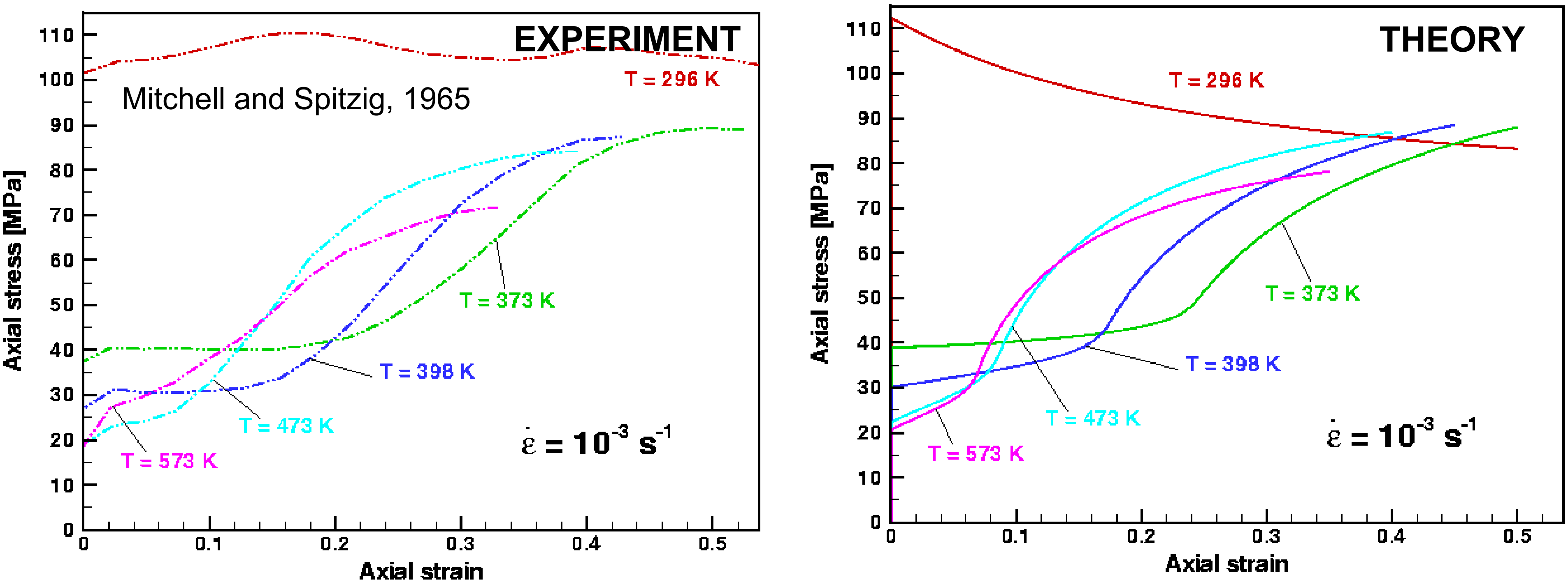
Pair annihilation



Dislocation multiplication

Ta single-crystal plasticity - Validation

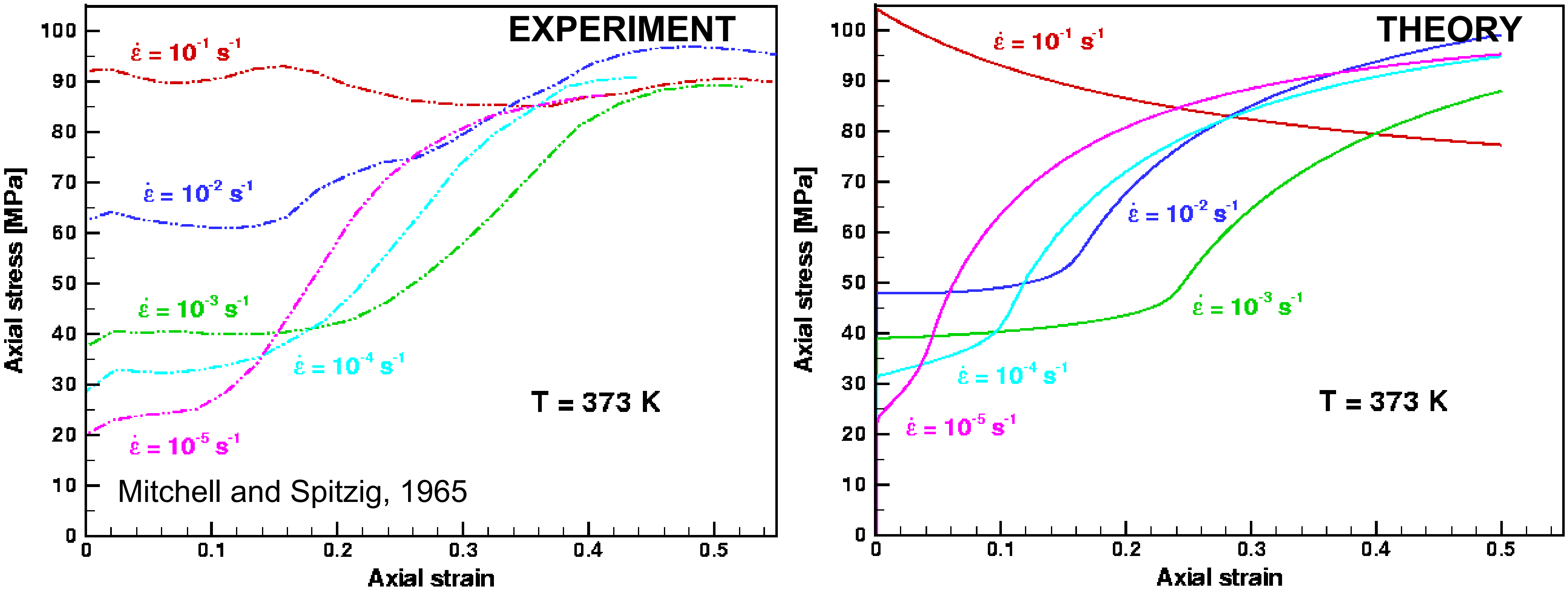
TEMPERATURE DEPENDENCE



(Cuitino, Stainier and Ortiz, 2001)

Ta single-crystal plasticity - Validation

STRAIN-RATE DEPENDENCE



(Cuitino, Stainier and Ortiz, 2001)

Ta single-crystal plasticity - Calibration

MATERIAL PROPERTY	FITTED FROM EXPERIMENT	COMPUTED BY ATOMISTICS
L^{kink}/b	13	17
E^{kink} [eV]	0.70	0.73
$U^{edge}/\mu\, b^2$	0.200	0.216
U^{edge}/ U^{screw}		1.77
E^{cross} [eV]	0.65	-

ATOMISTICS from WANG, STRACHAN, CAGIN and GODDARD

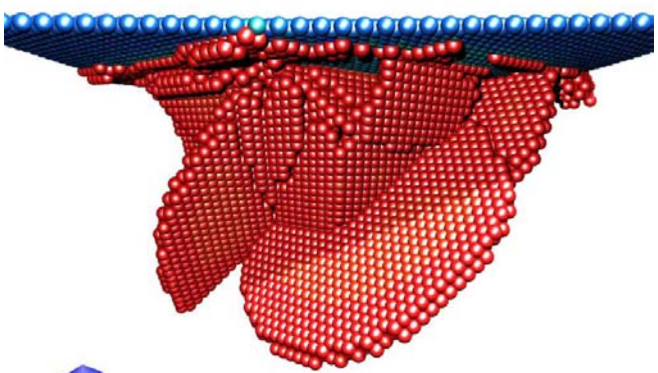
Multiscale modeling

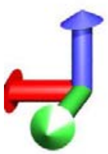
- Multiscale modeling leads to material parameters which quantify well-defined physical entities
- The material parameters for Ta have been determined independently in two ways:

Fitting | Atomistic calculations

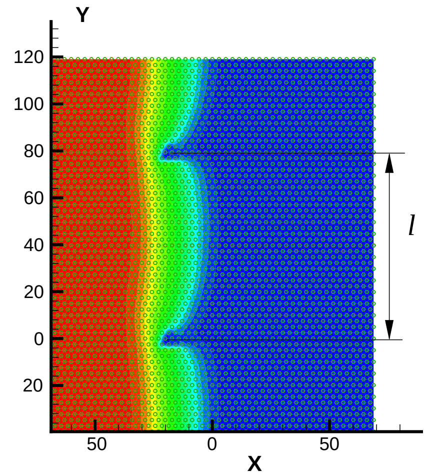
- **Both approaches have yielded ostensibly identical material parameters!**
- Same agreement with experiment would have been obtained if the parameters had been determined directly by simulation in the absence of data.
- This provides validation of modeling and simulation paradigm (as a complement to experimental science)

