Shock compression of molybdenum single crystals to 110 GPa: Elastic-plastic deformation and crystal anisotropy

Cite as: J. Appl. Phys. **127**, 205902 (2020); <https://doi.org/10.1063/5.0006559>

Submitted: 03 March 2020 . Accepted: 04 May 2020 . Published Online: 29 May 2020

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Submitted: 3 March 2020 · Accepted: 4 May 2020 ·

Published Online: 29 May 2020

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ABSTRACT

To investigate the role of crystal anisotropy on the elastic-plastic deformation of BCC single crystals at high shock stresses, molybdenum (Mo) single crystals were shock compressed along the [100], [111], and [110] orientations at elastic impact stresses between 20 and 110 GPa. Laser interferometry was used to measure shock wave velocities and particle velocity histories. Along the [100] and [111] orientations, elastic-plastic waves (two wave structure) were observed up to 110 GPa. Along the [110] orientation, the two wave structure was observed only up to 90 GPa. The measured elastic wave amplitudes were analyzed to determine crystal anisotropy effects, impact stress dependence, and the activated slip systems on the Hugoniot elastic limit. The findings from our work have provided insight into the role of crystal anisotropy on the elastic-plastic deformation under shock compression at high stresses.

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I. INTRODUCTION

Understanding material behavior under extreme conditions is important for many applications and scientific advances. Plate impact experiments utilizing uniaxial strain loading provide a unique approach to investigate the compressed state of a material at well-characterized, high stresses (~ 100 GPa). Experiments on single crystals are particularly beneficial for the following reasons: orientation of the loading direction and the slip systems are well-defined and that permits shear stress calculations on relevant slip systems; and complications arising from wave reflections at grain boundaries are avoided. Because of these benefits, we chose to study molybdenum (Mo) single crystals to gain insight into the elastic-plastic deformation mechanisms of BCC crystals under ~ 100 GPa shock stresses.

To date, shock wave experimental studies on single crystals have focused primarily on the elastic limit at low peak stresses. The anisotropy of the elastic limit was studied for molybdenum,^{1,2} tantalum,³ lithium fluoride,^{4–6} sodium chloride,⁷ magnesium,^{8,9} beryllium,¹⁰ and copper¹¹ at impact stresses on the order of ~ 10 GPa. Specifically, for BCC single crystals, there have been no studies that have investigated the elastic-plastic deformation under

shock compression to high stresses (~ 100 GPa). Thus, there is a need to conduct studies at ~ 100 GPa impact stresses, to fully understand the role of anisotropy and high impact stress on the elastic limit in shock compressed BCC single crystals. Also, a series of experiments with varying impact stress can enable an understanding of the impact stress dependence.

The objectives of this study were to investigate the elastic-plastic deformation and the anisotropic response of BCC single crystals shock compressed to high stresses that were more than an order of magnitude larger than the elastic limit and to determine the impact stress dependence (peak stress dependence) of the elastic limit for a broad range of impact stresses. Molybdenum was chosen for the following reasons. Molybdenum is a good representative of BCC metals, and it is available in the form of high-purity single crystals. Its elastic-plastic deformation under (quasi-) static loading has been well studied.^{12–25} The plastic deformation of Mo is dominated by the motion of screw dislocations.^{19–25} In BCC metals including Mo, due to its nonplanar structure, the mobility of screw dislocations is significantly lower compared to that of edge dislocations. Thus, the Peierls stress corresponding to a screw dislocation is ten times or more larger than that of an edge dislocation.

When the resolved shear stress (RSS) is smaller than the Peierls stress, thermally activated kink-pair formation and migration controls the plastic deformation. Above the Peierls stress, the mobility of dislocations due to phonon-drag controls the plastic deformation.²⁵ The temperature dependence and the strain-rate dependence of yield stress of Mo single crystals under static loading are attributed to the thermally activated kink-pair formation.

The governing deformation mechanism was found to be the dislocation slip on $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ systems.^{14–22} Some studies have also reported the activation of $\{123\}\langle 111 \rangle$ slip system, but those systems were only observed under small strains on the order of 0.1%, and $\{110\}\langle 111 \rangle$ became prominent as the strain increased.^{19,20} Therefore, in this study, we considered $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ slip systems as the candidates for the activated deformation mechanisms under shock compression.

