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# Temperature-dependent anisotropy in bond length of $\text{UO}_2$ as a result of phonon-induced correlations

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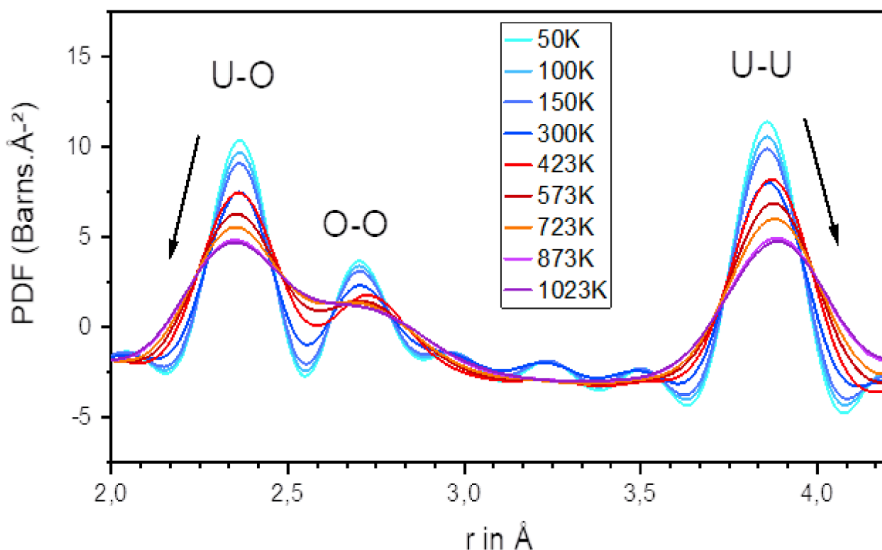
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Previous experiments on cubic  $\text{UO}_2$  have suggested that the temperature dependences of the nearest-neighbour U–O and U–U distances are different. We have acquired total-scattering neutron diffraction patterns out to  $Q=23.5 \text{ \AA}^{-1}$  for  $50 < T < 1023 \text{ K}$  and produced via Fourier transform a pair-distribution function PDF( $r$ ). The PDF( $r$ ) shows quite clearly that  $r(\text{U–O})$ , defined by the maximum of the U–O peak in the PDF( $r$ ), does in fact decrease with increasing temperature, whereas  $r(\text{U–U})$  follows the lattice expansion, as expected. We also observe that the  $r(\text{U–O})$  contraction accelerates continuously above  $T \approx 400 \text{ K}$ , consistent with earlier experiments by others. Furthermore, by analysing the eigenvectors of the phonon modes, we show that the  $\Delta_5(\text{TO}_1)$  phonon tends to separate the eight equivalent U–O distances into six shorter and two longer distances, where the longer pair contribute to a high- $r$  tail observed in the U–O distance distribution becoming increasingly anisotropic at higher  $T$ . These results have significance for a wide range of materials in which heavy and light atoms are combined in a simple atomic structure [1].



Neutron PDF( $r$ ) results from 50 to 1023 K. The  $r(\text{U–U})$  follows the thermal expansion, as it must. However, the  $r(\text{U–O})$  decreases with increasing temperature as a result of the phonon correlations. The  $r$ -space resolution is about  $0.16 \text{ \AA}$  (FWHM) for a  $Q_{\text{max}} = 23.5 \text{ \AA}^{-1}$ . Taken from Ref. [1]

[1] L. Desgranges *et al.* J. Physics: Condensed Matter **35** 10LT01 (2023)