Additional developments

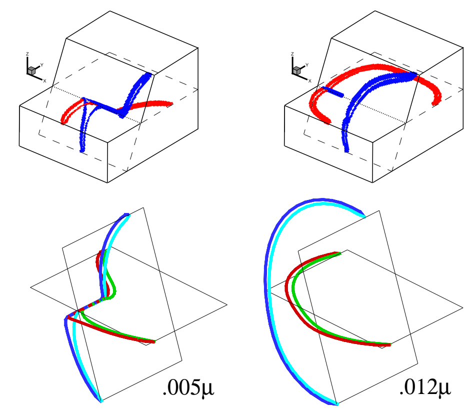




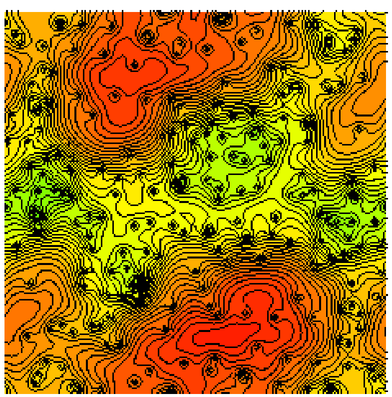
Nanoindentation
(J. Knap)



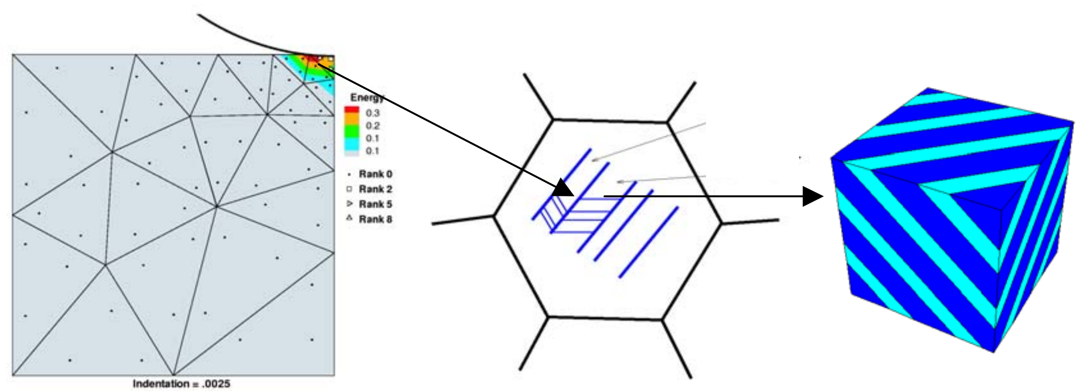
Dislocation/impurity
Interaction (R. Phillips)



Dislocation junctions
(R. Phillips)



