Extreme Deformation and Failure of Metals by Pulsed Lasers

Marc A. Meyers

Y.Z. Tang, C.-H. Lu, T. Remington, S. Zhao, E. Hahn UCSD E. M. Bringa, C. Ruestes, U. N. Cuyo, Argentina B. A. Remington, B. Maddox, H. S. Pullk, R. Rudd, LLNL

Funding: UCOP, DOE-NNSA

Laboratory for Laser Energetics (LLE), University of Rochester





- Energy up to 40,000 J
- 351 nm wavelength







http://www.lle.rochester.edu/

THE OMEGA TARGET CHAMBER





Source: http://www.llnl.gov/nif/project/lib_construction.html



Fundamental Questions

- Strength under extreme strain rates and pressures
- Dislocations in shock compression: homogeneous generation v. multiplication
- The slip/twinning transition
- Void nucleation and growth: defects and kinetics
 The search for the elusive supersonic dislocation

Lasers: time: ~1 ns strain rate: ~10⁹ s⁻¹ Molecular dynamics: time : ps strain rate: 10⁹ s⁻¹



Strength under Extreme Compression



X Ray Diffraction: Bragg(reflection) and Laue (transmission)



 b) time-resolved diffraction data Bragg

Uncompressed Uncompressed Time

Laue

UCSD

Meyers, Wark, Remington, Ravichandran et al., Acta Mat, 2001

Strength through Diffraction during Shock Compression



 $(\sigma_{12})_f = \gamma G = (\varepsilon_1 - \varepsilon_2) G = 435 MPa$

Pressure = 18 GPa Meyers, Wark, Remington, Ravichandran et al., Acta Mat, 2001

Highest Strain Rate for [001] Cu; P~100 GPa



W.J. Murphy, A. Higginbotham, G. Kimminau, B. Barbrel, E.M. Bringa, J. Hawreliak, R. Kodama, M. Koenig, W. McBarron, M.A. Meyers, B. Nagler, N. Ozaki, N. Park, B. Remington, S. Rothman, S. M. Vinko, T. Whitcher and J.S. Wark, J Phys : Condens. Matter, 22 (2010), 065404.



Dislocation Generation





Moving dislocations

Meyers, Remington, Wark, Ravichandran, et al. Acta mat. 2001 Meyers, Remington, Bringa, Jarmakani, in 'Dislocations in Solids,' Ed. J. P. Hirth, Vol. 15, 2010



FCC Metals:Generation of Partial Dislocation Loops







Predicted and Observed Dislocation Densities: FCC Ni





Stacking-Fault Formation above HEL: FCC Ni and Cu



Shock Compression and Unloading: FCC



BCC: Generation of Perfect Dislocations



MD predictions: Threshold for Dislocation nucleation: very high

Dislocation Multiplication: from Orowan to Kocks to Arsenlis/Barton

10

Dislocation Velocity, v_d (m/s)

Orowan

$$\dot{\gamma} = \frac{d\gamma}{dt} = Mb\rho \frac{\partial \ell}{\partial t} + Mb\ell \frac{\partial \rho}{\partial t} = Mb(\rho \upsilon_d + \ell \dot{\rho})$$

Kocks



Arsenlis/Barton

$$\rho = \rho(\dot{\varepsilon}_{p}, \upsilon_{d}) = \rho(P) = \frac{\dot{\varepsilon}_{p} - Mb\upsilon_{d}tR\dot{\varepsilon}_{p}}{\left(Mb\upsilon_{d} - \frac{Mb\upsilon_{d}tR\dot{\varepsilon}_{p}}{\rho_{sat}(\dot{\varepsilon}_{p})}\right)}$$



Simulation results from Deo et al. (2005) Simulation results Tang et al. (2010)

Fitting Curve



Grady-Kipp

 $\dot{\varepsilon} = 27.34 \times 10^{-36} \times P_{shock}^4$ Lu et al. Acta 2012

Homogeneous Dislocation Generation vs. Dislocation Multiplication: Tantalum (BCC)



Pressure (GPa)



