

Identification of distortions to the Ni atomic potential at 100 GPa with temperature measurements

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(Received 22 December 2025; accepted 10 August 2026; published 28 September 2026)

Characterizing the temperature of materials in high-energy-density (HED) experiments is a major gap in the benchmarking of HED matter, such as matter in the deep interiors of planets and low-mass stars. Extended x-ray absorption fine structure (EXAFS) spectroscopy is one of the few techniques capable of determining temperature at HED conditions, but the inferred EXAFS temperature depends upon the atomic potential, which itself is not measured. This work compares simultaneous EXAFS and self-emission temperature measurements [S. Boccato *et al.*, *J. Geophys. Res.: Solid Earth*, **122**, 9921 (2017)], to quantify the impact of atomic potentials implicit in the EXAFS temperature analysis. Traditional EXAFS analysis employing a harmonic potential produces systematically lower temperatures than from self-emission ($\sim 35\%$ at 100 GPa and 3000 K), while a sixth-order distortion to the pair potential recovers agreement between the two measurements. These results highlight and quantify the need and complexity of distortions or anharmonic corrections to atomic potentials at HED conditions.

DOI: [10.1103/qrck-lqpn](https://doi.org/10.1103/qrck-lqpn)

I. INTRODUCTION

Temperature is one of the crucial thermodynamic parameters defining a state of matter, but its determination at high-energy-density (HED) conditions is exceptionally difficult. Significant effort has focused on developing temperature measurements including the use of extended x-ray absorption fine structure (EXAFS) spectroscopy [1–8], inelastic x-ray scattering (IXS) [9], and streaked optical pyrometry (SOP) [10]. However, no work has been conducted on comparing multiple temperature measurements at HED conditions, meaning that there could be systematic issues with the temperature inference that have not yet been discovered. This work compares pyrometry and EXAFS spectroscopy, the latter of which uses modulations in the x-ray

absorption coefficient to constrain ion vibrations [11–13]. A range of different atomic potentials have historically been used in EXAFS analysis of HED matter, the simplest of which is a harmonic potential [2,14]. However, at temperatures $5\times$ the Debye temperature, third-order anharmonic effects become important [3] and even higher-order corrections are required for temperatures $\geq 8\times$ the Debye temperature [3,15]. Alternatively, molecular dynamics calculations can be used to directly infer temperature by modeling the ion motion in a simulated potential [5]. To quantify the systematic errors in EXAFS analysis of HED matter, we have compared simultaneous EXAFS and pyrometry measurements [16], for Ni from room temperature to the melt curve at pressures up to 100 GPa. By studying each of these atomic potentials, new insight can be gained into how to model atomic potentials at HED conditions.

In this work, we present a study of different EXAFS temperature analysis techniques by analyzing a Ni dataset with measured EXAFS spectra and self-emission temperatures [17]. The harmonic or second-order EXAFS analysis of these data systematically generates a lower temperature than the self-emission temperature with discrepancies up to $\sim 35\%$ at 100 GPa and 3000 K. A more tightly constraining or

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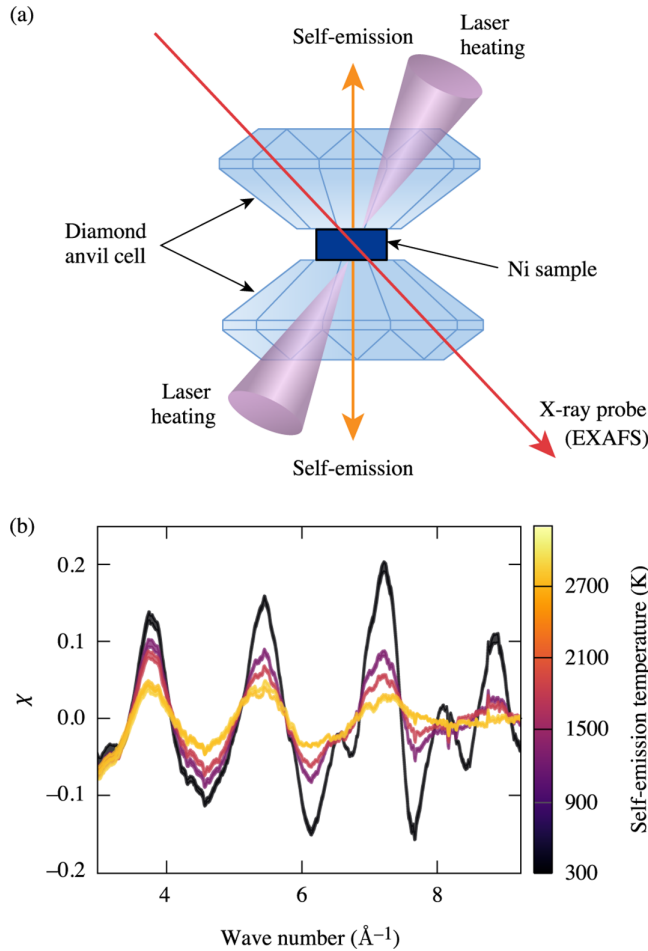


