LA-UR-20-20624

Approved for public release; distribution is unlimited.

Title: Elastic-Plastic Deformation of Molybdenum Single Crystals Shocked to 12.5 GPa

Author(s): Mandal, Anirban

Intended for: Send the slides to colleagues at WSU

Issued: 2020-01-22

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Elastic-Plastic Deformation of Molybdenum Single Crystals Shocked to 12.5 GPa

Anirban Mandal

**Committee Members: Dr. Yogendra M. Gupta (Chair)
Dr. David P. Field
Dr. Jow-Lian Ding**

**School of Mechanical and Materials Engineering
Washington State University, Pullman
June 28, 2016**

- **Introduction**
- **Motivation**
- **Background**
- **Objectives and Approach**
- **Experimental Results**
- **Analysis and Discussion**
 - Elastic wave amplitudes
 - Wave propagation simulations
- **Findings**

Introduction

Quasi-static compression (Uniaxial stress)

Elastic-perfectly plastic solid

Shock wave compression (Uniaxial strain)

- Above dynamic elastic limit, elastic-plastic two-wave structure seen
- Elastic wave decay indicates time-dependent plastic response
- Deformation mechanisms understood by analyzing measured wave profiles

Asay et al., JAP (1972)

Governing Equation + Material Response $\rightarrow$ Wave Profile

Motivation

- Studies on single crystals provide better insight
- Shock-induced deformation of BCC single crystals not well-understood
 - Lack of reliable and comprehensive elastic-plastic wave profile measurements: W^1 , Mo^2 , Ta^3
 - Material model to predict shock-induced deformation response not available
- Why Molybdenum?
 - Elastic-plastic deformation under compressive shock loading not studied previously
 - Well-studied under quasi-static loading; slip systems identified
 - Aerospace and defense applications involving dynamic loading due to high strength and refractory properties

¹Michaels, *Ph.D. thesis*, WSU (1972), ²Kanel *et al.*, *JAP* (1993); ³Whiteman *et al.*, *J Phys.* (2014)

Background & Objectives

- Quasi-static deformation at room temperature governed by screw dislocation slip
- Twins formed under laser shock loading
- Operative slip systems are $\{110\}\langle 111\rangle$ and $\{112\}\langle 111\rangle$ (also twin systems)
- $\{112\}$ slip exhibits twinning-antitwining asymmetry

Objective: Examine and understand shock-induced elastic-plastic deformation of Mo single crystals

- Examine effect of crystal orientation
- Compare elastic limits under shock and quasi-static loading
- Identify operative slip systems and gain insight into deformation mechanisms
- Develop a dislocation-based, continuum material model

Approach

- Careful characterization of single crystal samples (99.99% pure)
 - Initial dislocation density is $\sim 10^9 \text{ cm}^{-2}$ (Dr. Mukul Kumar, LLNL)
- Measure elastic-plastic wave profiles along [100], [111], [110]: 12.5 GPa elastic impact stress
- Effect of propagation distance or sample thickness ($\sim 0.3 - 2.3 \text{ mm}$)
- Perform 1D wave propagation calculations using a dislocation-based continuum material model to analyze wave profiles

Results: Wave Profiles

Strongly anisotropic, time-dependent material response

Results: Wave Profiles

Strongly anisotropic, time-dependent material response

Results: Wave Profiles

Strongly anisotropic, time-dependent material response

Results: Wave Profiles

Differences in elastic amplitude, stress drop and plastic profiles

Strongly anisotropic, time-dependent material response

Elastic Wave Attenuation

- Measurable attenuation only for [111] at distances examined
- Rapid elastic wave attenuation near impact surface
- No measurable attenuation beyond a threshold stress (elastic limit)

Decay rate and elastic limit depend on crystal orientation

Shear Stresses on Slip Planes

- Shear stresses (τ_{el}) on slip planes comparable at elastic limit
- τ_{el} is better measure of dynamic elastic limit for single crystals
- Decay rates proportional to $(\tau_{imp} - \tau_{el})$

Shear stresses on slip planes key to understanding shock-induced deformation of anisotropic materials

Elastic Limits: Shock and Quasi-static Loading

Exp. type	Longitudinal stress (GPa)			Shear stress on {110} (GPa)			Shear stress on {112} (GPa)		
	[100]	[111]	[110]	[100]	[111]	[110]	[100]	[111]	[110]
Uniaxial strain (Shock)	3.61	5.11	3.58	0.96	0.74	0.90	1.11	0.86	1.04
Uniaxial stress ¹ (Quasi-static)	0.05	0.18	0.20	0.02	0.05	0.08	0.02	0.06	0.09

Resolved shear stresses at dynamic elastic limit

- ~10 – 50 times larger than quasi-static values
- Comparable to Peierls stress ($\tau_p \sim 0.9$ GPa) of screw dislocations on {110} planes²
 - Screw dislocations on {110} planes likely govern deformation
 - Rapid decay for $\tau > \tau_p$; no measureable decay when $\tau \approx \tau_p$

Large difference between shock and quasi-static elastic limits is a consequence of large Peierls stress in Mo crystals

¹G. J. Irwin *et al.*, *PSS (a)* (1974); ²L. Hollang *et al.*, *Mater. Sci. Eng. A*, (2001)