Slip-Twinning Transition



$$\sigma_{s} = \sigma_{s}^{*} + C_{2}e^{-C_{3}T}\dot{\varepsilon}^{C_{4}T} + k_{s}d^{-1/2}$$

$$\sigma_T = \sigma_0 + m \left(\frac{Gb}{C_1}\right)^{1/2} \left[\frac{U^*}{RT} \ln \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right]^{1/q} d^{-1/2}$$



Slip-Twinning transition



Strength in Tension

Void growth in FCC (Cu) and BCC (Ta) metals



Spall Strength: Effect of Time





Void Seen in High Voltage TEM: KRATOS, NCEM 1 MeV



Christy, Pak, Meyers , Explomet Proc., 1986



Experimental Observation





Dislocation activity (slip) around growing voids



Meyers MA, Aimone CT. Prog in Matls Sci 1983;

Christy et al. Metallurgical Applications of Shock Wave and High-Strain-Rate Phenomena, Dekker 1986

Loading on [110] (z-axis)





Nanovoid growth:Marian, Knap, Ortiz







Marian, Knap, Ortiz, PRL, 93(2004)165503 Marian, Knap, Ortiz, Acta mat., 53(2005)2893

Void Growth Simulation-loading [110]

[110] strain direction along z-axis

Void Growth Simulation-loading [111]

[111] strain direction along z-axis





Loading on [111] Triplanar Loops



Hydrostatic tension-Tantalum Prismatic Loop Formation



Sequence of Shear Loop Emission in Ta

3.3 nm radius void, uniaxial compressive strain, strain rate 10⁸ s⁻¹



Stress for Dislocation Loop Emission

1. Creation of a new surface step during the emission process.

$$\tau_1 = \frac{2\gamma\rho b}{\pi[(\rho b)^2 + r^2]}$$

2. Stress required to generate and bow a dislocation loop to a radius R1 that is a fraction of the void radius *R*.

$$\tau = \frac{2\gamma}{\pi\rho b} + \frac{Gb(2-\nu)}{4\pi(1-\nu)R_{1}} \ln \frac{8mR_{1}}{e^{2}\rho b}$$

$$\frac{\sigma_{\nu M}}{G_{<111>}} = \frac{0.448\tau_{\max}}{G_{<111>}} = 0.448 \left[\frac{2\gamma}{G_{<11>}\pi\rho b} + \frac{b(2-\nu_{<11>})}{4\pi(1-\nu_{<11>})R_{1}} \ln \frac{8mR_{1}}{e^{2}\rho b} \right] \quad \text{BCC}$$

$$\frac{\sigma_{\nu M}}{G_{<112>}} = \frac{0.33\tau_{\max}}{G_{<112>}} = 0.33 \left[\frac{2\gamma}{G_{<11>}\pi\rho b_{p}} + \frac{b_{p}(2-\nu_{<112>})}{4\pi(1-\nu_{<112>})R_{1}} \ln \frac{8mR_{1}}{e^{2}\rho b_{p}} + \frac{\gamma_{SF}}{G_{<112>}b_{p}} \right] \quad \text{FCC}$$



Rice and Thomson , Phil Mag 1974

Stress vs. Void Size: MD and Analytical Prediction



Tang et al., Acta Mat 2012

Void Initiation at Tri-Vacancy: BCC Ta





 $\varepsilon = 11\%$



Tang et al. Acta Mat 2011

Experimental Evidence



Christy et al.



Void Shape Development



Nanocrystalline Copper: Tension



4 grains (D ~ 20nm) 1.3 million atoms Hydrostatic expansion Strain rate 10^9 /s

Bringa et al. Acta Mat. 2010


Tension of nanocrystalline Ta





Tensile failure of nanocrystalline Ta



High Velocity Dislocations: Nanoindentation as a Dislocation Source:Ta







Removal of Surface Layer and Shock Compression of Prismatic Loops







High Velocity Dislocations: Tantalum



High Velocity Dislocation: Silicon





Shock of 001 silicon using the SW potential P=35 GPa; Particle vel. 1.75 km/s; flyer plate velocity of 3.5 km/s.



[001] Si: Pressure ~60 GPa





Fundamental Questions: Answers?