FIG. 1. (a) Experimental setup highlighting how the DAC was heated from both sides and the self-emission temperature was also measured on both sides [17]. (b) Example normalized EXAFS χ at 97 GPa at a range of temperatures.

localized pair potential is required to bring the two temperatures into agreement. This is corroborated by *ab initio* molecular dynamics (AIMD) calculations, which also show a tighter pair potential than a harmonic oscillator. However, there is still a small systematic discrepancy ($\sim 10\%$) between the AIMD and self-emission temperatures even when accounting for potential systematic uncertainties in the self-emission temperatures [18].

II. EXAFS AND SELF-EMISSION MEASUREMENTS

The Ni EXAFS dataset was collected by compressing Ni foils in a diamond anvil cell (DAC) up to 100 GPa and laser heating the samples [17]. The EXAFS spectra were measured in the heated state and the temperature was determined from the sample self-emission. An example experimental setup and subset of the EXAFS spectra are shown in Fig. 1, and further details about the experiment can be found in Ref. [17]. Figure 2 shows the self-emission temperatures and pressures of the analyzed data with the assumed 10% error bar [17]. A subset of the published Ni dataset was chosen for this analysis to only include spectra with a long k -range to properly capture the damping in the EXAFS modulations at high wave number.

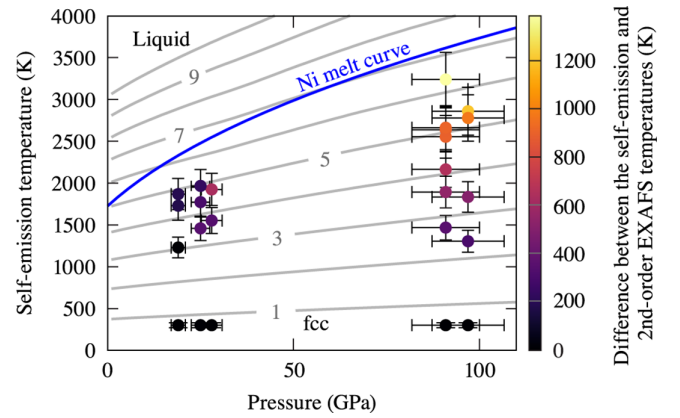


FIG. 2. Temperature and pressure of Ni data points [17] used for the EXAFS temperature analysis, where the Ni melt curve [17] is shown as the blue line. Each data point is colored by the difference between the self-emission temperature and the inferred harmonic EXAFS temperature analysis. Contours of the self-emission temperature divided by the Debye temperature are shown, where the density was computed using SESAME 3101 and the Debye temperature model is discussed in Sec. S2 of the Supplemental Material [27].

In this work, only solid Ni EXAFS spectra were considered and all EXAFS spectra were assumed to be face-centered cubic (fcc) Ni due to the experimental evidence of the stability of Ni fcc up to 402 GPa [19,20]. This stability of the fcc structure makes Ni an ideal candidate to study the EXAFS temperature extraction because the spectra will not be complicated by phase transitions.

