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**Supporting information for article:**

**Theoretical development and experimental validation on the  
measurement of temperature by extended X-ray absorption  
fine structure**

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### S1. Details of the temperature measurements

In Yakkobi's measurement methods (namely method1 and method2 in our article) the temperature determination expressions are as follows:

$$\sigma^2 = \frac{3\hbar^2}{Mk\Theta_D} \left[ \frac{1}{4} + \left( \frac{T}{\Theta_D} \right)^2 \int_0^{\Theta_D/T} dx \frac{x}{\exp(x)-1} \right] \quad (1)$$

$$\sigma^2 = \frac{\hbar}{M} \int d\omega \rho(\omega) \frac{\coth(\beta\hbar\omega/2)}{\omega} \quad (2)$$

$$\rho(\omega) = \frac{3\omega^2}{\omega_D^3} \left[ 1 - \frac{\sin(\omega r/c)}{\omega r/c} \right] \quad (3)$$

Formulas (1) and (2) are the uncorrelated and correlated Debye model, respectively, which contains Debye temperature  $\Theta_D$  or Debye frequency  $\omega_D$ , Yakkobi employed the Cowan's empirical model [1] to calculate these two quantities, while as mentioned in our article, this empirical model is quantitatively unreliable (for example, gold has a Debye temperature of 165K at normal pressure while the calculated Debye temperature is 360.03K according to Cowan's empirical model). Considering the samples were measured at normal pressure in our article, we have used the experimental values of  $\Theta_D$  and  $\omega_D$  instead of the calculated values from Cowan's empirical model when measuring the temperatures by method1 and method2, the experimental value of  $\Theta_D$  is 165K for Au, 470K for Fe, 380K for V and 420K for Ti at normal pressure [2].

The temperature determination formula (formula (S1)) of method1 was derived from a Debye model of atoms' oscillations in the cubic lattice, so this formula isn't suitable for dealing with titanium which has the hexagonal close packed (hcp) structure in our measurement condition. Thus we didn't give the measurement results of method1 for titanium.

Ping. Y's work has primarily focused on the much higher temperature range (3000K-6000K or even higher), their temperature determination formula was derived from the Einstein model:

$$\sigma_E^2 = \frac{\hbar}{M\omega_E} \coth\left(\frac{\hbar\omega_E}{2k_B T}\right) \quad (4)$$

Using the high temperature approximation  $k_B T \gg \hbar \omega_E$  and expand formula (4) to the first order the following expression could be obtained:

$$\sigma_E^2 \approx (k_B T) / (M \omega_E^2 / 2) = k_B T / k_{eff} \quad (5)$$

Then the results of Stern *et. al.* [3] has been employed:

$$\sigma^2 = \frac{k_B T}{k_{eff}} + 36(k_B T)^2 k_{3eff}^2 / k_{eff}^4 \quad (6)$$

$$\sigma_3 = 6(k_B T)^2 k_{3eff} / k_{eff}^3 \quad (7)$$

By combination of formulas (5) (6) and (7), the temperature determination formula in Ping Y's work has been obtained:

$$\sigma^2 = \sigma_E^2(T) + (\sigma_3 / \sigma_E^2(T))^2 \quad (8)$$

While in our article, the studied temperature range is rather lower as compared with Ping. Y's work, so the original expression of Debye-Waller factor without high temperature approximation  $k_B T \gg \hbar \omega_E$  has been employed. Specifically, the MSRD-temperature curves by method 3 (Fig. 2 in our article) were plotted according to formula (6) and the temperature measurement results (Fig. 3 and Table. 3 in our article) by method 3 were derived from the following formula:

$$\sigma^2 = \frac{k_B T}{k_{eff}} + 6\sigma_3 k_{3eff} / k_{eff} \quad (9)$$

## S2. Details of the molecular dynamic (MD) simulation and the reproduction of the MSRD

To examine if the MSRD values from the cumulant expansion are correct and have physical meanings, we have carried out the MD simulations of the thermal motions of the four kinds of metals at different temperatures and a standardized atmosphere (1 bar), the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [4] was employed in our MD simulations. The initial three

dimensions of simulation box and configurations for the four kinds of metals can be seen in table S1:

**Table S1** The initial three dimensions of simulation box and configurations for Au, Fe, V and Ti.

	Dimension x of the simulation box	Dimension y of the simulation box	Dimension z of the simulation box	lattice	Number of atoms	lattice symmetry
<b>Au</b>	20.4nm	20.4nm	20.4nm	50×50×50 fcc lattices	500000	f m3m
<b>Fe</b>	14.28nm	14.28nm	14.28nm	50×50×50 bcc lattices	250000	i m3m
<b>V</b>	15.15nm	15.15nm	15.15nm	50×50×50 bcc lattices	250000	i m3m
<b>Ti</b>	14.73nm	22.52nm	24.06nm	50×50×50 hcp lattices	500000	P 63/mmc

Periodic boundary condition have been adopted for the simulation boxes and the embedded-atom method (EAM) potentials were used to describe the interactions of atoms (Specifically, Au EAM potential model is employed from ref [5], Fe from ref [6], V from ref [7] and Ti from ref [8]), then the MD simulations were performed in isothermal-isobaric (npt) ensembles where the temperatures and pressures can be controlled to the given values by the thermostatting and barostatting algorithms. The timescales of the MD simulations are from 200 ps to 500 ps, we monitored the temperature, pressure and mean-squared displacement (MSD) of atoms during the simulations, and found that after about 5 to 10 ps relax time the systems had achieved the thermal equilibrium states, then we sampled the coordinates' information of atoms under thermal equilibrium for the following calculations of MSRDS.

We noticed that the Debye-Waller factor  $\sigma^2$  (or say the second order cumulant  $C_2$ ) is mainly sensitive to the parallel MSRDS, namely the projection of total MSRDS along the bond direction (ref [6]), so we calculated the parallel MSRDS from the MD

simulations' trajectories, the results and the second order cumulants fitted from EXAFS data are list in table S2:

**Table S2** The parallel MSRDs calculated from the MD simulations' trajectories and the second order cumulants fitted from EXAFS data.

		Parallel MSRD calculated from MD simulation ( $\text{\AA}^2$ )	C <sub>2</sub> fitted from EXAFS data ( $\text{\AA}^2$ )	Deviation
Au	300K	$1.35 \times 10^{-2}$	$1.46 \times 10^{-2}$ (fitted by third order expansion)	6.9%
	700K	$3.16 \times 10^{-2}$	$3.31 \times 10^{-2}$ (fitted by 4th order expansion)	4.4%
	1000K	$4.48 \times 10^{-2}$	$4.74 \times 10^{-2}$ (fitted by 4th order expansion)	5.4%
Fe	300K	$5.64 \times 10^{-3}$	$5.98 \times 10^{-3}$	5.6%
	500K	$9.60 \times 10^{-3}$	$9.55 \times 10^{-3}$	0.5%
	700K	$1.34 \times 10^{-2}$	$1.30 \times 10^{-2}$	2.6%
	900K	$1.68 \times 10^{-2}$	$1.67 \times 10^{-2}$	0.3%
	1100K	$2.01 \times 10^{-2}$	$2.08 \times 10^{-2}$	3.4%
V	300K	$8.40 \times 10^{-3}$	$8.90 \times 10^{-3}$	5.6%
	500K	$1.34 \times 10^{-2}$	$1.43 \times 10^{-2}$	6.5%
	700K	$1.83 \times 10^{-2}$	$2.02 \times 10^{-2}$	9.3%
Ti	300K	$8.70 \times 10^{-3}$	$8.34 \times 10^{-3}$	4.3%
	500K	$1.38 \times 10^{-2}$	$1.30 \times 10^{-2}$	6.2%
	700K	$1.91 \times 10^{-2}$	$1.80 \times 10^{-2}$	6%
	900K	$2.52 \times 10^{-2}$	$2.32 \times 10^{-2}$	8.7%

The parallel MSRDs produced by MD simulations matches the  $C_2$  values fitted from EXAFS data rather good (The smallest deviation is only 0.3%), so we indicates for Au, Fe, V and Ti crystals at our experimental temperature range, the cumulant expansion method can obtain meaningful and reliable  $C_2$  values.

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