- Strength under extreme strain rates and pressures?
- Great strides made up to 10 ¹⁰ s⁻¹
- Defect generation: dislocations
- Homogeneous dislocation generation; FCC dislocation multiplication; BCC
- •Twins in compression and tension?
- Twinning threshold, pressure and shear induced transformations.
- Tensile failure
- Void formation explained.
- Dislocation velocities: transonic/supersonic?
- Experiments January 30 in Omega



Conclusions Voids: I

- Special' Shear Loops Primary Mechanism of Void Growth, as postulated by Lubarda et al. (2004)
- Model FCC Metal: Copper
- New mechanisms for loop formation Bi-Planar and Tri-Planar Loops – identified by MD.
- Dislocation reactions and energetics for mono-planar, and bi-planar loops analyzed.
- Growth Kinetics of void modeled and compared with Cocks-Ashby.
- Density of geometrically-necessary dislocation loops calculated; consistent with observations
- Partial dislocation velocities: sub and transonic



Conclusions Voids: II

Model BCC Metal: Tantalum

- Three mechanisms identified:
 Shear loop formation
 Twinning
 Prismatic loop formation
- Dislocation velocities: subsonic
- Tension/Compression asymmetry
- Slip-twinning transition
- Void-size effect



Laser Shock Compression of Sandwich Micro-Nano-Micro Laminates

Marc A. Meyers , Vitali F Nesterenko, T. Weihs Ph. D. student: Chung-Ting Wei Collaboration: B. R. Maddox, B. A. Remington, LLNL

> Materials Science and Engineering University of California, San Diego

₹UCSD | Mechanical and Jacobs | Aerospace Engineering



Based on statistical mechanics supplemented by the SW potential.

(Lovelady & Oleynik, 2005)



Reactive Materials: Ni-Al Laminates







Schematic of Laser Experiment





After laser shock, the sandwich structure penetrated into the aero-gel in tube.
 Sandwich structure had fully developed irradiated crater and spall.
 Fragments were captured and stored in aero-gel,.



Dissembled Sandwich Structure





SEM Observation

Crater area (Irradiated surface)



Spallation area (included rear surface)





Reacted Nano-laminate (Rear surface of spall laminate)



Grain size varies from ~300 nm to ~800 nm.



SEM Observation

Crater BSE



<u>_____</u>

Crater SE image



Edge of the crater



Molten materials on the crater





Rear Surface of The Crater

Rear surface

Reacted nano-laminate







Зµm



Зµm

Spallation of 875 J Laser Irradiation





Evidence of Intermetallic reaction



After shock induced reaction, the nano-laminate turns to a granular intermetallic structure

The strong exothermic heat melted micro-laminate (both Ni and Al layers).

Reaction did not propagate



SEM Observation





Rear Surface of Irradiated Laminate



The irradiated laminate was shattered by a intensive laser shock, over 1300 J.

The spall was completely developed and peeled out off the rear surface of irradiated laminate.



Conclusions

✤ Laser shock did not generate reaction in microlaminate up to 1300

- Nanolaminate fully reacted at 650 J
- Granular intermetallic compounds with size ~200 nm to ~800 nm.
- Grain size decreases with increasing laser energy
- Spall surface has no reaction and molten materials. The fracture edge showed a clear ductile fracture. It implies that the spallation process is controlled by plastic flow.
- The inner surfaces of the sandwich structure show that strong exothermic heat from the intermetallic reaction of the nanolaminate can melt down the micro-laminate.
- However the reaction did not proliferate to the adjacent micolaminates.
- The irradiated surface shows molten pools, intermetallic densities and possible intermetallic grains.

Laser Spalling and Fragmentation in Vanadium





Dislocation Velocities: Ta



Spall Strength: Gas Gun, Laser, Theoretical <u>Maximum</u>



Future Work

Laser spall and fragmentation experiments

- Continued collaboration with Cavendish: Jan. 2011 visit
- Quantitative analysis of reaction products: granular intermetallics.
- Shock pressure simulation and analysis
- X-ray diffraction analysis
- TEM analysis (By using FIB, we can slice out a specific area and make a TEM samples; UCLA has capability

Additonal Slides: Not Shown



Conclusions: Deformation in Compression

- FCC Ni: dislocation generation at grain boundaries and emission into grains, and annihilation in opposite GB.
 Partial separation.
- Grain boundary sliding: decreases with increasing GS.