Regarding shock compression of Mo single crystals, prior studies provided comprehensive data at lower stress (~ 10 GPa) range.^{1,2} The present work has involved the stress range to significantly higher stresses (to 100 GPa and higher) and examined the stress dependence of the elastic limit. Thus, the present work has examined deformation issues not considered in the previous studies.

Specifically, the following questions are addressed in this study: How does the elastic wave amplitude under high impact stresses compare with the lower stress data? Does the elastic wave amplitude show dependence on the impact stress? What is the role of anisotropy at high stresses? What slip systems contribute to yielding at the elastic limit? Can high stress experiments distinguish between $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ slip systems?

To address the above questions, shock compression experiments were conducted on Mo single crystals along $[100]$, $[111]$, and $[110]$ orientations, and the impact stress was systematically varied from 23 GPa to 190 GPa. In this work, the primary focus was on the response of Mo single crystals near the elastic limit. Hence, results of higher impact stress experiments resulting in overdriven single waves are not discussed in any detail.

The experimental details are summarized in Sec. II, and the experimental results are presented in Sec. III. Section IV presents calculations of in-material quantities at the elastic limit, and comparison of results between experiments is discussed. The main findings from the study are summarized in Sec. V.

II. EXPERIMENTAL METHOD

Molybdenum single crystals were obtained from Accumet Materials Co. as cylindrical bars, approximately 30 mm in diameter. Each of the bars was oriented so that the longitudinal direction aligns with the $[100]$, $[111]$, or $[110]$ crystal orientation. A Mo sample was cut from each bar, and characterized under ambient conditions by measuring the density, the longitudinal sound speed, and the shear sound speed. The ambient properties are summarized in Table I.

The experimental configuration is shown in Fig. 1, and the experimental parameters are shown in Table II. Elastic impact stress (EIS) values in Table II provide a consistent approach to ensure that comparable longitudinal stresses are imparted along different crystal orientations, despite crystal anisotropy effects. The EIS values were determined as follows. Using a finite elasticity formulation,⁵ the Mo single crystal elastic Hugoniot was determined

TABLE I. Ambient properties of Mo single crystals.

Orientation	Density (g/cm ³)	Longitudinal sound speed (km/s)	Shear sound speed (km/s)
$[100]$	10.22 ± 0.06	6.746 ± 0.008	3.261 ± 0.005
$[111]$		6.319 ± 0.005	3.666 ± 0.014
$[110]^a$		6.432 ± 0.003	3.850 ± 0.004
			3.264 ± 0.004

^aAcoustic tensor corresponding to the wave propagation in the $[110]$ orientation in a cubic crystal has three distinctive eigenvalues.

for different crystal orientations.^{1,2} Utilizing the continuity of longitudinal stress and particle velocity at the buffer–Mo sample interface, the impactor (or buffer) Hugoniot^{26,27} and the Mo single crystal elastic Hugoniot (for each orientation) were combined to obtain the EIS values.

As shown in Fig. 1, the Mo sample was bonded to a buffer on the front surface and to a LiF optical window on the back surface. The orange arrow is the normal vector of the surface of the Mo sample, and the $[100]$, $[111]$, or $[110]$ orientation was aligned with this normal. The tilt crystal orientation was checked using Laue x-ray diffraction, and it was within 1.5° . The projectile was fabricated by molding the impactor into a polycarbonate base. The buffer and the impactor were always made from the same material to avoid wave reflections from the impactor–buffer interface. Materials were chosen to ensure a single overdriven shock wave in the buffer. There were four interferometry (Velocity Interferometer System for any Reflector; VISAR^{28,29}) probes: the center probe focused on the rear surface of the Mo sample and the three outer probes focused on the rear surface of the buffer. The particle velocity was measured at the Mo sample–LiF window interface using the center probe. By using the dual velocity per fringe (dual-VPF) configuration,³⁰ particle velocity measurements avoided complications due to fringe loss. The signals from the three outer probes were used to estimate the impact tilt. These data were also used to calculate the arrival time of the shock wave at the center of the front surface of the Mo sample, to enable shock velocity determination.

