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

- Dislocation cores
- Dislocation dynamics
- Subgrain structures, polycrystals
- Multiphysics, Multicomponent Systems

Time scale:
- hours
- minutes
- seconds
- microsec
- nanosec
- picosec
- femtosec

Distance scale:
- Å
- nm
- micron
- mm
- cm
- meters
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)

Mitchell and Spitzig, 1965

EXPERIMENT

THEORY

\[ \dot{\varepsilon} = 10^{-3} \, \text{s}^{-1} \]
Ta single-crystal plasticity - Validation

STRAIN-RATE DEPENDENCE

Mitchell and Spitzig, 1965

(Cuitino, Stainier and Ortiz, 2001)
## Ta single-crystal plasticity - Calibration

<table>
<thead>
<tr>
<th>MATERIAL PROPERTY</th>
<th>FITTED FROM EXPERIMENT</th>
<th>COMPUTED BY ATOMISTICS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L^\text{kink}/b$</td>
<td>13</td>
<td>17</td>
</tr>
<tr>
<td>$E^\text{kink}$ [eV]</td>
<td>0.70</td>
<td>0.73</td>
</tr>
<tr>
<td>$U^\text{edge}/\mu b^2$</td>
<td>0.200</td>
<td>0.216</td>
</tr>
<tr>
<td>$E^\text{cross}$ [eV]</td>
<td>0.65</td>
<td>-</td>
</tr>
</tbody>
</table>

**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

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 63 μm (~1.6 μm) on inner/outer surfaces
- \( V = 304 \text{ cc} \)

**HE:**
- LX-10 (RX-05-DE) 95% HMX / 5% Viton A \( \rho = 1.86 \text{ g/cc} \)
- LX-14 95% HMX / 5% Estane \( \rho = 1.83 \text{ g/cc} \)
- Total HE: 557 g

(Communicated by J. Belak, LLNL)
Fracture and fragmentation

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

Data from Hughes et al., 1997
Data from Coker and Rosakis, 2000

Hughes et al., 1997
Data from Coker and Rosakis, 2000