It is an open question whether the signature of temperature on thermal emission or EXAFS oscillations is well understood at HED conditions. The EXAFS temperature will constrain the bulk or interior ion temperature by measuring the effect of ion vibrations on the absorption spectra [21]. The self-emission measurements constrain the surface electron temperature by adopting a gray-body approximation [17]. For the self-emission or electron temperature, the samples were laser heated on both sides with a spot size of 20 μm . The EXAFS was measured using an x-ray spot size that was 2–3 times smaller than the laser heating spot [17], and the x-ray probe time began 50 ms after the laser probe was turned on [22]. One-dimensional thermal conduction calculations that solve the heat equation using a finite difference method [23,24] and assuming ambient Ni thermal conductivity [25], specific heat [26], and a density of 10.75 g/cm³ with fixed boundary temperatures of 3000 K show a steady-state temperature after hundreds of nanoseconds—well before the x-rays turn on. Therefore, there should not be a large temperature discrepancy between the surface and the bulk of the Ni perpendicular to the diamond culet surface. However, gradients in the sample parallel to the culet surface due to the uniformity in the laser heating and alignment of the x-ray probe with the laser heating probe could lead to differences in the temperatures between the self-emission and the EXAFS. Additional work [18] has shown some potential discrepancies with the self-emission temperature measurements due to the optics used during the experiment indicating that the self-emission Ni temperatures [17] could be 10% higher than the EXAFS temperatures.

For the EXAFS or ion temperature, the choice of the EXAFS atomic potential could lead to a systematic difference with the self-emission temperature. In the remainder of this work, we will focus the discussion on possible systematic issues with the EXAFS temperature inference.

III. EXAFS ANALYSIS

The Ni EXAFS spectra, shown in Fig. 1(b) and Sec. S1 of the Supplemental Material [27], were initially analyzed assuming the second-order EXAFS model to infer the second-order cumulant (C_2). The second-order EXAFS model is given by [6,12,28–31]

$$\chi(k) = S_0^2 \sum_j N_j \frac{F_{\text{eff},j}(k) e^{-2R_j/\lambda_j(k)}}{kR_j^2} \times \sin[2kR_j + \delta_j(k)] e^{-2k^2 C_{2,j}}, \quad (1)$$

where S_0^2 is the amplitude reduction factor, $\sum_j$ sums over each scattering path, R_j is the distance between atoms, N_j is the number of atoms in coordination shell j , $F_{\text{eff},j}$ is the scattering amplitude, δ_j is the phase shift, and λ_j is the electron mean free path. C_2 is the second-order cumulant of the effective distribution $P(r) = p(r)/r^2$, where $p(r)$ is the real distribution [12]. Details of the inference procedure and the fits to the data are discussed in Sec. S3 of the Supplemental Material [27].

A. Second-order potential

This second-order cumulant was first related to temperature using the correlated Einstein (CE) model [21], which assumes a second-order pair potential of the form

$$V(u) = \frac{1}{2} k_2 u^2, \quad (2)$$

where $k_2 = \mu \omega_E^2$, $\omega_E = \frac{3}{4} \omega_D$ is the Einstein frequency [21], $\omega_D = k_B \Theta_D / \hbar$ is the Debye frequency, Θ_D is the Debye temperature, $\hbar$ is Planck's constant (h) divided by 2π , μ is the reduced mass, and $u = r - R$ represents the variation from the nominal distance between atoms (R). From this potential, C_2 was related to temperature (T) [21,32,33]:

$$C_{2,\text{CE}} = \frac{\hbar}{2\mu\omega_E} \coth\left(\frac{\hbar\omega_E}{2k_B T}\right), \quad (3)$$

where k_B is the Boltzmann constant. For ions of the same mass, $\mu = m/2$, where m is the atomic mass. The Debye temperature for Ni was estimated using classical molecular dynamics calculations, discussed in Sec. S2 of the Supplemental Material [27].

The resulting harmonic EXAFS temperatures are shown in Fig. 3(a). In Fig. 3(a), the dashed black line corresponds to where these two temperatures would be equal. With increasing temperature, the EXAFS temperature from the harmonic CE analysis is systematically lower than the self-emission temperature. These results show a difference in the two temperatures of a few hundred kelvin for $T/\Theta_D \sim 3$ and the discrepancy is most pronounced for the highest pressures, reaching a discrepancy greater than 1000 K for $T/\Theta_D > 6$. Furthermore, an adjustment to the self-emission temperature by 10% [18] would not account for this discrepancy.