As shown in Table II, a total of 17 experiments were conducted in this work. Projectile velocities were systematically varied to achieve approximately 23, 67, 90, and 110 GPa impact stresses for each orientation. Experiments along the $[100]$ orientation are denoted as A1–A6; experiments along the $[111]$ orientation are

FIG. 1. Schematic of the plate impact experimental configuration.

TABLE II. Experimental parameters for the plate impact experiments.

Expt. number	Loading direction	Sample thickness (mm)	Impactor/buffer material	Impactor thickness (mm)	Buffer thickness (mm)	Window thickness (mm)	Impact velocity (km/s)	Elastic impact stress (GPa)	Impact tilt (mrad)
A1	[100]	2.019	1050Al	1.831	0.956	6.366	1.549	23.2	0.392
A2		2.010	C101Cu	1.717	0.924	6.363	2.099	65.7	2.61
A3		2.011	C101Cu	1.686	0.921	6.363	2.113	66.2	1.27
A4		2.030	C101Cu	3.058	0.921	6.362	2.680	89.1	3.05
A5		2.027	C101Cu	1.094	0.926	6.346	3.126	108.6	2.32
A6		2.030	C101Cu	1.109	0.923	6.397	3.291	116.1	4.80
B1	[111]	2.027	1050Al	1.842	0.915	6.366	1.595	23.9	0.55
B2		2.029	1050Al	1.803	0.916	6.342	1.599	24.0	0.30
B3		2.009	C101Cu	1.704	0.928	6.364	2.106	67.4	0.97
B4		2.043	C101Cu	3.052	0.925	6.055	2.710	93.7	4.99
B5		2.027	C101Cu	1.101	0.927	6.344	3.149	114.6	3.18
B7		3.499	C101Cu	1.102	0.921	6.362	2.806	98.1	8.76
B8		3.497	C101Cu	1.111	0.922	6.399	3.122	113.3	1.89
C1	[110]	2.021	1050Al	1.778	0.909	6.365	1.571	23.5	0.61
C2		2.018	C101Cu	1.708	0.934	6.360	2.110	67.0	1.28
C3		2.032	C101Cu	3.047	0.944	6.053	2.676	90.9	3.91
C4 ^a		2.029	C101Cu	1.097	0.920	6.054	3.151	112.9	4.33

^aThis experiment is excluded from the further discussion since the shock wave was overdriven, and the elastic limit was not observed.

denoted as B1–B5 and B7–B8; and experiments along the [110] orientation are denoted as C1–C4. Experiments (A2,A3), (A5,A6), and (B1,B2) represent pairs of experiments to check reproducibility. The sample thickness was kept constant at nominally 2 mm, except for experiments B7 and B8, which used 3.5 mm thick samples. These two experiments were conducted to examine elastic wave amplitude decay with propagation distance. The projectiles were launched using a powder gun in experiments A1–A3, B1–B3, and C1–C2. A two-stage light gas gun was used in the remainder of the experiments.

Along the [110] orientation, when the impact stress was above 90 GPa, shocks in the Mo single crystals were overdriven and the single wave was observed (Experiment C4). Since the primary focus in this work was on the behavior at the elastic limit, the results for the experiment were excluded from the further discussion.

III. EXPERIMENTAL RESULTS

In this section, the measured velocity profiles at different impact stresses are compared, and the findings for each orientation are summarized. The measured velocity profiles for 2 mm thick samples along [100], [111], and [110] orientations are shown in Figs. 2, 3, and 4, respectively. In each plot, the time is divided by the sample thickness to compensate for slight differences in sample thicknesses, to enable elastic shock velocity comparisons between experiments. As noted previously, results from experiments with overdriven, single waves are not shown in the figures. Results from the 3.5 mm thick samples (B7 and B8) are shown in Sec. III D.

The elastic shock velocity and the measured particle velocity at the elastic limit are reported in Table III along with calculated in-material quantities in Sec. IV.

A. [100] orientation

Figure 2 shows that in experiments A1–A6, the two wave structure—an elastic wave trailed by a plastic wave—was observed. In all of the velocity profiles shown in Fig. 2, the relaxation behind the elastic wave was observed. This is a consequence of the large plastic strain rate due to a rapid and significant increase in

FIG. 2. Measured particle velocity for the [100] orientation.