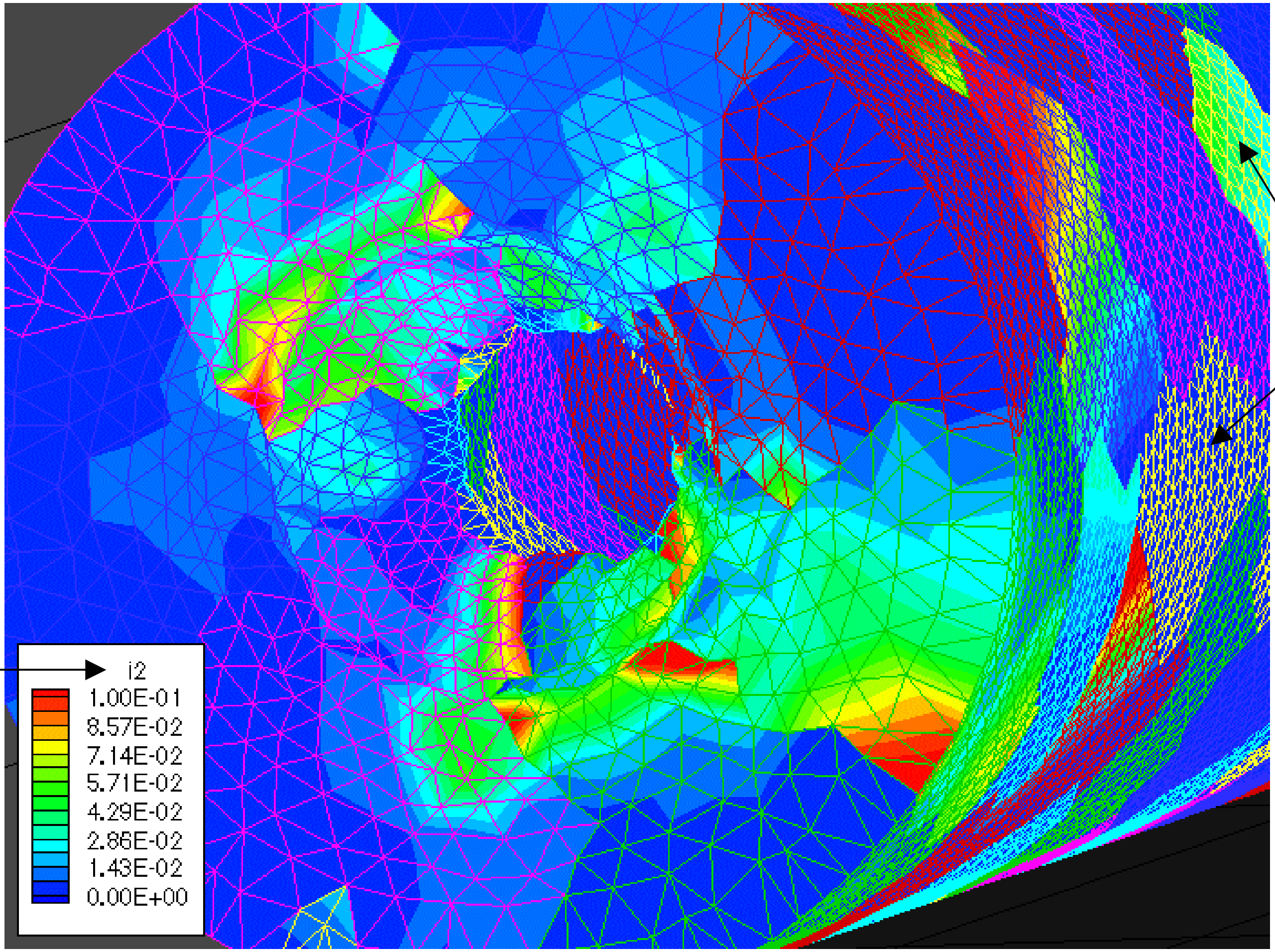
Dislocation dynamics
(M. Koslowski,
A.M. Cuitino and M. Ortiz)



Subgrain structures
(S. Aubry, M. Fago
And M. Ortiz)

