

Thermoelastic instabilities in rare-earth perovskites $REScO_3$ ($RE = Nd, Sm, Tb, Dy$)

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Materials with perovskite-type structure are well known for undergoing series of phase transitions during temperature or pressure change, wherein the tilt-scheme of the network of corner-connected octahedra typically changes with respect to an untilted cubic parent structure. Rare-earth scandate perovskites ($REScO_3$, $RE = Pr-Dy$) defy this trend, as they crystallize at temperatures above 2000 °C [1] in an orthorhombic structure ($Pnma$) and do not undergo any known phase transitions when cooled to room temperature. Due to their high chemo-physical stability and because their lattice parameters can be tuned by (partly) exchanging the RE [2], they are widely used as substrate materials for epitaxial growth of other perovskites.

The thermoelastic properties of substrates are of great importance as they can be used to estimate interfacial stress that may develop between substrate and thin-film during temperature change. Thus, we used resonant ultrasound spectroscopy and inductive gauge dilatometry to determine the elastic stiffnesses and thermal expansion coefficients of single crystal $NdScO_3$, $SmScO_3$, $TbScO_3$ and $DyScO_3$ in situ from 103 K to 1673 K [3]. The elastic stiffness coefficients are indicative of high internal consistency, e.g. $c_{11} > c_{33} > c_{22}$ and $c_{66} > c_{44} > c_{55}$ hold for all crystal species at room temperature. With increasing charge density caused by decreasing RE -radius, the crystal species become stiffer. The anisotropy of the elastic behavior approaches tetragonal symmetry with rising temperature, which is probably caused by decreasing structural tilt as the orthorhombic phases approach hypothetical tetragonal phases [3].

The shear resistance c_{44} has anomalous positive temperature coefficients at low temperatures; the relevant temperature ranges are shifted to lower temperatures with increasing RE -radius (Fig. 1). This resembles the characteristic behavior of the critical parameter of an orthorhombic to monoclinic phase transition involving shear of the (100)-plane. $c^{[101]}$ and $c^{[011]}$ are two effective resistances of plane waves propagating parallel [101] and [011] with respective displacement vectors subparallel [-101] and [0-11] that have positive temperature coefficients at low temperatures in the case of $TbScO_3$ (Fig. 1). This is indicative of at least one additional competing structural instability for $TbScO_3$ which may activate a phase transition involving shear of the (120)-plane. Only magnetic phase transitions at very low temperatures are known for these $REScO_3$, so increasing pressures may be required to activate phase transitions associated with these instabilities [3].

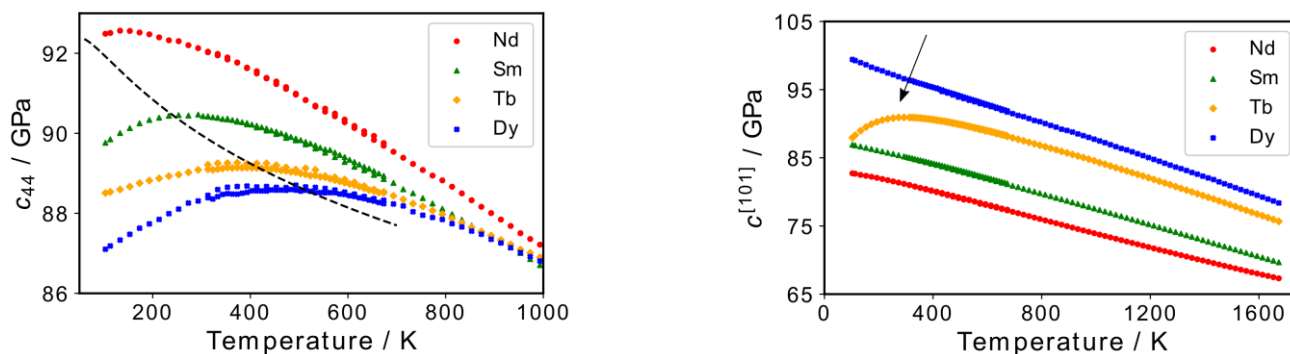


Figure 1. Temperature-dependent stiffnesses c_{44} and $c^{[101]}$ of $REScO_3$ designated by their RE in the key.

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