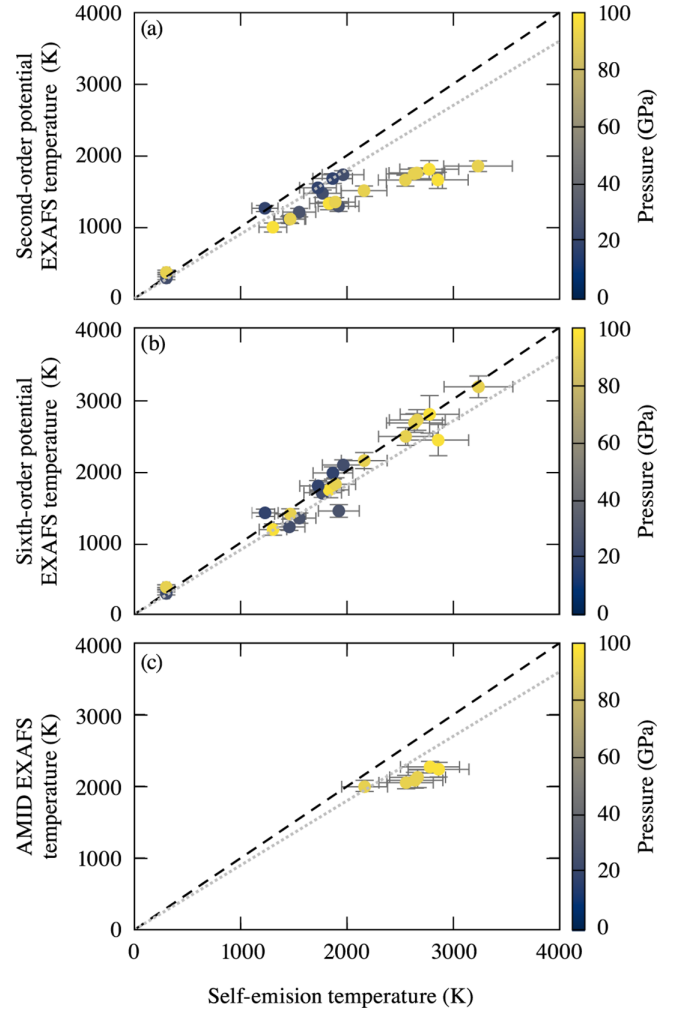


FIG. 3. Comparison of the EXAFS and the self-emission temperatures showing how the sixth-order potential provides the best agreement. (a) Second-order EXAFS analysis shows systematically lower EXAFS temperatures, (b) sixth-order potential EXAFS brings the two temperatures into agreement, and (c) AIMD EXAFS analysis shows systematically lower EXAFS temperatures, where the color corresponds to the pressure in GPa. Only a few points were analyzed with the AIMD surrogate model due to the reduced temperature and density AIMD ranges. The dashed black line corresponds to where the EXAFS and self-emission temperatures would be equal. The dotted gray line represents the correction to the self-emission temperature measurements [18], where the data would sit on this line if the self-emission temperatures were 10% lower.

This discrepancy between the EXAFS and self-emission temperatures is most likely due to the assumption of a harmonic pair potential. There are two other possible explanations for the discrepancy: (1) The second-order EXAFS analysis does not extract the true underlying C_2 or (2) the Debye temperature is not correct. First, from previous studies of Ni synthetic spectra [6], it was found that the second-order EXAFS analysis can capture the width or C_2 of the real distribution. Second, increasing the Debye temperature to bring the higher temperature data into agreement with the self-emission temperature would result in a discrepancy at ambient temperature. Therefore, it is unlikely that the discrepancy between

the self-emission and EXAFS temperatures is solely due to an issue with the Debye temperature, but instead due to the assumption of a harmonic potential.