Wave Profile Calculations: [100] Loading

Dislocation model (Winey & Gupta, 2006)

$${}^{\alpha}\dot{\gamma}^p = b^{\alpha} N_m^{\alpha} \bar{v}$$

$${}^{\alpha}\bar{v} = v_s \exp[-D/({}^{\alpha}\tau - \tau_0)]$$

$${}^{\alpha}\dot{N}_m = \begin{cases} M^{\alpha}\dot{\gamma}^p, & \text{for } {}^{\alpha}\tau < \tau_c \\ M^{\alpha}\dot{\gamma}^p + \underbrace{A({}^{\alpha}\tau - \tau_c)^{\alpha}\dot{\tau}}_{\text{'nucleation' term}}, & \text{for } {}^{\alpha}\tau \geq \tau_c \end{cases}$$

- Regenerative multiplication alone cannot explain measured profiles
- 'Nucleation' term required to match measured wave profiles
- $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ systems could not be distinguished
- Work hardening was not required to match wave profiles

Calculations provide insight into rapid elastic wave attenuation

Wave Profile Calculations: [111] Loading

- Good match at small propagation distances, but not at large distances
- Structure likely due to a second yielding on the operative slip systems

Shear stress and shear strain histories provide insight into observed features

Wave Profile Calculations: [110] Loading

- Kink in the plastic profiles results from yielding of non-equivalent slip systems of {110} or {112} family
- Shear stresses on slip systems at kink approach shear stress values at elastic limit

Role of $\{112\}$ Slip Asymmetry

- For [110] loading, $\{112\}$ systems yield in both twinning and anti-twinning sense
- Asymmetry provides somewhat better match following kink
- [100] and [111] profiles are not affected by slip asymmetry

Asymmetry provides likely distinction between $\{110\}$ and $\{112\}$ slip

Is Twinning Responsible for Rapid Attenuation?

Shear stresses at the elastic limit

Longitudinal stress (GPa)			Shear stress on {112} slip systems (GPa)			Shear stress on {112} twin systems (GPa)		
[100]	[111]	[110]	[100]	[111]	[110]	[100]	[111]	[110]
3.61	5.26	3.58	1.11	0.88	1.04	0.55	0.88	1.04

- Shear stresses on twin systems at elastic limit different for [100]
- Twinning alone cannot account for the kink
- Kink in [110] profiles not captured without 'nucleation term'

Dislocation slip responsible for rapid attenuation, not twinning

Findings

- **Mo single crystals shocked to 12.5 GPa elastic impact stress along [100], [111], [110] orientations**
 - **Material response time-dependent and displays crystal anisotropy effects**
- **Elastic wave attenuation and elastic limits depend on crystal orientation**
 - **Shear stresses (τ) on operative slip systems provide key insight into orientation dependence**
 - **Shear stresses (τ_{el}) at elastic limit better measure of material strength for anisotropic crystals**
- **τ_{el} comparable to Peierls stress (τ_p) of screw dislocations**
 - **Deformation governed by screw dislocations**
 - **Rapid attenuation for $\tau > \tau_p$; no measureable decay when $\tau \approx \tau_p$**
 - **Large difference between shock and quasi-static elastic limits is a consequence of large Peierls stress in Mo crystals**

Findings (*contd.*)

- **Wave profile calculations**
 - **$\{110\}\langle 111 \rangle$ and/or $\{112\}\langle 111 \rangle$ slip systems are operative; they could not be distinguished conclusively**
 - **Regenerative multiplication alone cannot account for rapid attenuation**
 - **Attenuation likely governed by a dislocation generation mechanism operative for $\tau > \tau_{el}$; physical justification was not established**
 - **No significant work hardening under shock loading**

Most comprehensive and detailed study of elastic-plastic wave profiles in a shocked BCC crystal

TABLE III. List of $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ slip systems.

Index (α)	$\{110\}\langle 111 \rangle$ type	Index (α)	$\{112\}\langle 111 \rangle$ type
1	$(110)[\bar{1}11]$	13	$(\bar{1}2\bar{1})[111]$
2	$(110)[\bar{1}1\bar{1}]$	14	$(2\bar{1}\bar{1})[111]$
3	$(\bar{1}10)[111]$	15	$(\bar{1}\bar{1}2)[111]$
4	$(\bar{1}10)[11\bar{1}]$	16	$(1\bar{1}2)[\bar{1}11]$
5	$(101)[\bar{1}11]$	17	$(2\bar{1}\bar{1})[\bar{1}11]$
6	$(101)[\bar{1}\bar{1}1]$	18	$(12\bar{1})[\bar{1}11]$
7	$(\bar{1}01)[111]$	19	$(\bar{1}21)[11\bar{1}]$
8	$(\bar{1}01)[1\bar{1}1]$	20	$(2\bar{1}1)[11\bar{1}]$
9	$(011)[1\bar{1}1]$	21	$(\bar{1}\bar{1}2)[11\bar{1}]$
10	$(011)[\bar{1}\bar{1}1]$	22	$(\bar{1}12)[1\bar{1}1]$
11	$(0\bar{1}1)[\bar{1}11]$	23	$(21\bar{1})[1\bar{1}1]$
12	$(0\bar{1}1)[111]$	24	$(\bar{1}2\bar{1})[1\bar{1}1]$