FIG. 3. Measured particle velocity for the [111] orientation.

dislocation density, similar to that discussed in earlier studies.^{5,6,11} Except for A2, the elastic shock velocity increased with increasing impact stress. Also, the measured particle velocity at the elastic limit followed the same trend.

In experiment A5, during the unloading behind the elastic wave, an abrupt drop in the particle velocity was observed. This abrupt drop was not observed in the repeat experiment A6 nor in other experiments. Therefore, this anomalous experiment is not included in the detailed discussion.

FIG. 4. Measured particle velocity for the [110] orientation.

B. [111] orientation

Figure 3 shows that in experiments B1–B5, a two wave structure was observed. Similar to the [100] orientation, the particle velocity at the elastic limit increased as the elastic impact stress increased. Also, the relaxation behind the elastic wave was observed, which was an indication of the time dependence. Regarding experiment B1 and the corresponding repeat experiment B2, the results were well-reproduced. In these two experiments at 23 GPa impact stress, considerable kinks were observed between the elastic and plastic shock waves around time/thickness = 0.18, apart from the relaxation. There were some differences observed in the features between the elastic and the plastic shock wave, but the elastic shock velocities and the particle velocity at the elastic limit were within the experimental uncertainties.

C. [110] orientation

Figure 4 shows that in experiments C1–C3, a two wave structure was again observed. As mentioned earlier, along the [110] orientation, two wave structure was only observed up to 90 GPa impact stress. This observation is different from the other orientations. In all of the velocity profiles shown in Fig. 4, the relaxation behind the elastic limit was observed, but in experiment C3, there was only a slight relaxation due to the small time separation between the elastic and the plastic shock wave. In experiment C1, considerable kink was observed during the rise of the plastic shock wave, around time/thickness = 0.175. The measured particle velocity at the elastic limit slightly increased with increasing impact stress. The dependence on the impact stress was smaller along the [110] orientation.

D. 3.5 mm thick sample experiments along the [111] orientation

The measured wave profiles from experiments B7 and B8, for 3.5 mm thick sample experiments along the [111] orientation, are shown in Fig. 5. For comparison, the measured velocity profiles for the 2 mm thick sample experiments (B4 and B5) with nominally the same impact stress are shown in Fig. 6. We note that time units are in μs .

By comparing Figs. 5 and 6, one can observe the difference in the profiles during the release behind the elastic wave, that is, an effect of the time separation between the two waves (elastic and plastic shock) due to the difference in the sample thickness. The measured particle velocity at the elastic limit was comparable in 90 GPa impact stress experiments (B4 and B7). However, for 110 GPa impact stress experiments (B5 and B8), the measured particle velocity at the elastic limit was lower in the 3.5 mm thick sample experiment B8.

IV. ANALYSIS AND DISCUSSION

Similar to impedance matching procedures and the Rankine–Hugoniot jump conditions used previously,^{1,2} in-material particle velocity, longitudinal stress, and density were calculated at the elastic limit for each experiment. They are referred to as the in-material quantities. Known Hugoniot relation for the LiF window³¹ was used in the calculation. Table III summarizes the

TABLE III. Calculated in-material quantities at the elastic limit.