B. Higher-order potential

To improve the agreement between the EXAFS and self-emission temperatures, higher-order pair potentials were explored. As shown in Fig. 3(a), the second-order EXAFS and self-emission temperatures agree at ambient conditions; however, at high temperatures, the second-order EXAFS temperature is lower than the self-emission temperature with a larger discrepancy at higher pressures. Therefore, at low temperatures, the pair potential is reasonably described by a harmonic potential, but at higher temperatures when the atomic motion can access more of the atomic potential, a deviation from a harmonic potential is required. This is further emphasized in Fig. 4(a), which shows C_2 from the second-order model and the data at 91 GPa. Only data along one isobar are shown because the figure assumes a density of 11 g/cm³, which is close to this dataset. The data and the second-order model are consistent at ambient conditions but then diverge at higher temperatures. This implies that the pair potential should be more tightly binding than a harmonic potential at these higher temperatures because a more tightly binding potential would confine the atomic motion more, leading to higher temperatures for a given second-order cumulant.

Continuing the expansion out to a third-order potential would allow the wave functions to expand more at a given temperature, increasing the discrepancy between the EXAFS and self-emission temperatures. A third-order potential model has been previously used to analyze iron at HED conditions [3] and a summary of the third-order model is shown in Sec. S4 of the Supplemental Material [27]. Using this third-order potential model, the resulting relationship between the second-order cumulant and temperature is shown in Fig. 4(a) as the dashed green line. This third-order model would result in even lower temperatures for a given second-order cumulant value further increasing the discrepancy.

To expand the potential to higher order, we turned to directly solving for the wave functions of higher-order potentials. An n th-order potential of the form

$$V(u) = \frac{1}{2}k_2u^2 + \kappa_n k_2 u^n \quad (4)$$

was assumed, where $k_2 = \mu\omega_E^2$. By construction, only the n th-order term (κ_n) is added, mitigating the risk of introducing many free parameters for higher orders. To solve for the wave functions of this potential and ultimately the relationship between C_2 and temperature, we employed the phase method [34], which numerically solves for the energy levels (E_n) and wave functions (ψ_n) of a given potential (V). From the wave functions, the partition function is given by $Z(\beta) = \sum_n e^{-\beta E_n}$, where $\beta = \frac{1}{k_B T}$, and the real distribution (p) can be computed using

