

Crystal structure and temperature of tantalum dynamically compressed to hundreds of gigapascals

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(Received 22 August 2025; revised 11 September 2026; accepted 16 September 2026; published 19 October 2026)

We determine the crystal structure and temperature of tantalum ramp and shock ramp compressed to hundreds of gigapascals at the National Ignition Facility. With x-ray diffraction, we find that tantalum remains in the body-centered-cubic structure with no evidence for the proposed *Pnma* phase up to ramp-compression stresses of $531.7^{+21.3}_{-18.7}$ GPa. In separate experiments measuring single-shot extended x-ray absorption fine structure (EXAFS) at the L_3 edge, we find that tantalum's temperature agrees well with radiation-hydrodynamics calculations incorporating strength models for ramp and shock-ramp compression to ~ 200 GPa, but not ~ 400 GPa. The discrepancy at ~ 400 GPa can plausibly be explained by underestimated ablation-plasma x-ray heating, with the magnitude of this heating increasing with laser irradiance. These results constitute the highest-stress structural determination for Ta, the first *L*-edge EXAFS thermometry in ramp and shock-ramp experiments, and a stringent benchmark of hydrodynamic models. They validate *L*-edge EXAFS as a robust platform for thermometry in dynamic compression and underscore the need for careful ablator design in future high-pressure studies.

DOI: [10.1103/klbh-bmb1](https://doi.org/10.1103/klbh-bmb1)

I. INTRODUCTION

Laser-driven compression with precise laser pulse shaping has transformed high-pressure condensed matter research by enabling quasi-isentropic compression of solids up to hundreds or thousands of gigapascals, avoiding the significant entropy generated in shock compression. This advance has enabled numerous key insights including mapping iron's melting curve to 1000 GPa [1] and observing diamond-phase carbon's metastability to 2000 GPa [2]. It has also revealed other properties like measuring compressibility beyond 2000 GPa [3,4], dramatic lead strengthening near 400 GPa [5], and observation that thermal conduction can significantly alter the sample state [6]. Despite these remarkable advances, one of the grand challenges in this field remains accurately determining temperature, a key state variable governing compressibility, phase stability, transformation kinetics, strength, and transport properties.

Several methods exist for thermometry of dynamically compressed solids. Each offers advantages, but all have tradeoffs in sensitivity, model assumptions, or experimental difficulty. Optical pyrometry measures thermal emission from the skin depth of the surface (in opaque samples like

metals), relies on often unknown emissivity, can be compromised by thermal transport into surrounding layers, is insensitive to the bulk where gradients may occur, and has a floor around 3000 K for the nanosecond timescale of laser-driven experiments. Neutron-resonance spectroscopy is a potentially powerful technique that requires few assumptions but is largely not used due to a lack of viable neutron sources [7,8] and the few available, appropriate isotopes [9]. Forward-scattering (collective scattering regime) inelastic x-ray scattering is another promising approach with low model dependence, but generating sufficient signal requires hundreds to thousands of measurements for a single state [10,11], which has so far not been reported in a dynamic compression setting. X-ray diffraction (XRD) Debye-Waller analysis infers temperature from Bragg-peak intensities but requires detailed analysis and is often complicated by sample texture [12] and grain size (for both small and large grains). X-ray thermal diffuse scattering is a promising new technique for dynamic compression [13] but requires the very high signal-to-noise currently only available at x-ray free-electron laser (XFEL) sources. There are currently no XFEL facilities with a sufficiently powerful laser to ramp compress a sample to 100 GPa or higher. In contrast, temperature can be determined from extended x-ray absorption fine structure (EXAFS) by measuring the damping of EXAFS oscillations. EXAFS yields temperature in a single shot, is applicable to many elements, and is mostly insensitive to texture or grain size, especially for unpolarized x-rays and rolled foil samples. However, temperature extraction requires either assuming a model form [14–16] or performing large-scale calculations [6] that account for important effects and properties like anharmonicity and the

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phonon density of states. One of the requirements for the approach using large-scale simulations is knowledge of the crystal structure.

Tantalum is an ideal material for this study because of its remarkable stability in the body-centered-cubic (bcc) phase over a broad pressure (P) and temperature (T) range. Room-temperature diamond-anvil-cell (DAC) experiments find tantalum stays in the bcc phase when compressed up to 310 GPa [17,18]. Laser-driven ramp compression measurements also report tantalum remains in the bcc structure up to 260 GPa [19]. Shock-Hugoniot XRD measurements likewise report observing bcc up to and along the melt curve from incipient melt at 254(15) GPa through completion at 317(10) GPa [20]. *Ab initio* electronic structure calculations predict tantalum remains stable in the bcc phase up to 1000 GPa [21–24], yet there are no published measurements above 317 GPa. However, density-functional metadynamics calculations by Yao *et al.* [25] suggest a $Pnma$ phase may become thermodynamically preferred at multi-100 GPa pressures and elevated temperature.

The EXAFS oscillations we aim to measure arise from self-interference of photoelectrons emitted by x-ray absorption just above an absorption edge: the oscillation wavelength encodes interatomic distances, while the amplitude is damped by thermal vibrations and structural disorder. Determining the temperature with Debye or Einstein models can be effective [14], but this additionally requires knowledge of other properties like the Debye temperature, which is often not known at high pressure. We therefore choose to use first-principles molecular dynamics (FPMD) calculations. While FPMD naturally accounts for anharmonicity and the full phonon spectrum with no need for the Debye temperature, it still requires knowledge of the sample's crystal structure, which can be independently measured with x-ray diffraction (XRD).

Despite the structural simplicity, there are significant challenges associated with measuring tantalum EXAFS. While K -edge EXAFS generally produces large amplitude features, K -edge measurements become increasingly impractical for period 5 and heavier elements due to their high absorption edge energies. For tantalum (period 6), the K edge is at 67.4 keV, where it is hard to design a spectrometer with sufficient resolution and there are a lack of suitable x-ray sources. So, while the EXAFS amplitude is lower, we choose to probe the L_3 edge (9.881 keV, and the largest edge jump of the L series) where there are suitable spectrometers [26] and x-ray sources [27]. Tantalum's relatively low heat capacity and short x-ray attenuation length tighten the balance between generating sufficient signal and limiting concurrent heating by the probe [28] and ablation-plasma-generated x-rays. Plastic work heating can be another significant heat source, where for strong materials like tantalum [29] it is expected to contribute up to many hundreds K at these pressures. Absorption of x-rays emitted both from the ablation plasma and the probe x-rays is yet another thermal source, which will induce an asymmetric heating in the sample biased towards the laser drive side. Heating of this sort can be mitigated with the use of heat shield layers, which is common for experiments in the hundreds of gigapascal pressure regime but typically reduces signal levels. A final effect is the role of conduction, which

could increase or decrease the sample temperature depending on the state and properties of adjacent layers. Recent work by our team has found that conduction can play a large role [6], but the impact of conduction in dynamic compression is an active area of research and must be considered on a case-by-case basis.

