

We thank the reviewers for taking the time to review the manuscript and for their constructive comments. We have addressed each individual comment below. We believe that all comments have been appropriately addressed, and that the manuscript has improved due to these revisions.

- It's not clear how the volume averaged value of thermal expansion is calculated. Since there are a,b,c three directions that are different in expansion, what is "L" in eq. 1 in terms of volume averaged?

We acknowledge the confusion and we have refined the manuscript to better describe the procedure. The text now reads: "and L is the length of the individual lattice constant or averaged lattice constant (cube root of the volume) at a given temperature". This matches the description from the experimental efforts on volumetric linear thermal expansion.

- Page 3: "Such a supercell is sufficiently large to preclude defect-defect interactions." Is there any support for this claim? The interstitial interactions can be long range. The supercell size needs to be checked to confirm that the size is large enough, especially given that the settings of Lx, Ly, Lz are quite different (Figure 1).

Scoping studies on supercell size had been previously conducted utilizing 0 K DFT simulations. Such work had shown that a 180-atom supercell (5x3x3 unit cells) was sufficiently large to preclude defect-defect interactions. The determining factor to identify an absence of defect-defect interactions was the defect formation energy. The supercell was formed to be as close to cubic as possible, without increasing the supercell size to proportions that are no longer computationally feasible for this type of study. Huang and Wirth (Huang, G.-Y. and Wirth, B. (2011). *J. Phys.: Cond. Mat.* 23, 205402) published results of a convergence study that corresponded with our findings for defect formation energy. They stated that larger supercells are required for migration barrier calculations, which are not performed in this work. Such indications have been included in the manuscript.

- Why 400K seems to be a transition point? The authors may want to provide some insights into this observation instead of simply stating it.

Currently, we do not have an explanation for the transition behavior. This was the attempted goal in pursuing both radial distribution function and electronic structure variations with temperature. We assumed that some insight would be gained from these analyses; however, we were left somewhat empty-handed. Thus, we noted the transition, performed additional analyses to try to uncover causation, but found no tangible explanation.

- Figure 6: why does the defect formation energy increase with temperature (high temperature range)? It looks counter intuitive. For example, with increasing temperature and volume increase, it is expected the formation energy of interstitials will decrease.

It is not uncommon for defect formation energies to decrease with increasing temperature. Such behavior has been computationally shown in hcp and bcc Zr (Mendelev, Phil. Mag. Vol. 90

(2010) 637), and bcc U (Beeler, J. Nuclear Materials 545 (2021) 152714), for example. While volume is increasing with temperature, atomic vibrations are also increasing and potentially negate the additional available volume from thermal expansion. It should be noted that these are formation energies, and only account for the potential energy changes, not for entropies.

- Figure 5: potential reasons for the discrepancy between the calculations and experiment?

There are numerous reasons that the computational and experimental results would not exactly correspond, including impurities in the material, effects from underlying microstructure, defect concentrations, inaccuracies in the fundamental computational theories, etc. However, the agreement observed in Fig. 5 is considered quite good, if imperfect. An additional sentence noting potential sources of error has been included.

- Equation 4: the squared doesn't make sense.

This equation has been modified to more clearly illustrate the described relationship. As an example, the relationship itself is outlined in [Farrance I, Frenkel R. *Clin Biochem Rev.* 2012;33(2):49-75]. However, we feel this relationship is sufficiently ubiquitous to not require explicit citation.