Expt. number	Loading direction	Sample thickness (mm)	Elastic impact stress (GPa)	Elastic shock velocity (km/s)	Measured particle velocity (km/s)	In-material quantities		
						Particle velocity (km/s)	Longitudinal stress (GPa)	Density (g/cm ³)
A1	[100]	2.019	23.2	6.79 ± 0.17	0.0954 ± 0.001	0.057 ± 0.001	3.98 ± 0.11	10.307 ± 0.003
A2 ^a		2.010	65.7	6.76 ± 0.14 ^b	0.0877 ± 0.001	0.053 ± 0.001	3.64 ± 0.09	10.300 ± 0.002
A3		2.011	66.2	6.82 ± 0.14 ^b	0.0975 ± 0.001	0.059 ± 0.001	4.08 ± 0.10	10.308 ± 0.003
A4		2.030	89.1	6.87 ± 0.07	0.103 ± 0.002	0.061 ± 0.001	4.31 ± 0.07	10.312 ± 0.002
A5 ^a		2.027	108.6	6.99 ± 0.13 ^c	0.119 ± 0.002	0.071 ± 0.001	5.08 ± 0.11	10.325 ± 0.003
A6		2.030	116.1	7.01 ± 0.13 ^c	0.0963 ± 0.001	0.058 ± 0.001	4.12 ± 0.09	10.305 ± 0.002
B1	[111]	2.027	23.9	6.52 ± 0.15	0.172 ± 0.002	0.105 ± 0.002	6.96 ± 0.19	10.387 ± 0.005
B2		2.029	24.0	6.58 ± 0.15	0.167 ± 0.002	0.101 ± 0.002	6.78 ± 0.19	10.379 ± 0.005
B3		2.009	67.4	6.59 ± 0.13 ^b	0.187 ± 0.002	0.113 ± 0.002	7.60 ± 0.19	10.398 ± 0.005
B4		2.043	93.7	6.73 ± 0.07	0.198 ± 0.002	0.120 ± 0.002	8.23 ± 0.13	10.405 ± 0.003
B5		2.027	114.6	6.96 ± 0.12 ^c	0.214 ± 0.003	0.128 ± 0.002	9.13 ± 0.20	10.412 ± 0.005
B7	[110]	3.499	98.1	6.79 ± 0.04	0.199 ± 0.002	0.120 ± 0.002	8.31 ± 0.11	10.404 ± 0.003
B8		3.497	113.3	6.98 ± 0.07 ^c	0.200 ± 0.002	0.120 ± 0.002	8.54 ± 0.14	10.399 ± 0.003
C1	[110]	2.021	23.5	6.48 ± 0.15	0.0999 ± 0.001	0.060 ± 0.001	4.00 ± 0.11	10.316 ± 0.003
C2		2.018	67.0	6.42 ± 0.13 ^b	0.104 ± 0.002	0.063 ± 0.001	4.15 ± 0.10	10.322 ± 0.003
C3		2.032	90.9	6.63 ± 0.07	0.106 ± 0.002	0.064 ± 0.001	4.32 ± 0.07	10.319 ± 0.002

^aThese experiments are excluded from further discussions due to the inconsistencies mentioned above.

^bImpactor bowing correction of 4.1 ± 2 ns is applied.

^cImpactor bowing correction of 2.0 ± 2 ns is applied.

elastic shock velocity, the measured particle velocity (Mo–LiF interface) at the elastic limit, and the in-material quantities.

Results from 2 mm thick sample experiments are discussed in Secs. IV A and IV B, and results from 3.5 mm thick sample experiments are compared with corresponding 2 mm thick sample experiments in Sec. IV C.

FIG. 5. Measured particle velocity in 3.5 mm thick sample experiments along the [111] orientation.

A. Elastic wave amplitude anisotropy

By comparing the results from 2 mm thick sample experiments in Table III, a positive correlation between the elastic wave amplitude and the impact stress is observed, except for experiment A2. In experiment A2, the in-material quantities and the measured

FIG. 6. Comparison of 3.5 mm thick sample experiments with corresponding 2 mm thick sample experiments.

particle velocity were not consistent with the other [100] experiments and the difference between the repeat experiment A3 was beyond the experimental uncertainties. Experiment A2 is, therefore, not included in further discussions. This inconsistency might be attributed to the scatter between samples, but we cannot conclusively determine the cause. We note that larger scatter between [100] oriented samples was also reported in Ref. 1.

Figure 7 shows the plot of the elastic wave amplitude against the impact stress along each orientation for 2 mm thick sample experiments. The data from lower stress impact experiments with comparable thickness (2.3 mm) samples^{1,2} are also shown for comparison. A linear fit—only for the present work—is superposed onto the results along each orientation.