Here we present results of XRD and EXAFS measurements taken at Lawrence Livermore National Laboratory's National Ignition Facility (NIF) from ramp and shock-ramp compressed tantalum. Our XRD measurements show that tantalum remains in the bcc structure up to $531.7^{+21.3}_{-18.7}$ GPa under ramp-compression conditions. Our EXAFS measurements show that the temperature agrees well with predictions from hydrodynamics and radiation-hydrodynamics calculations with strength models near 200 GPa, but reveal a significant discrepancy at ~ 400 GPa. The temperature on the pure ramp compression experiment to $170.2^{+5.8}_{-5.9}$ GPa is significantly hotter than the expected temperature on the principal isentrope, which can be explained by including the effects of plastic work heating predicted by strength models designed to characterize tantalum's strength under similar conditions [29–31] and x-ray absorption heating. At ~ 400 GPa, our measurements indicate higher temperatures than radiation-hydrodynamics predictions, potentially due to greater-than-expected heating from absorption of ablation-plasma x-rays. Our measurements provide both the highest-pressure structure determination for tantalum and the first temperature determination in ramp and shock-ramp compression using L -edge EXAFS. These results bolster recent tantalum strength results [29] while highlighting the critical importance of sample design when using high-power lasers to compress to hundreds of gigapascals or higher.

II. SETUP AND METHODS

We performed both XRD and EXAFS measurements of ramp and shock-ramp compressed tantalum using the NIF's high-power lasers. The XRD measurements were made using the TARget Diffraction *In Situ* (TARDIS) platform [28,32], and the EXAFS measurements used the setup shown in Fig. 1, similar to Sio *et al.* [6,33], but with a spectrometer optimized for tantalum's L_3 edge (9.881 keV) [26]. In both experiment types, tailored laser pulses ramp or shock-ramp compress a (3.0–5.2)- μm -thick tantalum sample to hundreds of GPa peak stress. The samples are ramp compressed over ~ 10 –20 ns to the peak stress, which is maintained for several nanoseconds and the sample is probed by x-rays emitted from a laser-heated foil. For XRD measurements, elastically scattered, narrow-band He_α line emissions from a Zn or Zr foil are recorded on MS-type Fujifilm image plates. The drive lasers that generate the high stress are focused on the sample using the standard 1-mm continuous phase plates (CPPs) available at NIF, arranged in a 2×2 tile pattern designed for TARDIS experiments [19]. For EXAFS measurements, continuum x-rays emitted from the Ti foil [27] are transmitted through the sample, spectrally resolved by the high-resolution absorption x-ray spectrometer (HiRAXS) [26,34], and recorded on SR-type Fujifilm image plates. The drive lasers are focused on the sample using continuous phase plates with all 16 lasers overlapped in a single 3.2-mm diameter spot.

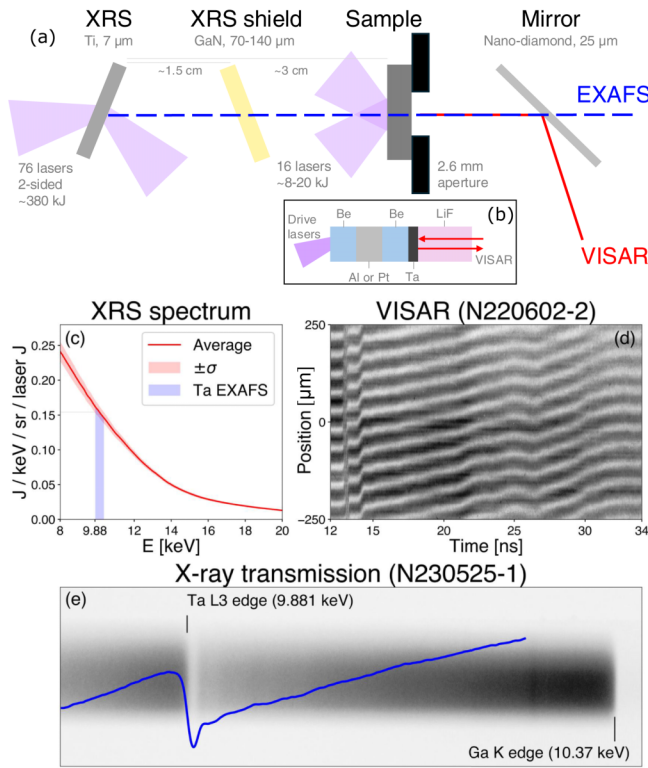


FIG. 1. Tantalum EXAFS experimental setup at the National Ignition Facility. The full target includes the x-ray source (XRS), the XRS shield, the sample sandwich, and significant shielding (not shown). (b) Shows the detailed sample stack. It is driven by 16 beams (2 shown in purple). Up to 76 beams are incident on both sides of the Ti XRS [2 shown in purple in (a)] whose spectrum, measured by the NIF Survey Spectrometer [37], is shown in (c). A mirror behind the physics package enables simultaneous velocity measurements of the Ta-LiF interface using VISAR (red line) with example data shown in (d). X-ray transmission through the physics package (dashed blue line) is measured by the HiRAXS x-ray spectrometer, with example data shown in (e). The grayscale image shows the raw data and the blue curve is the sum across the signal region.

We use a multilayer “sandwich” target consisting of an ablator, a heat shield, a pusher, the sample layer, and a dual-purpose tamper or window layer [see Figs. 1(b) and 2(b)]. The ablator absorbs the laser, converting the pulse shape into a shaped stress wave. The heat shield filters out x-rays that do not contribute signal while transmitting probe x-rays. The pusher layer separates the sample from the heat shield (that could be hot from x-ray absorption); it has reasonably similar impedance to the window or tamper (to reduce reverberations needed to efficiently equilibrate the pressure), high x-ray transmission, and sufficient stiffness to support ramp compression. The tamper or window maintains pressure in the sample. In both sample design drawings [Figs. 1(b) and 2(b)], the layers are not to scale and the aspect ratio is exaggerated to show the thin sample layers; layer thicknesses are listed in the Supplemental Material [35]. For XRD measurements, the ablator, pusher, and tamper are diamond (which becomes opaque, but reflects from the rear surface), with a gold heat shield deposited on the ablator’s pusher side.

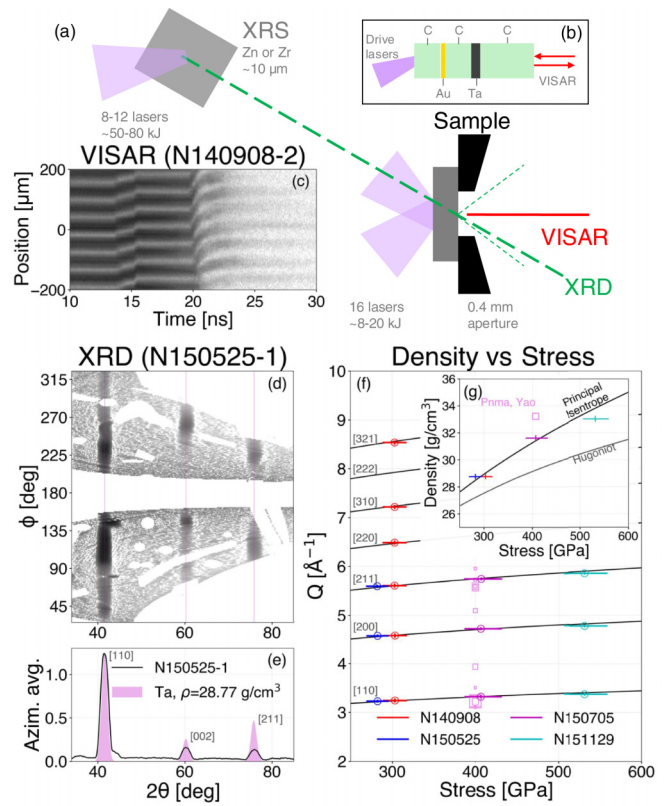


FIG. 2. XRD configuration and sample data. (a) Shows a sketch of the setup. (b) Shows the sample design. (c) Shows example VISAR data from shot N140908-2. (d) Shows the background subtracted XRD data from shot N150525-1 projected into polar coordinates and (e) shows the azimuthally averaged lineout. The first three bcc reflections are clearly seen as is a narrow spot from the diamond carbon layers at slightly higher 2θ than the [110] bcc tantalum reflection at $\sim 41^\circ$. (f) Shows a comparison of experimentally measured reflections and the expected positions of the bcc reflections calculated from the principal isentrope [4]. The circle markers show the position of the reflections and the crosses indicate the error bars. The predicted diffraction reflection positions from the proposed $Pnma$ structure are shown as pink squares at 400 GPa sized proportionally to the relative expected powder diffraction signal. (g) Shows density vs stress for each XRD shot and the density value for $Pnma$ when the lattice parameters are adjusted to match the two strongest $Pnma$ features to the XRD data.

