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An approach towards Zero Thermal Expansion

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Most materials expand upon heating due to the anharmonic nature of lattice vibrations. However, some exhibit the rare phenomenon of volume contraction with increasing temperature, known as negative thermal expansion (NTE). Even rarer are zero thermal expansion (ZTE) materials, which show negligible dimensional changes with temperature. ZTE materials hold significant technological promise, particularly in precision applications.

ZTE is often achieved by combining NTE and positive thermal expansion materials in composites, though these may suffer from thermal instability due to their inhomogeneous nature. Alternatively, ZTE can result from tuning the NTE properties of a single-phase material through controlled elemental substitution.

This presentation focuses on the development of such ZTE materials. We investigated the intermetallic R_2Fe_{17} series (R = rare earth) and $PbTiO_3$-based ceramics, both of which exhibit NTE below their Curie temperatures. By intuitively analyzing the NTE mechanisms and selectively substituting elements to weaken them, we achieved ZTE behavior over wide temperature ranges. We calculated the thermal expansion via unit-cell volume measurements at various temperatures using a temperature-dependent X-ray diffractometer. Notably, $Ho_2Fe_{16}Cr$ exhibits near-zero expansion from cryogenic temperatures to well above room temperature. Additionally, several ceramic compounds demonstrate ZTE within the broad range of RT ± 150 K.

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