$$p(T, r) = \sum_n \frac{e^{-\beta E_n} \psi_n(r)^2}{Z}. \quad (5)$$

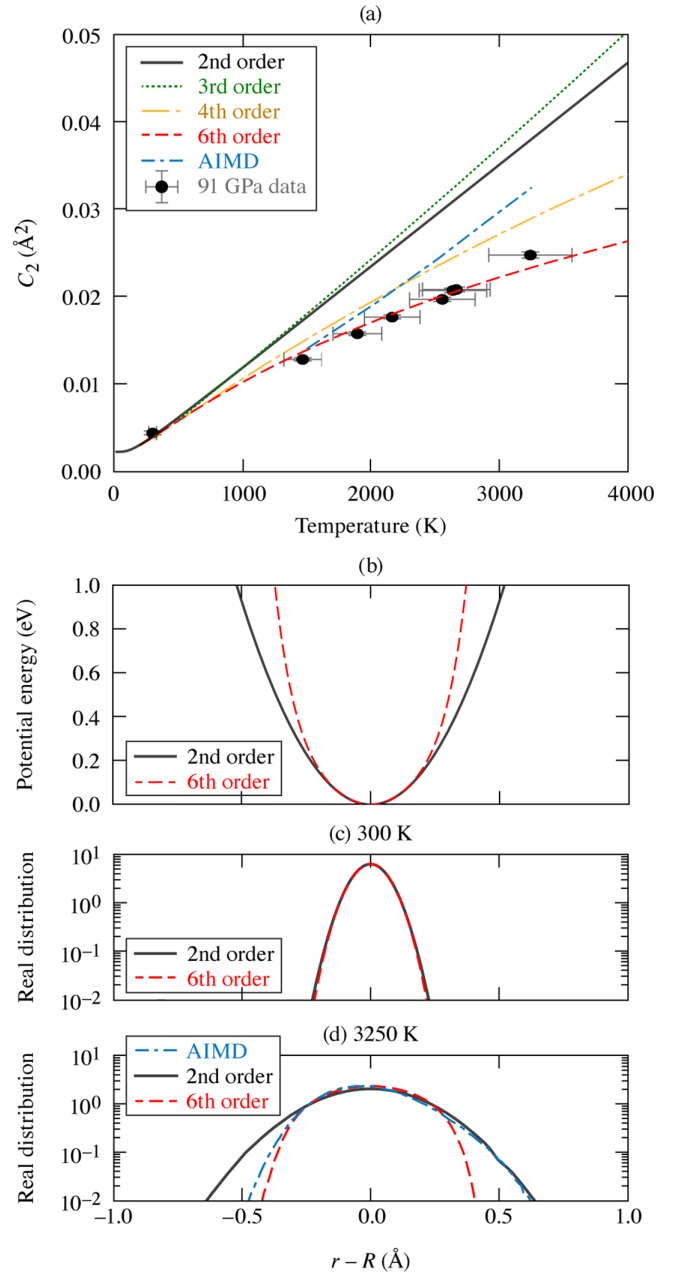


FIG. 4. (a) The second-order cumulant (C_2) as a function of temperature highlighting how the sixth-order potential model is most consistent with the data: the harmonic (black line), third order (green dotted line), fourth order (orange dash-dotted line), sixth order (red dashed line), and AIMD (blue dash-dotted line). These cumulants were calculated for a density of 11 g/cm³, $\omega_E = 4.9261 \times 10^{13}$ Hz, $\kappa_4 = 1 \text{ Å}^{-2}$, and $\kappa_6 = 25 \text{ Å}^{-4}$. The third-order potential was computed assuming $C_3 = 1.6 \times 10^{-3} \text{ Å}^3$ at 3000 K [6]. (b) Comparison of the second-order (solid black) and sixth-order (dashed red) potentials. (c) Real distribution for the harmonic (solid black) and modified pair potential (dashed red) at 300 K. (d) Real distribution for the harmonic (solid black), modified pair potential (dashed red), and AIMD (dash-dotted blue) at 3250 K.

From the real distribution, the second-order cumulant is given by [12]

$$C_2(T) = \int (r - R)^2 p(T, r) dr. \quad (6)$$

Even-order potentials were considered to more tightly constrain the motion and gain an idea of what potential shape would generate EXAFS temperatures that are consistent with the self-emission temperature. The results for a fourth-order potential are shown in Fig. 4(a), where κ_4 was assumed to be $1 \text{ \AA}^{-2}$ because this brought the fourth-order potential into agreement with the second-order potential at ambient conditions. However, this fourth-order potential does not constrain the ion motion enough and would still result in temperatures that are too low. Therefore, a sixth-order potential was considered, where κ_6 was assumed to be $25 \text{ \AA}^{-4}$ because this brought the sixth-order potential into agreement with the second-order potential at ambient conditions. This sixth-order model constrains the ion motion enough to become consistent with the data at all temperatures. A comparison of this sixth-order potential with the harmonic potential is shown in Fig. 4(b), showing how the sixth-order potential is a tighter potential because the sixth-order potential has a higher potential energy further away from the origin. The real distributions for the harmonic and sixth-order potentials are shown in Figs. 4(c) and 4(d) for 300 and 3250 K, respectively. As expected, at low temperatures, the two potentials are indistinguishable, but at higher temperatures, the sixth-order pair potential results in a more tightly constrained real distribution relative to a second-order potential.

The results of the sixth-order potential analysis are shown in Fig. 3(b), where the second-order cumulant as a function of temperature was computed using Eq. (6) with the lowest ~ 40 wave functions. The results show good agreement between the EXAFS and self-emission temperatures as shown in Fig. 3(b), while maintaining consistency with the ambient temperature data points. For this temperature model, κ_6 was determined empirically from the data to be $5 \text{ \AA}^{-4}$ for datasets with pressures less than 30 GPa and $25 \text{ \AA}^{-4}$ for datasets above 90 GPa. The need for the larger κ_6 term for the higher-pressure data indicates a larger deviation from the harmonic potential with increasing pressure.