For EXAFS measurements, the ablator and pusher are beryllium, the tamper or window is lithium fluoride (LiF, which remains transparent in our experiments), and the heat shield is either aluminum or platinum foil. The XRD experiments were performed before we knew about the potential for heating effects in thin samples from conduction from diamond components revealed by Sio *et al.* [6]. The EXAFS targets also avoided diamond because their shock-ramp loading paths are difficult to realize through diamond’s large and complex elastic response [36], whereas the earlier XRD targets were designed for nominally pure ramp loading.

In both EXAFS and XRD experiments, we determine the ramp stress by applying the method of characteristics [38,39] to the velocities measured by NIF’s velocity interferometer for any reflector (VISAR) [40] system. In EXAFS experiments,

this velocity is recorded at the Ta-LiF interface [see Figs. 1(a), 1(b), and 1(d)] and in XRD experiments it is recorded at the diamond tamper's free surface [see Figs. 2(a)–2(c)] [41]. We use the known $P - \rho$ equations of state for diamond [42] and tantalum [4], where ρ is the density. The shock stress in shock-ramp EXAFS shots is determined via impedance matching with the LiF tamper or window, using known Hugoniot relations [43–45]. In all cases, errors are propagated using the Monte Carlo method.

We determine the temperature in EXAFS experiments by comparing the measured spectra to synthetic spectra generated for bcc tantalum at fixed densities over a range of temperatures. The synthetic spectra are produced using atomic configurations obtained from first-principles molecular dynamics (FPMD) simulations, performed with the Vienna *ab initio* simulation package (VASP) [46] within finite-temperature density functional theory (DFT) [47,48] using the PBEsol generalized gradient approximation (PBEsol-GGA) [49]. Further details on the computational methods and convergence tests, including those related to system size effects and the choice of pseudopotential, are provided in the Supplemental Material [35]. The synthetic EXAFS are calculated using the FEFF code (version 10.0.0) [50] for between 2000–4000 FPMD snapshots to ensure thermal and numerical convergence.

Temperature is extracted by minimizing the sum of squared residuals between the measured and synthetic EXAFS signals over $k = 3.6$ – 3.95 to $9.6 \text{ \AA}^{-1}$. Uncertainty is quantified by separating statistical uncertainty at fixed processing from systematic uncertainty associated with data reduction and instrumental parameters. To propagate these systematic effects, we use Latin hypercube sampling to generate an ensemble of physically plausible analysis configurations using LARCH [51]. Each ensemble member specifies a complete set of analysis parameters, including the normalization windows, background-removal parameters, mask locations, and instrumental broadening. The raw data are then reprocessed for each configuration, producing an independent $\chi(k)$ extraction and temperature estimate. Instrumental broadening is included by convolving the synthetic spectra before comparison with the data. We exclude members with significant low- R or high- R $|\chi(R)|$ content to limit sensitivity to unphysical signal components and poorly constrained high- k structure. Further details of the sampling ranges, ensemble construction, and filtering criteria are provided in the Supplemental Material [35]. While we compare our results to hydrodynamics and radiation-hydrodynamics calculations below, the temperature determinations are not dependent on them in any way.

III. RESULTS

A. XRD

We measured x-ray diffraction from tantalum ramp compressed to between $282.3^{+9.0}_{-9.4}$ and $531.7^{+21.3}_{-18.7}$ GPa across several experiments (Table I). Figure 2(d) shows background-subtracted XRD data projected into polar coordinates where diffraction reflections form lines of constant 2θ (vertical), where θ is the Bragg angle. Here we can see three clear powder diffraction features that correspond to the [110], [200],

TABLE I. Results of XRD experiments.

Shot	Stress (GPa)	Density (g/cm^3)
N140908-2	303.1(+9.9, –10.0)	28.77 (0.16)
N150525-1	282.3(+9.0, –9.4)	28.77 (0.16)
N150705-5	407.0 (+20.7, –15.6)	31.62 (0.17)
N151129-2	531.7 (+21.3, –18.7)	33.04 (0.18)

and [211] planes of the bcc structure. Two narrow diffraction features at $2\theta \simeq 43^\circ$, $\phi \simeq [80^\circ, 140^\circ]$ originate from the diamond pusher or window layers. The azimuthally averaged lineout [Fig. 2(e)] shows reasonable qualitative agreement between the measured relative signal level of each peak given the textured nature of the sample, which is evident in the data in Fig. 2(d), and the potentially elevated temperature.

Figure 2(f) overlays the measured scattering-vector magnitudes Q of the observed features (determined with individual Gaussian fits) from each shot with their expected bcc positions using the known tantalum $P - \rho$ equation of state [4]. The 3–6 visible reflections in each diffraction pattern confirm the bcc structure in all probed conditions. We also plot the expected *Pnma* reflections at 400 GPa [pink squares in Fig. 2(f)], with lattice constants from Yao *et al.* [25]. The *Pnma* structure clearly disagrees with our data. Peak-position uncertainties combine the Gaussian fit error and the $\sim 0.2^\circ$ nominal calibration accuracy of TARDIS [32], which is the dominant factor. These uncertainties are propagated through to produce the reported density uncertainties.

Figure 2(g) plots our measured bcc densities against the corresponding pressures, showing reasonable agreement with the principal isentrope. The 293-K isotherm is visually indistinguishable from the principal isentrope on the scale of the figure [4]. For reference, we also overlay the $P - \rho$ curve for the principal Hugoniot. The *Pnma* structure proposed by Yao *et al.* [25] does not align with any of our peaks; to illustrate this, we manually adjusted the lattice constants so that the two strongest *Pnma* reflections coincide with our data. The resulting density (pink square) lies well above the expected value for those shot conditions and implies a significant lattice distortion compared to the reported structure.

B. EXAFS

We recorded EXAFS from both ramp and shock-ramp compressed tantalum. The ramp shots are designed to have a minimal initial shock and thus follow a low-temperature, quasi-isentropic compression path. Shock-ramp shots introduce a controlled initial shock, raising the entropy and temperature, followed by ramp compressing along an elevated isentrope to roughly the same final density. The goal of the shock-ramp shots is to demonstrate temperature sensitivity at nearly constant density with our challenging approach of measuring L_3 -edge EXAFS.