Figure 7 shows that the elastic wave amplitude increases linearly with the elastic impact stress. The elastic wave amplitude is significantly larger along the [111] orientation compared with other orientations, and the dependence on the elastic impact stress is also larger along the [111] orientation. Along [100] and [110] orientations, the elastic wave amplitude shows a slight increase, but the dependence on the elastic impact stress is minimal. The equation for the linear fit along the [111] orientation is provided below,

$$\text{Above 23 GPa: } \sigma_x^{el} = 0.023\sigma^{imp} + 6.25 \text{ (GPa)}. \quad (1)$$

The elastic wave amplitudes at the lowest impact stress^{1,2} do not match well with the extrapolations from the present results. This difference is most pronounced for the [111] orientation and is well beyond the combined experimental scatter from the previous work and the present work. At present, we are unable to explain the rapid increase in the elastic wave amplitude—between the two lowest impact stresses—in Fig. 7.

FIG. 7. Elastic wave amplitude vs impact stress for the three different orientations. The data from lower stress impact experiments^{1,2} at a comparable sample thickness of 2.3 mm are shown with markers "x."

Since all of the experiments in the present work were conducted with a constant sample thickness, the differences in the elastic wave amplitudes imply that the change of the elastic wave amplitude with the propagation distance depends on the crystal orientation. Also, the larger elastic wave amplitude along the [111] orientation means that the decrease from the impact stress imparted to the Mo sample is smaller along the [111] orientation. These observations are consistent with the observation at the lower impact stress.^{1,2}

The anisotropic response is manifested in terms of the elastic shock velocity as well. In Table III, for 23, 66, and 90 GPa impact experiments, one can observe that the elastic shock velocity was higher along the [100] orientation compared to [111] and [110] orientations, which were comparable.

B. Resolved shear stress at the elastic limit

To better understand the anisotropy effects seen in Fig. 7 and to gain insight into the slip systems governing elastic-plastic deformation in Mo single crystals, the maximum resolved shear stresses (RSS) on {110}<111> and {112}<111> slip systems—at the elastic limit—were calculated following the approach in Ref. 32. The results are shown in Figs. 8 and 9. As in Fig. 7, the data from the lower impact stress experiments^{1,2} (for comparable thickness samples) are shown for comparison. A linear fit to the present data is shown for each orientation. The black horizontal line in both figures represents the corresponding Peierls stress of screw dislocations on each family of planes.²¹ The Peierls stress is the resolved shear stress required for dislocations to overcome the energy barrier without thermal effects under the ambient pressure.

In Figs. 8 and 9, one can observe the same trend as in Fig. 7. RSS at the elastic limit increases linearly with increasing elastic

FIG. 8. Resolved shear stress at elastic limit on {110}<111> slip system (data from 2 mm thick sample experiments). The data from lower stress impact experiments^{1,2} at a comparable sample thickness of 2.3 mm are shown with markers "x."

FIG. 9. Resolved shear stress at elastic limit on {112}⟨111⟩ slip system (data from 2 mm thick sample experiments). The data from lower stress impact experiments^{1,2} at a comparable sample thickness of 2.3 mm are shown with markers “x.”

impact stress. Along the [111] orientation, RSS showed a strong increase, while only a slight increase was observed along [100] and [110] orientations. This is expected because the RSS is proportional to the longitudinal stress. However, the differences in the RSS at the elastic limit among different orientations are smaller compared to the differences in the corresponding longitudinal stress (elastic wave amplitude) in Fig. 7. The difference between the RSS and the corresponding Peierls stress reported in earlier work²¹ is smaller for the {110}⟨111⟩ slip system than for the {112}⟨111⟩ slip system.

As mentioned in Sec. I, when the RSS is greater than the Peierls stress, phonon-drag controls the plastic deformation.²⁵ In our case, Figs. 8 and 9 show that the RSS was larger than the Peierls stress. Thus, we will not consider the temperature dependence that arises in the thermally activated kink-pair formation. Reference 25 also reports on the pressure dependence of the Peierls stress. In our case, the pressure (or mean stress) at the elastic limit can be calculated from the elastic constants³³ and the elastic wave amplitude by considering the uniaxial strain loading condition. The pressure is given by

$$P = \frac{1}{3}(\tilde{C}_{1111}\epsilon_{11} + \tilde{C}_{2211}\epsilon_{11} + \tilde{C}_{3311}\epsilon_{11}) = \frac{\tilde{C}_{1111} + \tilde{C}_{2211} + \tilde{C}_{3311}}{3\tilde{C}_{1111}}\sigma^{el}, \quad (2)$$

where

$$\tilde{C}_{ijkl} = R_{im}R_{jn}R_{ko}R_{lp}C_{mnop}. \quad (3)$$

In Eq. (3), R_{ij} is a rotation tensor corresponding to each loading orientation.