Multiscale Ta model: VTF Simulation

Slip activity

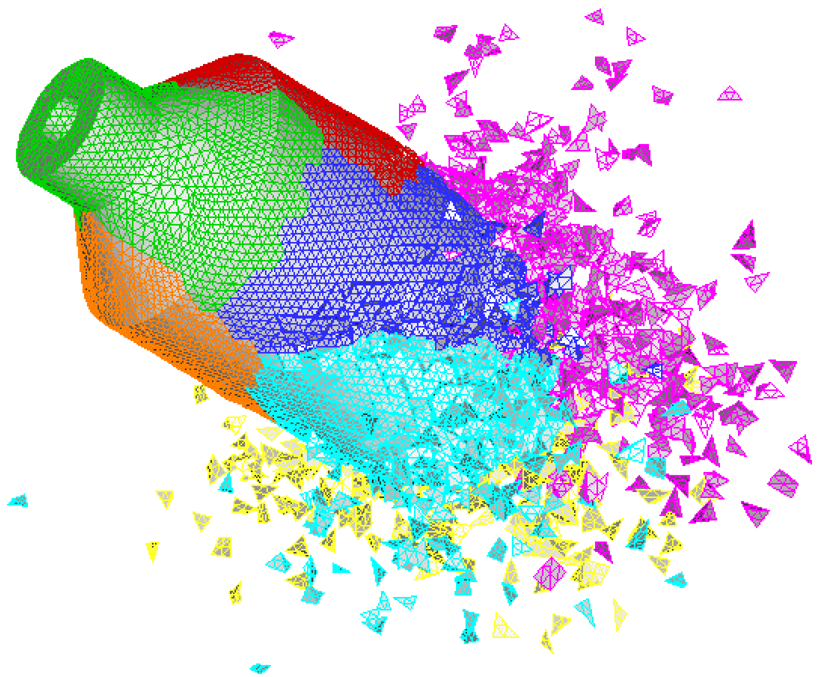


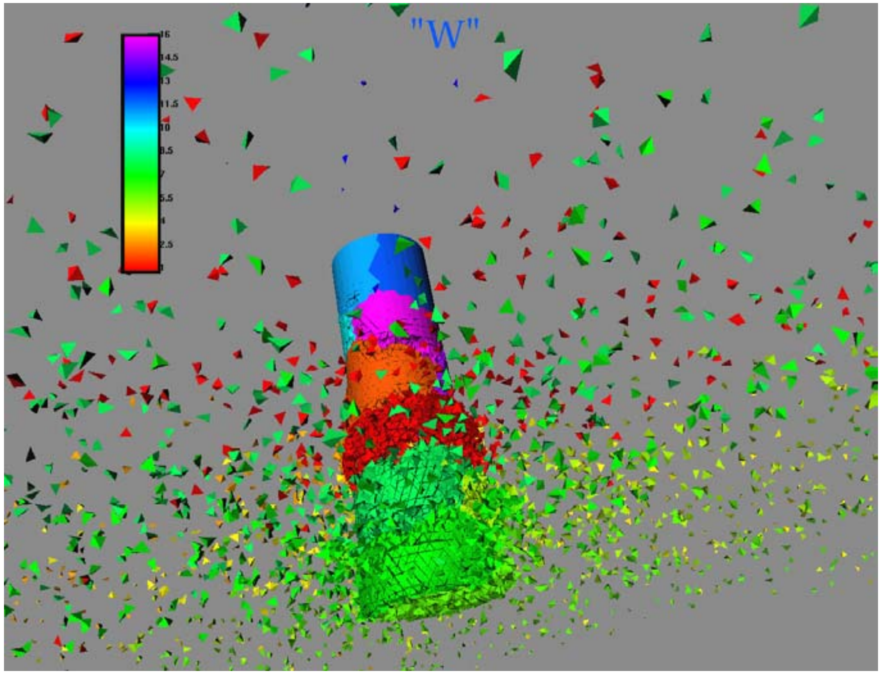
grains

VTF calculations using multiscale Ta model

(Radovitzky, Cuitino, 2001)

Fracture and fragmentation





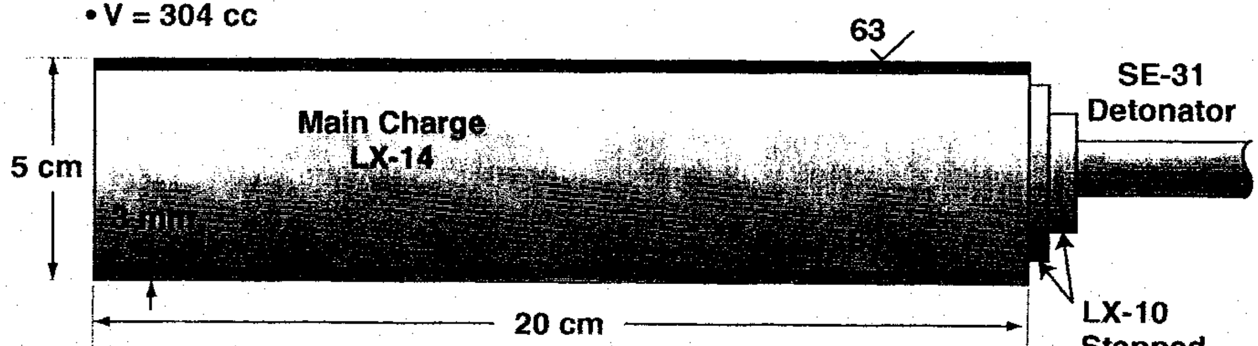
Parallel calculations of fragmentation of steel canister

(Radovitzky, Knap, Pandolfi)

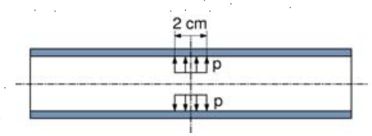
Fracture and fragmentation - Validation

PB-X Cylinder / HE Assembly

CYLINDER:
- 1045 Steel, heat treated prior to machining
- Surface finish is 63m (~1.6 µm) on inner/outer surfaces
- V = 304 cc



HE:
- LX-10 (RX-05-DE) 95% HMX / 5% Viton A — ρ = 1.86 g/cc
- LX-14 95% HMX / 5% Estane — ρ = 1.83 g/cc
- Total HE: 557 g