Figure 3 shows the delivered laser pulse profiles, Ta-LiF measured and simulated interface velocities, and extracted ramp stresses for the EXAFS shots at ~ 200 GPa (the ~ 400 GPa shot is not shown due to VISAR signal loss). The simulated velocities are calculated with radiation-hydrodynamics calculations (see Supplemental Material [35]

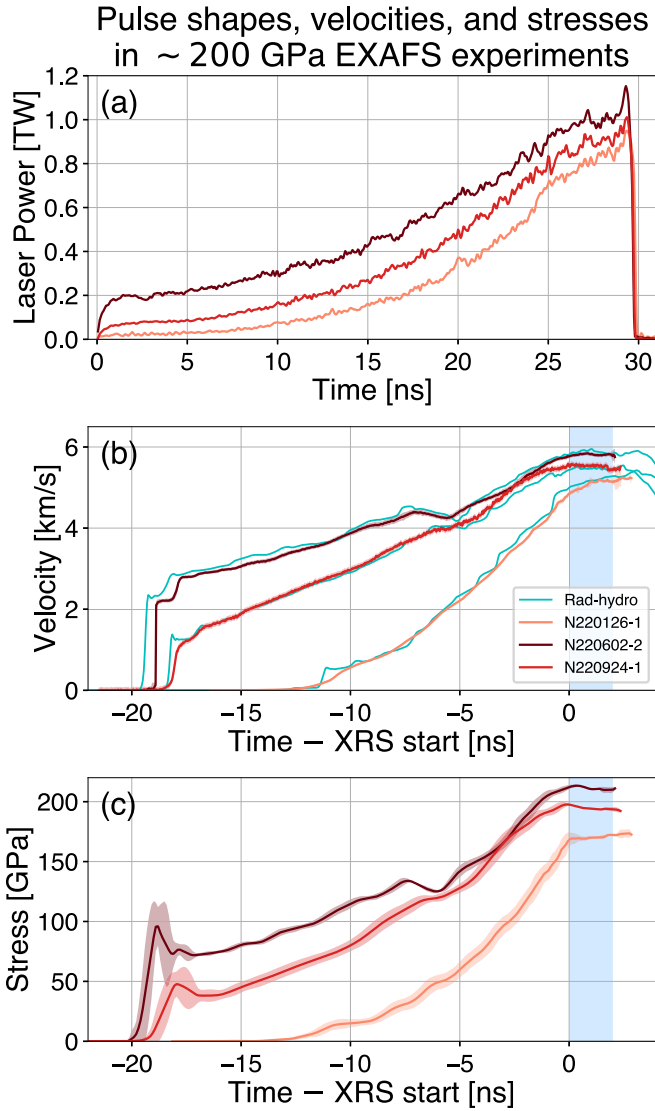


FIG. 3. Laser pulse shapes (a), tantalum and lithium fluoride interface velocity histories (b), and tantalum stress histories (c) in each of the three EXAFS experiments near ~ 200 GPa. The laser pulse shape in (a) is plotted against absolute time, while velocities and stresses are plotted against time relative to the start of XRS emissions on a common axis. The XRS probe time is shown in light blue shading. The cyan curves in (b), labeled “Rad-Hydro,” show the radiation-hydrodynamics calculations that are matched to each experiment. (c) Shows stress histories from the characteristics analysis used to determine the stress at the probe time; the initial shock stress determination is done with impedance matching and not shown here.

for more information) and show reasonable agreement with the corresponding measurements. The velocity and stress histories are shown in Figs. 3(b) and 3(c) on a timescale relative to the probe time, for clarity; the probe time is indicated by the shaded blue regions. The numerical values for shock and ramp stresses are given in Table II.

Figure 4 shows the results of our EXAFS shots and temperature determination. Figure 4(a) shows $\chi(k)$ for each shot, stacked vertically; orange markers show the full data range

TABLE II. Results of EXAFS experiments. Shock pressures correspond to the mean and standard deviation; ramp pressures correspond to the median with uncertainties given by the 16th and 84th percentiles of the sampled distribution, which is asymmetric.

Shot	Shock (GPa)	Ramp (GPa)	Temperature (K)
N220126-1	~ 0	170.2(+5.8, -5.9)	1250–1750
N220602-2	125.1 (3.9)	211.9(+7.2, -7.2)	3000–4000
N220924-1	53.6 (4.2)	196.4(+6.6, -6.6)	2000–3000
N230525-1	~ 0	397 (+15, -13) ^a	4000–5000

^aValues are from radiation-hydrodynamics calculations due to VISAR data loss. See Supplemental Material [35] for more information.

and green markers show the region used in our analysis. The low- k regions ($k < k_{\text{low}}$, with shot-dependent values of k_{low} ranging from 3.60 – $3.95 \text{ \AA}^{-1}$ as listed in the table in the Supplemental Material [35]), are excluded because the EXAFS approximation fails. A few local regions in $k = 5$ – $10 \text{ \AA}^{-1}$ are masked to remove image plate defects. The narrow shaded band around each dataset is the $\pm 1\sigma$ envelope from the preprocessing ensemble. Figure 4(a) also shows synthetic EXAFS calculated from FPMD trajectories at a range of temperatures at the density of each shot, with the center of the best-fit temperature range highlighted in black; temperature steps of ~ 250 K were used for N220126-1 and steps of 500 K for the remaining shots. Figures 4(b)–4(e) show the corresponding normalized profile misfit versus temperature, as described below.

Figure 4(b)–4(e) show the temperature determination results from the EXAFS data. For each shot, we compute the sum of squared residuals, $S(T, \Delta E)$, between the measured $\chi(k)$ and the synthetic spectra. Here $\chi(k)$ is the EXAFS oscillation function, which isolates the fine-structure signal from the absorption edge jump; ΔE is a shift applied to the synthetic spectrum that accounts for uncertainty in the absolute edge energy E_0 in FEFF. The plotted quantity is the profile misfit normalized by its 95% confidence threshold $\Delta S/S_{95}$. At each temperature T , the profile misfit is defined as $\Delta S(T) = S(T) - S_{\text{min}}$, where S_{min} is the minimum misfit at the best-fit temperature. The 95% threshold is defined as $S_{95} = 3.84 \sigma^2$, where $\sigma^2 = S_{\text{min}}/(N_k - 2)$ is the residual variance at the best fit and N_k is the number of k points. For each preprocessing-ensemble member, the range satisfying $\Delta S/S_{95} \leq 1$ defines the 95% statistical confidence interval at fixed processing. Repeating this analysis across the preprocessing ensemble gives a distribution of confidence intervals that also reflects the systematic uncertainty associated with data-reduction choices. The reported temperature range for each shot encompasses these intervals and therefore includes both the statistical uncertainty and the spread across the preprocessing ensemble. The numerical resolution is limited by the temperature spacing of the FPMD simulations. Each panel shows results for both the masked k range (green) and the full k range (orange); their agreement provides a robustness check on the inferred temperature. The resulting temperature ranges are listed in Table II.