Among our experiments, the maximum pressure at the elastic limit, achieved in experiment B5, was 5.9 GPa. Based on the second order polynomial fit to the pressure dependence reported in Ref. 25, the Peierls stress at a pressure of 5.9 GPa is only 5% larger than that at ambient pressure. Thus, for our discussion regarding the elastic limit, the pressure dependence of the Peierls stress is not a significant factor.

The RSS plots in Figs. 8 and 9 suggest the activation of the {110}⟨111⟩ slip system at the elastic limit. This inference assumes that the RSS value falls in the vicinity of the threshold for activating deformation mechanism. In the lower stress study,^{1,2} it was not possible to distinguish between the two possible slip systems. However, in this work, the considerable difference between the RSS and the Peierls stress on the {112}⟨111⟩ slip system points to the activation of the {110}⟨111⟩ slip system.

We also note that the Peierls stress for edge dislocations in Mo obtained using Finnis–Sinclair potential is 25 MPa³⁴ and is significantly smaller than the RSS shown in Figs. 8 and 9. This supports the view that the plasticity in BCC crystals at high impact stresses are governed by the motion of screw dislocations. This inference is consistent with the past studies under quasistatic loading.^{19–25}

C. Comparison with 3.5 mm thick samples

As discussed in Secs. IV A and IV B, the elastic wave amplitude along the [111] orientation showed significant dependence on the impact stress. Since time-dependent behavior was observed in the velocity profiles (Figs. 2–6), this dependence cannot be attributed entirely to the impact stress; the effect of propagation distance on the elastic wave amplitude needs to be considered. Toward this end, the results for 3.5 mm thick samples (experiments B7 and B8) are compared with corresponding 2 mm thick samples (experiments B4 and B5).

As shown in Table III, for ~95 GPa impact stress experiments (B4 and B7), measurable decay was not observed in the elastic wave amplitude with propagation distance. For ~110 GPa impact stress experiments (B5 and B8), the elastic wave amplitude at a propagation distance of 3.5 mm was 7% lower than at 2 mm. This difference indicated that the elastic wave amplitude—at the highest stress—had not fully decayed at a propagation distance of 2 mm.

V. SUMMARY

To investigate the elastic–plastic deformation of BCC single crystals under shock compression to high stresses, Mo single crystals were subjected to shock loading along [100], [111], and [110] orientations to impact stresses ranging between 20 and 110 GPa. The present work focused on the response near the elastic limit. The significant findings are summarized below.

- Along [100] and [111] orientations, a two wave structure was observed up to 110 GPa impact stress. Along the [110] orientation, a two wave structure was observed only up to 90 GPa impact stress.
- The elastic wave amplitude increases with the elastic impact stress. The elastic wave amplitude is significantly larger along the [111] orientation compared with other orientations, and the

dependence on the impact stress is most pronounced along the [111] orientation.

- In the high stress range examined in the present work, the decay rate of the elastic wave amplitude depends on the crystal orientation and is smaller along the [111] orientation. This is consistent with the observations at lower stress.^{1,2}
- Compared with the lower stress data,^{1,2} the elastic wave amplitudes in the present work are higher. The increase from the lower stress data is maximum for the [111] orientation. However, we are unable to explain the cause of this large increase.
- At the elastic limit, the difference between RSS and the corresponding Peierls stress is smaller on the {110}<111> slip system than on the {112}<111> slip system. This suggests the activation of the {110}<111> slip system at the elastic limit.

ACKNOWLEDGMENTS

We would like to thank Nate Arganbright, Kurt Zimmerman, and Yoshi Toyoda for their help in designing and conducting experiments. We would also like to thank Dr. Michael Winey for his help in obtaining known Hugoniot relations and for useful discussions. This work was supported by the DOE/NNSA (Award No. DE-NA0002007).

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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