Critical issues for Mo$_5$Si$_3$ as an ultra-high-temperature material include the understanding of the structure and the reduction of high anisotropy in the coefficient of thermal expansion (CTE). In Mo$_5$Si$_3$, the CTE along the $c$-direction is more than twice that in the $a$-direction. We address these issues by x-ray powder diffraction and by first-principles calculations where we examine the physical origin for the high CTE anisotropy. The x-ray powder diffraction data was collected on (Mo,Nb)$_5$Si$_3$ samples using two different diffractometers with different high temperature furnace designs. Parallel beam optics and a low temperature gradient in the furnace improved the experimental precision dramatically. The anisotropy is due to an elastically more rigid basal plane and a higher anharmonicity along the $c$-axis. This higher anharmonicity along the $c$-axis is attributed to the existence of [001] Mo chains in the D$_{8m}$ structure of Mo$_5$Si$_3$. As these chain structures are modified (by alloying additions) or eliminated (by structural modification from D$_{8m}$ to D$_8$), we found significant changes in the CTE anisotropy. Additions of Nb up to approximately 40 at. % reduced the anisotropy. At higher Nb concentrations the CTE increased until the structure changed to that of Nb$_5$Si$_3$ and the CTE anisotropy decreased.

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