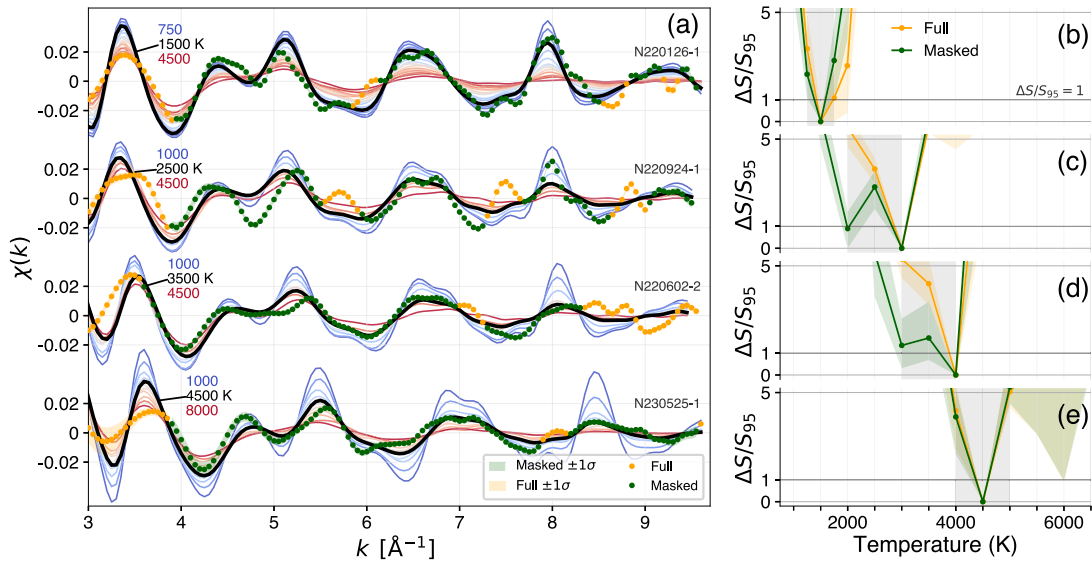


FIG. 4. Measured and synthetic EXAFS for each shot are shown in (a), stacked vertically and labeled by shot ID. The full extracted $\chi(k)$ is plotted in orange, with the subset retained for thermometry after applying that member's exclusion windows overplotted in green; visible orange points are therefore those excluded from the fit. The narrow shaded band around the data is the $\pm 1\sigma$ envelope from the preprocessing ensemble. Thin colored curves are synthetic EXAFS computed from FPMD trajectories at a range of temperatures, colored by temperature (blue $\rightarrow$ red, cool $\rightarrow$ warm). The black curve corresponds to the center of the reported temperature range. (b)–(e) Show the normalized profile misfit $\Delta S/S_{95}$ versus temperature for each shot. For each preprocessing-ensemble member, $\Delta S/S_{95} \leq 1$ defines the 95% statistical confidence interval at fixed processing; the horizontal gray line marks this threshold. Green curves use the masked k range and orange curves use the full k range. Shaded bands show the $\pm 1\sigma$ spread across the preprocessing ensemble. The shaded gray box in each of (b)–(e) marks the reported temperature range, which encompasses the statistical confidence intervals across the preprocessing ensemble.

IV. DISCUSSION

In this discussion, we first consider the structural implications of the XRD and EXAFS measurements, emphasizing the lack of evidence for a *Pnma* phase in compressed tantalum. We then discuss the advantages of EXAFS for probing local structure at higher pressures, where diffraction measurements become increasingly difficult. Finally, we examine the thermal state of the samples by comparing the EXAFS-derived temperatures with radiation-hydrodynamics calculations and estimating the relative roles of plastic work, ablation-plasma x-ray absorption, XRS heating, and conduction.

A. Structure determination

We conclude that tantalum remains bcc under the conditions explored in this work and find no evidence for the proposed *Pnma* structure. Our attempts to fit the reported *Pnma* structure to our observed diffraction data reveal several insurmountable inconsistencies: matching more than one measured diffraction peak simultaneously requires $\sim 10\%$ distortions of the b/a or c/a lattice ratios. In these distorted *Pnma* fits, the resulting density significantly disagrees with the measured $P - \rho$ relationship from Gorman *et al.* [4]; this density difference is equivalent to that expected when compressing from ~ 400 to 500 GPa (see Fig. 2). Even when the *Pnma* lattice is scaled isotropically to force a single peak into alignment, the computed density is still significantly too high. Additionally, we are not able to match the reflection we identify as the [200] bcc line. Finally, our EXAFS measurements at all conditions agree well with the bcc phase and have

significant differences with the reported *Pnma* structure (see Fig. S17 in Supplemental Material [35]).

B. EXAFS signal scaling at high density

While XRD is a powerful probe of long-range crystalline order, its application at laser-driven dynamic compression facilities becomes increasingly challenging as pressure is pushed into the TPa regime [2,52]. Reaching these pressures demands higher drive energy and a stronger x-ray source to probe the compressed state, both of which raise the background. Additionally, the image plate detectors must sit close to the ablation region, where background is inherently high; signal-to-background ratios of 0.1 or lower are common for XRD on TARDIS.

Unlike diffraction implementations, which require detectors to be positioned near the laser-target interaction region and therefore experience substantial background, the NIF EXAFS platform uses a geometry that strongly suppresses background. The x-rays are reflected by the spectrometer crystal before detection, allowing the detector to be positioned more than 1 m from the interaction point. This geometry allows substantial shielding to be placed along the line of sight to the detector, yielding low background levels (~ 0.2 PSL/pixel for our tantalum measurements). Indeed, we observe no significant difference in background between the ~ 200 and ~ 400 GPa EXAFS experiments. A similar insensitivity to driver-generated background was reported for the ~ 400 and ~ 1000 GPa copper EXAFS experiments by Sio *et al.* [6]. EXAFS offers a route that is at once more robust to this background and sensitive to the local atomic environment.

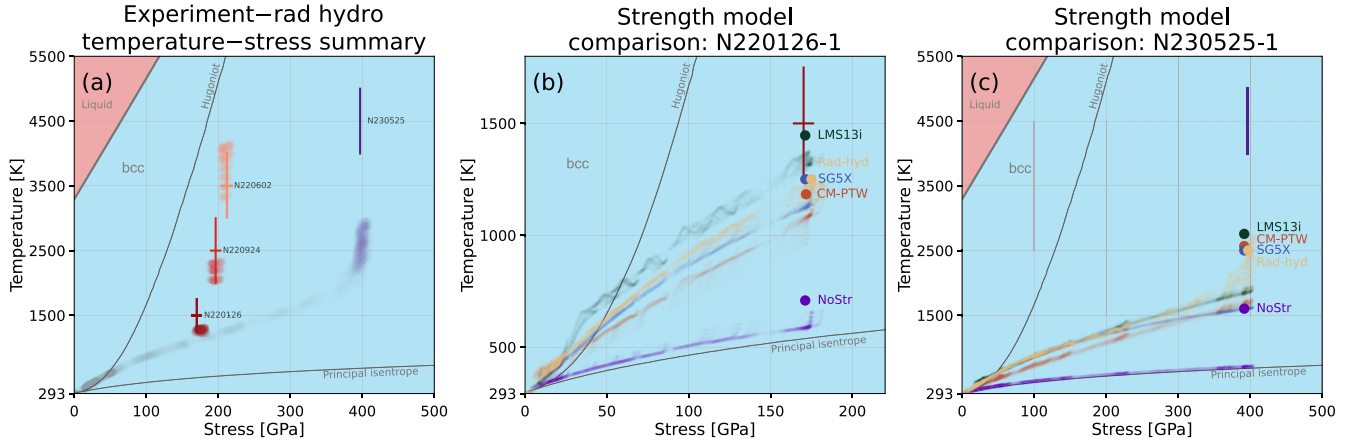


FIG. 5. Ta stress and temperature determined from VISAR/EXAFS measurements compared with predictions from radiation hydrodynamics and hydrodynamics calculations. Crosses in (a) show the experimentally determined conditions for all four EXAFS measurements. Colored markers show the stress and temperature conditions during the x-ray probe predicted by radiation hydrodynamics using the SG5X strength model [53] (see main text). (b), (c) Compare the EXAFS measurements at $170.2^{+5.8}_{-5.9}$ GPa and ~ 400 GPa, respectively, with hydrodynamics predictions obtained using different strength models. Faint colored markers show the calculated stress-temperature trajectories, while the larger solid markers indicate the mean conditions during the probe. The solid markers include shot-dependent temperature corrections for ablation-plasma heating and concurrent x-ray-source heating, which vary with the drive conditions and sample configuration (see main text). The melt curve in (a) and (c), shown by the gray boundary separating the red and blue regions, is from Kraus *et al.* [20] and is plotted assuming that pressure and longitudinal stress are equal.