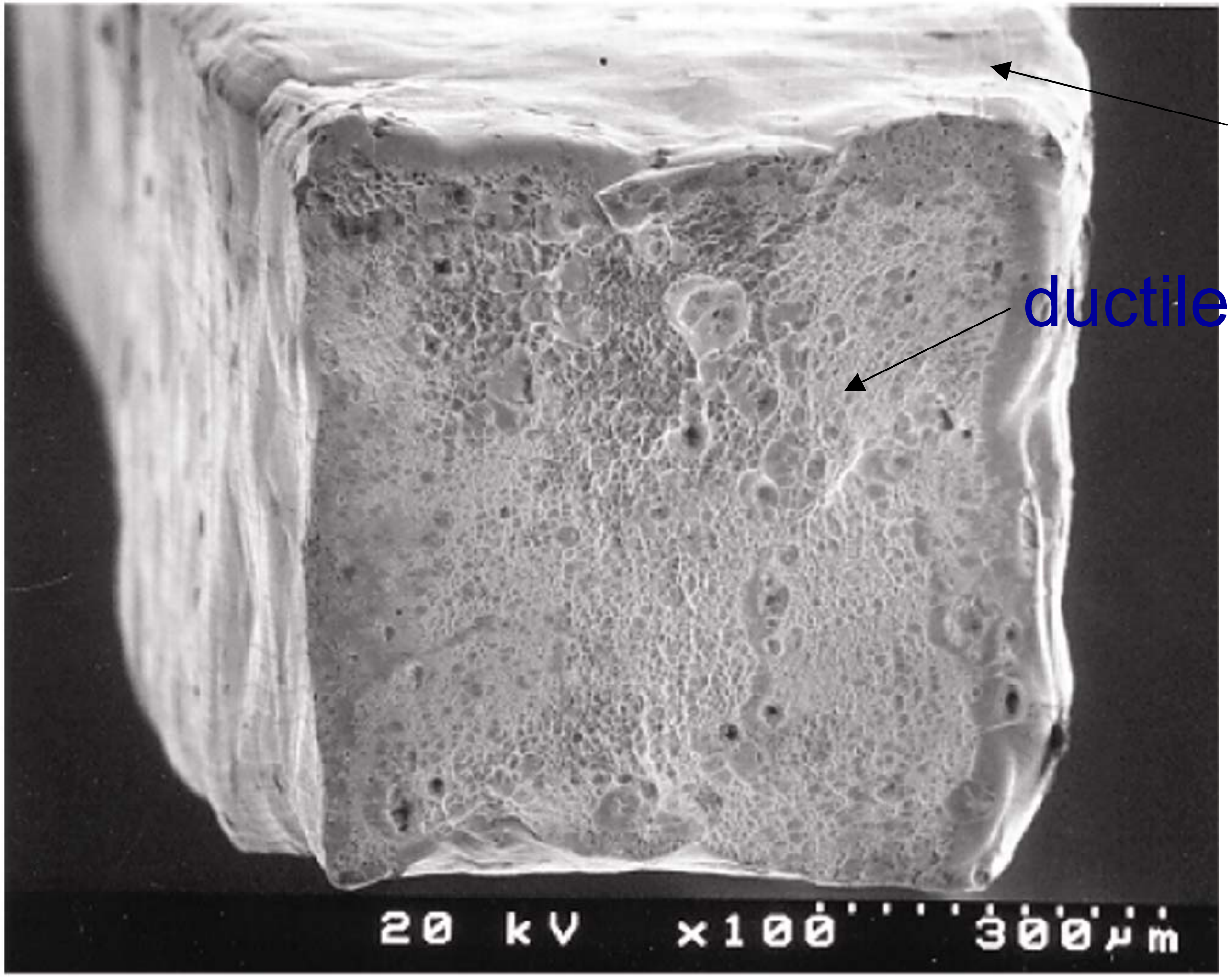
ENERGETIC MATERIALS CENTER

LLNL - JDM - 3/6/01 - 4

Ted Orzechowski DNT/Adiv and John Molitoris CMS/HEAF

(Communicated by J. Belak, LLNL)