BCC Ta: In compression, plasticity, in the form of both GB sliding and dislocation activity, occurs.
Inverse Hall-Petch from 2.5 to 30 nm, due to the decreasing role played by GB shear as GS increased.


Molecular Dynamics (MD): II BCC Metals (Ta)

- Potential: Extended Finnis-Sinclair Potential for Ta
- Boundary Condition: Periodic Boundary Conditions along three directions
- Sample size: 20 ~ 66 nm in length (0.4 M ~16 M atoms)
- Strain rate: 10⁷ s⁻¹ ~ 10¹⁰ s⁻¹, Loading along
 [100] orientation
- Void: Pre-existing, spherical, with radii between 0.15 and 30 nm
- Simulator: LAMMPS, Common Neighbor Analysis (CNA) as defect filter



Sequence of Shear Loop Emission in Ta

3.3 nm radius void, uniaxial compressive strain, strain rate 10⁹s⁻¹



Twinning planes and directions





Dislocation Velocities: MD Predictions









Ni G. S. = 10 nm Uniaxial Compression to 23 GPa and Release



Tantalum Sample preparation: Voronoi Tesselation



66*66*66 nm, *d*=27.3 nm



66*66*66 nm, *d*=872 nm



Uniaxial tensile strain-Twnning

3.3 nm radius void, uniaxial tensile strain, strain rate 10⁹s⁻¹



Compression of nanocrystalline Ta: GB shear

Grain rotation



Compression of nanocrystalline Ta: GB shear



Stage I: Initiation by Vacancy Diffusion



In-plane Dislocation loops

Partial In-plane Dislocations

$$\vec{b}_1 = rac{a}{2} \, [ar{1}01] \Rightarrow \vec{b}_{p1} = rac{a}{6} \, [ar{1}ar{1}2] \, ; \vec{b}_{p2} = rac{a}{6} \, [ar{2}11]$$

$$ec{b}_2 = rac{a}{2} \, [ar{1}10] \Rightarrow ec{b}_{p3} = rac{a}{6} \, [ar{1}2ar{1}] \, ; ec{b}_{p4} = rac{a}{6} \, [ar{2}11]$$

$$\vec{b}_{p1} + \vec{b}_{p3} = \frac{a}{6} \left[\bar{1}\bar{1}2 \right] + (-)\frac{a}{6} \left[\bar{1}2\bar{1} \right] = \frac{a}{2} \left[0\bar{1}1 \right]$$

$$ec{b}_{p2}+ec{b}_{p4}=rac{a}{6}\,[ar{2}11]+(-)rac{a}{6}\,[ar{2}11]=0$$





Traiviratana et al. Acta Mater 2008;56:3874

Void Growth Simulation-loading [001]

[001] strain direction along z-axis





Bi-planar Dislocation loops



Bi-planar Dislocation loops











Traiviratana et al. Acta Mater 2008;56:3874

Loading on [110] (z-axis)











Bi-planar Dislocation loops

Perfect Dislocation – Bi-Planar Interaction





 $(\bar{1}\bar{1}\bar{1}\bar{1})$

Modeling of Nanovoid Growth

Lubarda et I. Acta mat 2004. Marian , Knap, Ortiz. Phys Rev Lett 2004; Acta Mat 2005 Traiviratana et al. Acta Mater 2008. Meyers et al. J Mater 2009. Bringa et al. Acta Mater 2010.



Bi-planar Dislocation loops

Partial Dislocation – Bi-Planar Interaction

$$\vec{b}_{1} = \frac{a}{2} [\bar{1}01] \Rightarrow \vec{b}_{p1} = \frac{a}{6} [\bar{1}\bar{1}2]; \vec{b}_{p2} = \frac{a}{6} [\bar{2}11]$$
$$\vec{b}_{2} = \frac{a}{2} [\bar{1}10] \Rightarrow \vec{b}_{p3} = \frac{a}{6} [\bar{1}2\bar{1}]; \vec{b}_{p4} = \frac{a}{6} [\bar{2}11]$$
$$\frac{a^{2}}{2} > \frac{a^{2}}{6} + \frac{a^{2}}{6} = \frac{a^{2}}{3}$$
$$\vec{b}_{p1} + \vec{b}_{p3} = \frac{a}{6} [\bar{1}\bar{1}2] + (-)\frac{a}{6} [\bar{1}2\bar{1}] = \frac{a}{2} [0\bar{1}1]$$
$$\vec{b}_{p2} + \vec{b}_{p4} = \frac{a}{6} [\bar{2}11] + (-)\frac{a}{6} [\bar{2}11] = 0$$