In this sense EXAFS is not simply a substitute for XRD, but a complementary diagnostic, and one potentially well suited to multi-TPa conditions.

To understand how EXAFS signal amplitude scales with density and pressure, we examine the EXAFS equation:

$$\chi(k) = \sum_j \frac{N_j S_0^2 F_j(k)}{k R_j^2} e^{-2k^2 \sigma_j^2} e^{-2R_j/\lambda(k)} \sin[2kR_j + \delta_j(k)]. \quad (1)$$

Here k is the photoelectron wave number, N_j is the coordination number of the j th shell, S_0^2 is the passive electron reduction factor, $F_j(k)$ and $\delta_j(k)$ are the scattering amplitude and phase shift, respectively, R_j is the half-path length (interatomic distance), σ_j^2 is the mean-square relative displacement, and $\lambda(k)$ is the photoelectron mean-free path.

Under compression, the interatomic distance scales approximately as $R_j \propto \rho^{-1/3}$, so the geometric prefactor $1/R_j^2$ increases as $\rho^{2/3}$, directly enhancing the EXAFS amplitude. The remaining terms depend more weakly on density along an isentrope. The Debye-Waller damping term

$$e^{-2k^2 \sigma_j^2}, \quad \sigma_j^2 \sim \frac{T}{\Theta^2}$$

changes slowly because both the temperature T and the Debye temperature Θ increase with density. Similarly, the mean-free-path damping term

$$e^{-2R_j/\lambda(k)}$$

changes slowly along an isentrope: compression reduces R_j while the accompanying temperature rise shortens λ , so the overall damping varies only weakly with density. As a result, the dominant density dependence arises from the geometric prefactor, leading to an overall increase in EXAFS amplitude with pressure. Although the exact balance is material

dependent, this favorable scaling suggests that EXAFS could remain an effective probe of local atomic structure into the multi-TPa regime.

C. Comparison with hydrodynamics and radiation-hydrodynamics predictions

A key goal of this work is to benchmark the temperature predictions of one-dimensional (1D) radiation-hydrodynamics calculations commonly used for designing and interpreting laser-driven dynamic compression experiments (for example, when constructing phase diagrams). In addition to treating mechanical and thermal transport, these calculations model radiation generation and transport, including the x-rays generated in the ablation plasma and their transport into the sample layers. However, by treating the ablation plasma as an infinite plane, these calculations omit transverse radiation losses. This simplification enhances the modeled x-ray flux into the sample and is therefore generally expected to overestimate those contributions.

Figure 5(a) compares our VISAR/EXAFS-derived temperature-stress points (shaded red and purple crosses) with predictions from one-dimensional radiation-hydrodynamics calculations (shaded red and purple markers). The vertical portion of each cross shows the corresponding temperature uncertainty, and the horizontal portion shows the stress uncertainty. Only the vertical portion is shown for N230525-1 because the stress could not be determined directly from the data, although an estimate is reported in Table II. Translucent black dots show the full predicted compression history of N230525-1 as a guide.

Figures 5(b) and 5(c) compare the EXAFS-derived temperatures with predictions obtained using different strength models. Faint colored markers show the calculated stress-temperature trajectories, while the larger solid markers show

the mean conditions during the x-ray probe. For each experiment, calculations using SG5X provide a common baseline between the radiation-hydrodynamics and hydrodynamics approaches. The difference between their temperatures during the probe defines the ablation-plasma radiation-heating correction, which is applied to the hydrodynamics prediction for each strength model. We also include the shot-dependent heating from the concurrent XRS probe, calculated from the measured XRS emission (Fig. 1) using a calibrated throughput model [28] and the sample absorption. Thus, the solid markers from the hydrodynamics calculations include both the ablation-plasma and XRS heating corrections, whereas the radiation-hydrodynamics predictions, which already include ablation-plasma heating, receive only the XRS correction. The faint trajectories do not include either correction, accounting for their apparent offset from the corresponding solid markers.

The EXAFS-derived temperatures agree well with the radiation-hydrodynamics predictions for the three shots reaching peak stress near 200 GPa. However, a clear disagreement emerges at ~ 400 GPa, where the temperature inferred from EXAFS (4000–5000 K) is substantially higher than predicted by the radiation-hydrodynamics calculations (2200–2700 K). This range corresponds to the median temperatures from the scan of radiation-hydrodynamics calculations used to determine the stress (see Table II and Supplemental Material [35]). Next, we examine the role of different potential heating mechanisms in our experiments.

D. Sources of heating

1. Plastic-work heating contributions

To evaluate the sensitivity of the predicted temperatures to plastic-work heating, we performed hydrodynamics calculations using four different strength treatments: no strength (NoStr); the Steinberg-Guinan model [53] with the yield stress and maximum yield-stress limit multiplied by five (SG5X); the calibrated Preston-Tonks-Wallace model [29] (CM-PTW); and the Livermore multiscale model [31] (LMS13i). These calculations are driven using the ablator-surface pressure history extracted from the corresponding radiation-hydrodynamics simulation. The CM-PTW and LMS13i calculations use the Sesame equation of state for Ta, whereas the remaining calculations use LEOS 735; we expect this difference to have little effect on the predicted temperatures.

At ~ 200 GPa [Fig. 5(b)], the data are consistent with the SG5X and LMS13i predictions, while the CM-PTW calculation lies slightly below the experimental uncertainty range but remains close to the other high-temperature estimates. At ~ 400 GPa [Fig. 5(c)], the different strength models produce a spread of a few hundred kelvin in predicted temperature, but even the highest-temperature prediction remains approximately 2000 K below the center of the EXAFS-derived temperature range.

2. Absorption of ablation-plasma emissions

The radiation-hydrodynamics calculations for N230525-1 predict an approximately 700-K temperature increase near peak stress [Fig. 5(a)] from absorbed ablation-plasma x-rays.

