

STRUCTURAL AND THERMAL EXPANSION OF Mo-Si COMPOUNDS: THEORY AND EXPERIMENT

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Critical issues for Mo_5Si_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_5Si_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 $(\text{Mo,Nb})_5\text{Si}_3$ 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 $D8_m$ structure of Mo_5Si_3 . As these chain structures are modified (by alloying additions) or eliminated (by structural modification from $D8_m$ to $D8_l$), 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_5Si_3 and the CTE anisotropy decreased.

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