There are a wide range of different pair potentials that would result in the agreement shown in Fig. 3(b). Higher temperatures or pressures may also result in the need for further modifications to the pair potential because the atoms will sample additional portions of the potential. Future work should include identification of the family of potentials that produce the same EXAFS temperature by including the impact of lattice vibrations along different crystal lattice vectors [33] or extracting more information about the real distribution from the EXAFS spectra [6]. However, this result highlights the need for a more constraining potential, which is surprising at these extreme conditions. Previous work suggests that the potential should become less constraining at HED conditions [3], allowing the atoms to spread out further for a given temperature. The need for a tighter potential would significantly impact the equation of state of the material. For example, a tighter pair potential would lead to a smaller specific heat than estimated by the Dulong-Petit limit [35].

C. *Ab initio* molecular dynamics potential

To investigate a potential that includes the effect of all neighboring atoms, the EXAFS spectra were also directly

analyzed with AIMD calculations [5]. From these calculations, the ion positions were input into FEFF [36] to generate the synthetic EXAFS spectra at the given condition. By generating a grid of spectra from 10.25 to 11.75 g/cm³ and 1500 to 3250 K, a surrogate EXAFS model was built and fit to the EXAFS data [5]. Details on the AIMD calculations are discussed in Sec. S5 of the Supplemental Material [27] and the inferred temperatures are shown in Fig. 3(c).

The AIMD analysis improves the temperature agreement relative to the harmonic analysis. However, there is still a discrepancy between the AIMD and self-emission temperatures. If the self-emission temperatures were lowered by 10% [18], there would still be a systematic offset between the EXAFS and self-emission temperature on the order of $\sim 10\%$. This is possibly because the AIMD potential is not as constraining as the sixth-order potential, resulting in a wider real distribution [shown in Fig. 4(d)]. It is interesting that the AIMD real distribution resembles the tighter distribution at the left side, while overlapping with the harmonic distribution at the right side as shown in Fig. 4(d). This wider real distribution results in larger cumulants at a given temperature, where this discrepancy is largest at the highest temperatures as shown in Fig. 4(a). Studying different exchange functionals in the AIMD analysis may help reduce the discrepancy between the self-emission and AIMD temperatures. These results indicate additional corrections are needed in either the self-emission or the AIMD analysis to bring the two temperatures into agreement.

IV. CONCLUSIONS

In this work, we analyzed a Ni EXAFS dataset with a corresponding self-emission temperature to characterize different EXAFS temperature analysis techniques. EXAFS temperatures inferred using a second- or third-order pair potential are systematically lower than the self-emission temperature. Better agreement is found for both an analytic sixth-order pair potential and ion positions from AIMD simulations, suggesting that a tighter pair potential (compared to second or third order) is needed at these extreme conditions. There is no guarantee that the pair potential supported here is universal for all materials or at all conditions, emphasizing the need to investigate other materials using the method presented in this paper. Furthermore, additional optimization of the AIMD calculations is needed to bring the AIMD EXAFS temperatures into agreement with the self-emission temperatures. Future work should include developing the techniques to further constrain the pair potential by extracting the full real distribution from the EXAFS spectrum [6], and continuing to cross-benchmark temperature measurements with available HED temperature diagnostics, including EXAFS, IXS [9], or dynamic SOP [10]. These steps are critical to improve the ability to measure temperature and better constrain the thermodynamic parameters of compressed materials.

ACKNOWLEDGMENTS

The authors thank Richard Briggs and Ruggero Giampaoli for the contributions acquiring the Ni data. This material is based upon work supported by the Department of

Energy [National Nuclear Security Administration] University of Rochester “National Inertial Confinement Fusion Program” under Award No. DE-NA0004144. The support of DOE does not constitute an endorsement by DOE of the views expressed in this paper. Funding for this research was provided by the Center for Matter at Atomic Pressures (CMAP), a National Science Foundation (NSF) Physics Frontiers Center, under Award No. PHY-2020249. G.H. and N.A. were supported by the National Nuclear Security Administration via Grant No. NA0004078. N.A. was also supported by the National Science Foundation via Grant No. DMR-2202124. This collaborative work was partially supported under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344. S.A. thanks the Generalitat Valenciana for the CIDEGENT Grant No. CIDEXG/2022/6.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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