Fracture and fragmentation



necking

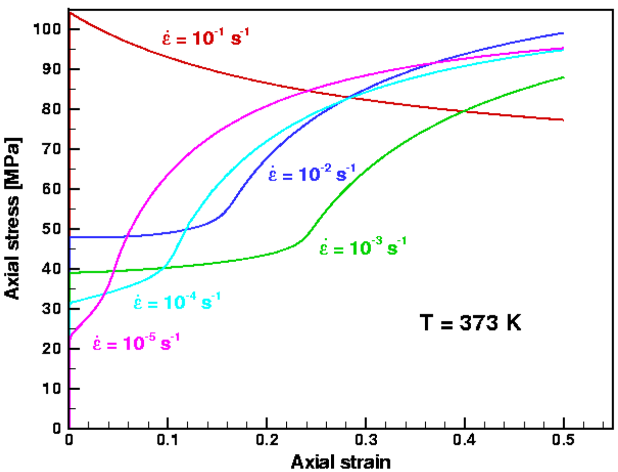
ductile fracture

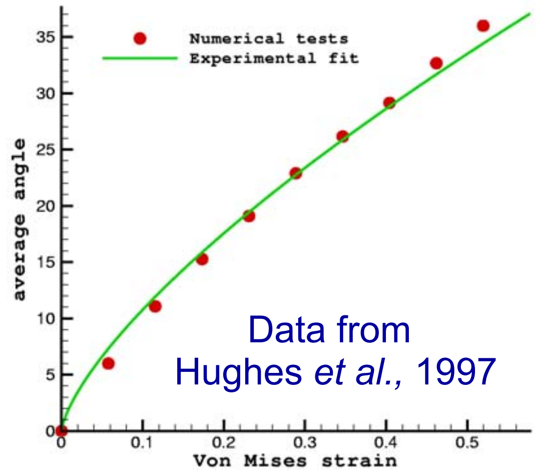
Courtesy of Rich Becker, 2001

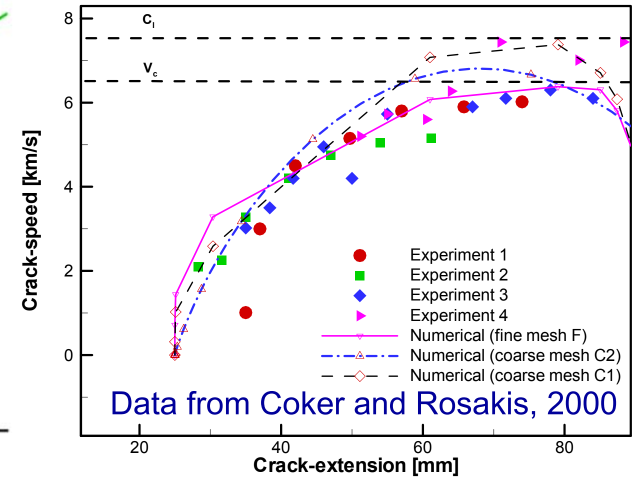
Fracture and fragmentation

- Objectives:
  - *Multiscale modeling of ductile fracture, spall*
  - *Numerical simulation of fragmentation, coupling to plasticity*
- Nucleation: MC model of vacancy aggregation in bulk, at grain boundaries (A. Cuitino, M. Koslowski)
- Nanovoids: QC, phase field simulations of nanovoid growth (J. Knap, M. Koslowski)
- Microvoids: Continuum porous plasticity model (K. Weinberg)
- Fragmentation and spall: Spall elements for localizing damage to surfaces (A. Mota, J. Yang)

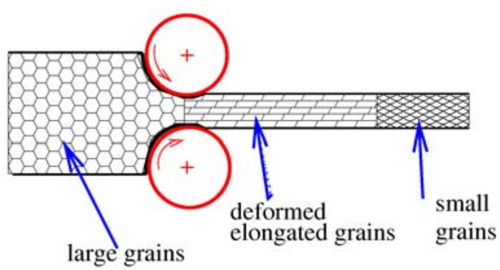
Validation tests

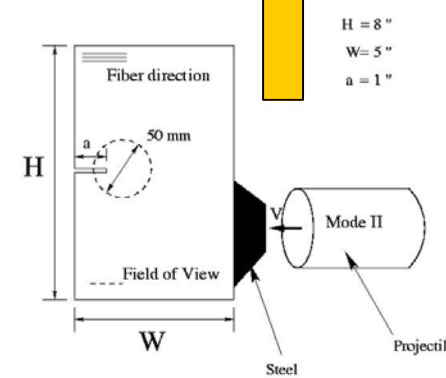






Uniaxial tension test





Uniaxial test | Subgrain structures | Dynamic fracture