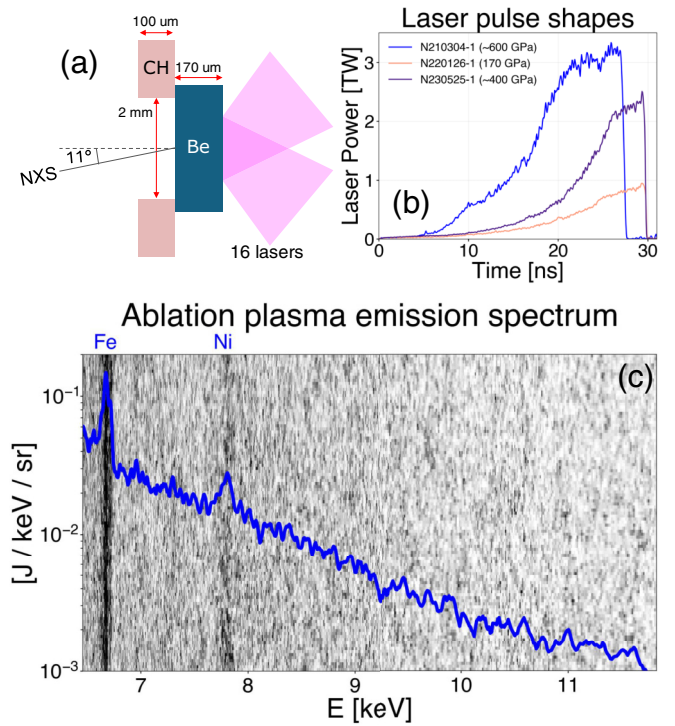


FIG. 6. Summary of experiment N210304-1, which measured the x-ray spectrum emitted by a laser-driven beryllium ablator. (a) Target geometry. (b) Laser pulse used for N210304-1 compared with those used in the 170.2 GPa and ~ 400 GPa ramp-compression EXAFS experiments. (c) Time-integrated spectrum recorded by the NIF x-ray spectrometer (NXS). The raw spectral data are shown in grayscale, and the averaged spectrum is shown by the blue curve. The spectrum is background subtracted and absolutely calibrated using the throughput model of Thorn *et al.* [54].

This contribution is included in the strength-model comparisons discussed above, but the resulting temperatures remain approximately 2000 K below the observed value. If this remaining difference is attributed primarily to underestimated radiative heating, the total contribution would need to be approximately 2700 K. Several approximations could affect this estimate in competing directions. The one-dimensional planar geometry likely overestimates the heating by preventing lateral radiation escape from the finite focal spot. Conversely, laser-plasma instabilities are not modeled, and the ablator is treated as pure beryllium despite containing approximately 0.01–0.03 wt.% Fe and Ni, both of which could increase the x-ray emission incident on the sample through enhanced continuum and characteristic line emission. These competing effects highlight the difficulty of quantitatively modeling the radiation heating and motivate this study.

We therefore performed a dedicated experiment, N210304-1, to measure the x-ray spectrum produced by the high-pressure drive lasers. Its laser pulse was designed to reach peak stresses of approximately 600 GPa in support of a different campaign, but the resulting emission provides a relevant reference spectrum for this study. Figure 6(a) shows the target geometry, a 170- μm -thick, 3-mm-diameter beryllium foil mounted on a plastic aperture, and Fig. 6(b) compares the laser pulse with those used in the 170.2 GPa and ~ 400 GPa

ramp-compression EXAFS experiments. Sixteen NIF beams were used in all cases, but N210304-1 employed standard 1-mm CPPs in the 2×2 tile pattern used on TARDIS rather than the 3.2-mm CPPs in a single overlap pattern used for the EXAFS experiments. Its total laser energy and irradiance were each roughly twice those of the ~ 400 GPa EXAFS experiment.

Figure 6(c) shows the time-integrated emission between approximately 6.5 and 12 keV recorded by the NIF x-ray spectrometer (NXS) [54,55], which viewed the ablator surface at 11° from its normal. The emission is dominated by a strong bremsstrahlung continuum with He_α lines from the Fe and Ni impurities noted above. Excluding the line regions, we fitted the continuum with

$$S_{\text{ref}}(E) = A_{\text{ref}} \exp\left(-\frac{E}{T_{\text{rad,ref}}}\right), \quad (2)$$

where E is the x-ray energy in keV, $S_{\text{ref}}(E)$ is the time-integrated emitted energy per unit photon energy per steradian, A_{ref} is a normalization constant with the same units as S_{ref} , and $T_{\text{rad,ref}}$ is the fitted radiation temperature expressed in keV. We then extrapolated Eq. (2) over 1–40 keV to estimate the unmeasured portion of the spectrum.

To apply this reference spectrum to N230525-1, we assumed that the total emitted x-ray energy scales linearly with drive laser energy and that the radiation temperature scales with irradiance as $T_{\text{rad}} = T_{\text{rad,ref}}(I/I_{\text{ref}})^p$, where I is the irradiance. We adopt $p = \frac{2}{3}$, following the ablation-pressure scaling predicted by coronal-absorption models [56], and assume that the plasma temperature, and therefore the hardness of the emitted x-ray spectrum, follows the same irradiance dependence ($P_e \propto T_e$). The rescaled spectrum was assumed to originate from a disk the size of the laser focus and was propagated through the target stack using energy-dependent attenuation; the energy deposited in each tantalum volume element was converted to a temperature increase using its ambient density and heat capacity, following previous work [28]. Averaged over the tantalum layer, the predicted temperature increase is ~ 1740 K, comparable in magnitude to the ~ 2700 K total ablation-plasma radiation contribution required to reconcile the measured temperature with the hydrodynamics prediction. However, the inferred heating is sensitive to the assumed spectral scaling: choosing $p = \frac{1}{2}$, which produces a harder rescaled spectrum, increases the predicted heating to ~ 3000 K, sufficient to account for the observed discrepancy.

There is additional uncertainty in extrapolation beyond the NXS measurement range, the assumed location and extent of the emitting plasma, the treatment of the time-integrated spectrum, hot-spots in laser focus due to CPP use, use of different laser pulse shapes between shots, uncertainties in target geometry and material properties, and the NXS throughput model, which is calculated rather than directly measured [54]. We therefore estimate the absolute heating values to be accurate only to within a factor of 2–3. Even so, this treatment shows that absorbed ablation-plasma x-rays could plausibly account for the temperature discrepancy on N230525-1. Enhanced shielding or alternative ablator materials, two-dimensional radiation-hydrodynamics modeling, and direct spectral measurements under comparable drive conditions with broader

energy and temporal coverage would provide more stringent tests of this explanation.

3. Estimate of conduction

Our previous results at ~ 400 GPa on copper showed an additional heating of ~ 3300 K when the sample was sandwiched between a diamond pusher and window [6] compared with experiments at similar pressures using aluminum and lithium fluoride. This extra heating was attributed to thermal conduction from the surrounding diamond layers, which are themselves heated by plastic work. Because the XRD experiments in this work also used a diamond-sandwich design that is expected to provide a comparable heat source, it is important to consider whether the thermal state of the tantalum samples could also be influenced by conduction. In contrast, the tantalum EXAFS experiments deliberately avoided diamond components in the sample stack; as a result, they are not expected to experience heating from thermal conduction.

In the absence of sufficiently detailed data, we make a scaling argument to estimate the possible effects of thermal conduction in our XRD experiments. Conductive heating is diffusion limited, with a characteristic penetration depth given by the thermal diffusion length $L \sim \sqrt{\alpha\tau}$, where α is the thermal diffusivity and τ is the duration of heating; in metals at ambient conditions, L is of order $0.1\text{--}1\ \mu\text{m}$ for a 10-ns duration. The magnitude of conductive heating is further governed by the temperature difference between the diamond and the sample. Using LEOS table 735 for Ta and 291 for Cu, tantalum is expected to be ~ 400 K hotter than copper on the principal isentrope (1220 K versus 824 K), a difference that is small compared with the ~ 3300 K heating observed in copper when adjacent to diamond layers; consequently, the temperature difference driving the conduction should be of similar magnitude for each.

