

MS27-2-12 Phase transitions and thermal expansion in a niobium oxyfluoride solid solution
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Abstract

The control of thermal expansion is key for any engineering materials which undergo significant temperature changes, for instance by improving thermal shock resistance or reducing strain in solid oxide fuel cells.[1, 2] ReO₃-type structures, such as ScF₃, can exhibit negative thermal expansion through thermally-induced octahedral tilting.[3] Many ReO₃-type trifluorides and oxyfluorides also show an octahedral tilting pressure phase transition, from Pm-3m to R-3c.[4] The octahedral tilting, therefore, creates a clear link between the temperature-pressure behaviour of ReO₃-type structures.[5] The variable oxidation state of niobium in NbO₂F allows the formation of a ReO₃-type oxygen-fluorine solid solution.[6] This provides an excellent model system for exploring the impact of anionic composition on physical properties. Initial ab initio calculations predict the pressure phase transition is strongly dependent on anionic composition. A similar dependence is therefore expected for thermal expansion, opening the potential for control of thermal expansion through anion doping.

A full pressure-temperature phase diagram for both pure and fluoride-doped NbO₂F has been measured experimentally at the ESRF. Combining ab initio predictions with X-ray diffraction at extreme conditions provides insight into the fundamental relationship between anionic composition, thermal expansion and pressure phase transitions. This presents a new pathway for the design of functional mixed-anion materials with controllable pressure and temperature responses.

References

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Figure 1: The (a) Pm-3m and (b) R-3c phase of NbO₂F