$$\frac{a^2}{6} + \frac{a^2}{6} = \frac{a^2}{3} > \frac{a^2}{18}$$





Traiviratana et al. Acta Mater 2008;56:3874

Loading on [111] (z-axis)





Conclusions: Deformation in Tension

- FCC Cu: dislocation generation at grain boundaries leads to void formation at GBs.
- BCC Ta: decohesion of GBs occurs before plasticity, due to flow stress exceeding grainboundary cohesion strengh at the imposed strain rate (~10⁸ s⁻¹).





First Generation

Janus Laser facility in Lawrence Livermore National Lab





Laser Shock Eperiments: First Generation

Bilayer Thickness	8ns Laser Energy	Laser Intensity (8ns)	3ns Laser Energy	Laser Intensity (3ns)	
5µm	229 J	2.56 × 10 ¹² (W/cm ²)	107 J	3.18 × 10 ¹² (W/cm ²)	
5µm			430 J	1.28 × 10 ¹³ (W/cm²)	
30µm	24J	2.68 × 10 ¹¹ (W/cm ²)	105 J	3.13 × 10 ¹² (W/cm ²)	
30µm	409J	4.56 × 10 ¹² (W/cm ²)	421 J	1.25 × 10 ¹³ (W/cm ²)	



Second Generation: OMEGA Laser Facility



Shot #	Shot # SRF shot ID Configuration		ation	Target IDs		On-target energy				
					H7-H14	H3-H1	8	H7-H14	H3-H18	
1	32511	59039	Recovery/VISAR		19 VISAR	23 <110>		600.6	625.2	
2	32745	59040	Recovery/VISAR		20 VISAR	24 <110>		351.8	352.5	
3	32746	59041	Recovery/VISAR		21 VISAR	27 <100>		501.8	505.4	
4	32747	59042	Recovery/VISAR		22 VISAR	30 <111>		682.7	525.2	
5	32510	59043	Recovery/Recovery		25 <110>	28 <123>		476.9	489.0	
6	32748	59044	Recovery/Recovery		29 <123>	40 <rl></rl>		633.0	653.0	
7	32749	59045	Recovery	/Recovery	32 <poly></poly>	35 <na< td=""><td>ino></td><td>509.3</td><td>495.0</td><td></td></na<>	ino>	509.3	495.0	
8	32750	59046	Recovery	/Recovery	33 <poly></poly>	36 <na< td=""><td>no></td><td>362.2</td><td>351.9</td><td></td></na<>	no>	362.2	351.9	
9	32751	59047	Recovery	/Recovery	31 <poly></poly>	37 <na< td=""><td>ino></td><td>657.2</td><td>650.7</td><td></td></na<>	ino>	657.2	650.7	
10	32752	59049	Recovery	/Recovery	34 <poly></poly>	38 <na< td=""><td>ino></td><td>837.4</td><td>662.9</td><td></td></na<>	ino>	837.4	662.9	
11	32753	59050	Recovery	/Recovery	26 <110>	39 <na< th=""><th>ino></th><th>661.5</th><th>842.7</th><th></th></na<>	ino>	661.5	842.7	
12	32754	59051	Recovery	/Recovery	41 <rl></rl>	42 <rl< th=""><th>></th><th>875.3</th><th>1305.3</th><th></th></rl<>	>	875.3	1305.3	
Sample		Laser energy		Recovery						
Tube-18 65		3J/3.7 ns			Complete Spall					
Tube-19 875J		J/3.7 ns			Complete Spall					
Tube-20		1305J/3.7 ns		Shattered		UCSD				

Capsule and Target Configuration

Laser arrangement



Vent Hole on this side



5 mm long Alignment Fibers (1 mm overlap with recovery tube) *Only one fiber (drawing shows 2)



Second Generation

Sample Capsule