Tantalum's ambient thermal diffusivity is 4.9 times lower than copper's, implying that for the same temperature gradient and time scale, tantalum's diffusion length is smaller by a factor of ~ 2.2 . The characteristic timescale of the tantalum experiments is also shorter, with laser pulse durations of 17–25 ns for Ta compared with ~ 30 ns for Cu, although this difference is partially reduced in the sample as the pressure ramp steepens during propagation. The tantalum samples were also thinner ($3.7\text{--}5.2\ \mu\text{m}$) than the $6\text{-}\mu\text{m}$ copper samples used by Sio *et al.*, partially compensating for the reduced diffusion length by decreasing the distance over which heat must propagate to heat the sample.

Combining these factors, the fraction of the sample heated scales as L/d , where d is the sample thickness. The lower diffusivity and shorter drive reduce this fraction by $(1/2.2)\sqrt{21/30} \approx 0.38$, while the thinner Ta samples increase it by $6/4.5 \approx 1.33$, for a net ratio of ≈ 0.5 relative to copper. Applying this ratio to the ~ 3300 K of conductive heating inferred for copper by Sio *et al.* [6] gives an average temperature increase of ~ 1650 K in the tantalum XRD experiments, although the magnitude will depend on the high-pressure thermophysical properties of the materials and the specific compression history. At 400 GPa, this corresponds to approximately 15% of tantalum's melting temperature [20]. Additional uncertainties associated with interfacial thermal

TABLE III. Summary of the inferred temperature contributions for each EXAFS experiment. Heating from the x-ray source (XRS) is calculated from the measured x-ray spectrum. Heating from plastic work and absorption of ablation-plasma x-rays is obtained from hydrodynamics and radiation-hydrodynamics calculations constrained by the measured velocimetry. The final column gives the ablation-plasma heating predicted by the scaled-spectrum model. The final two columns are alternative estimates of the same contribution and are not additive. All values are temperature increases in kelvin.

Shot	XRS meas.	LMS13i strength	Ablation rad-hydro	Ablation model
N220126-1	63	542	56	10
N220602-2	62	513	126	120
N220924-1	58	623	267	60
N230525-1	222	900	686	1740

resistance and the presence of epoxy layers are beyond the scope of this study.

By contrast, the EXAFS sample design was similar to the Al/Cu/LiF configuration studied by Sio *et al.*, for which the measured Cu temperature agreed with radiation-hydrodynamics calculations to within approximately 200 K. Although the present experiments used a beryllium rather than an aluminum pusher, neither material is expected to undergo the substantial plastic-work heating inferred for diamond under ramp compression. Moreover, the initial shock is expected to produce a larger temperature rise in tantalum than in the adjacent Be and LiF layers. The resulting temperature gradients would therefore tend to drive heat out of, rather than into, the tantalum. Thermal conduction may consequently produce some cooling of the Ta sample, but a much smaller magnitude than the rise observed for the diamond sandwich design.

E. Heating contribution summary

We estimate the individual contributions from XRS heating, plastic-work heating, and radiation absorption in our EXAFS experiments by combining measurements with values extracted from radiation-hydrodynamics and hydrodynamics calculations. These results are summarized in Table III.

The first column gives values for heating by absorption of the XRS determined by calculating the energy deposited in the sample from the measured x-ray spectrum using ambient properties. The value for N230525-1 is several times higher than those for the other shots because slightly more transparent x-ray shielding was used to improve the EXAFS signal-to-noise ratio. The second column gives strength heating by the LMS13i strength model calculated by the difference in temperature between the hydrodynamics simulations using the LMS13i and no-strength models during the probe time. The strength models affect the hydrodynamics and could in turn change the amount of heating, but we expect these differences to be negligible. The third column gives heating by absorption of radiation from the ablation plasma, which is determined by calculating the difference between the hydrodynamics and radiation-hydrodynamics calculations using the SG5X strength model, the only model considered here that

is available in our radiation-hydrodynamics code. The final column gives the alternate values for ablation-plasma heating determined by our model using $p = \frac{2}{3}$.

The values in Table III demonstrate that, despite the experimental challenges posed by tantalum, EXAFS measurements can be performed without substantial heating from the probe x-rays. They also show that both plastic-work heating and ablation-plasma heating increase with drive strength. For N230525-1, however, the heating predicted by the radiation-hydrodynamics calculations, even allowing for reasonable variations in the strength model, remains well below the observed temperature excess. In contrast, the larger ablation-plasma contribution inferred from the measured and scaled x-ray spectrum is similar magnitude as the discrepancy. This mechanism should therefore be considered carefully in experiments at high pressure, particularly for thin samples, materials with low heat capacity, and experimental requirements that preclude effective heat shielding.

The implications extend beyond the present experiments. Ablation-plasma x-ray emission is intrinsic to high-power laser drives, and the resulting sample heating depends on laser irradiance, ablator composition, target geometry, and sample properties. Our results show that one-dimensional radiation-hydrodynamics calculations can underestimate this contribution, with direct consequences for phase-boundary determinations, equation-of-state and strength inferences, melt-curve measurements, and assessments of metastability and phase transition kinetics. Materials with low heat capacity and short x-ray attenuation lengths are likely to be especially susceptible. The effect may be reduced through thicker or higher-Z heat shields and lower-irradiance pulse shapes, although these approaches introduce tradeoffs in drive efficiency and target complexity. Because direct measurements of ablation-plasma emission remain scarce, experiments whose conclusions depend sensitively on the thermal state should include an independent temperature constraint whenever possible.

V. CONCLUSION

We have used the XRD and EXAFS platforms at the NIF to determine the crystal structure and temperature of tantalum ramp and shock-ramp compressed to hundreds of GPa pressure. Using XRD, we have determined that tantalum ramp compressed up to $531.7^{+21.3}_{-18.7}$ GPa remains in the body-centered-cubic structure, with no evidence for any other structure including the proposed *Pnma*. Combining EXAFS measurements with FPMD calculations shows good agreement with one-dimensional radiation-hydrodynamics calculations (including strength models and concurrent XRS heating) at ~ 200 GPa, but reveals significantly higher temperatures than predicted at ~ 400 GPa. This discrepancy can plausibly be explained by underestimation of ablation-plasma x-ray heating in the calculations. These results validate *L*-edge EXAFS as a robust platform for temperature measurements under extreme dynamic compression and highlight the need for improved modeling at very high pressures. By extending dynamic-compression EXAFS thermometry from *K*-edge measurements in mid-Z materials to *L*-edge measurements, this approach provides access to high-Z materials such as

tantalum, for which the K edge is at an impractically high energy. This work also highlights the importance of considering x-ray emissions from the ablator, including trace impurities even when using nominally low atomic number ablaters like beryllium. This study marks our team's second application of EXAFS thermometry on dynamically compressed samples at the NIF, and both investigations have uncovered unexpected phenomena that underscore the critical importance of accurate temperature measurements in this field.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. During preparation of this manuscript, the authors used ChatGPT 5.5

and Claude Opus 4.8 and 5.0 to assist with editing for clarity, concision, and organization and with modifying Python analysis scripts. For manuscript editing, the tools were provided with author-written text and specific revision instructions. All suggested language was reviewed and revised as necessary by the authors. AI-assisted modifications to analysis scripts were evaluated through direct inspection of the source code, comparison with independently calculated or known results where applicable, and bounding and sensitivity studies. The authors verified all resulting text, code, analyses, and conclusions and take full responsibility for the content of the manuscript.

DATA AVAILABILITY

The data that support the findings of this article are openly available [57].

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