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Interplay of cation disorder and thermoelastic properties of $MgGa_2O_4$

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Transparent semiconducting oxides are materials suitable for a wide variety of optoelectronic applications, such as UV-LEDs, Schottky diodes, high voltage transistors and transparent thin film transistors. Spinel structure $MgGa_2O_4$ was recently shown to have an appropriate carrier concentration and bandgap for such applications and it can be grown using various techniques from the melt as relatively large crystals[1]. Furthermore, it has a high chemo-physical stability and its conductivity can be controlled by adjusting the atmosphere during the growth process[1], making it an excellent candidate for future applications. However, spinel-like materials often exhibit anomalies in their physical properties at higher temperatures due to changes of their cation ordering (normal/inverse spinel). In fact, both heat capacity[1] and thermal diffusivity[2] of $MgGa_2O_4$ were shown to behave anomalously as a function of temperature.

We studied this issue by direct investigation of the cation ordering of annealed samples using single crystal X-ray diffraction. Additionally, we used inductive gauge dilatometry and resonant ultrasound spectroscopy to determine thermal expansion and the complete set of elastic constants, respectively, from 103 K to 1673 K to assess correlations between the changing structure and properties.

Thermal expansion and most stiffness coefficients show a discontinuity in their temperature dependence at about 820 K. Furthermore, the cation disorder is independent of temperature up to about 820 K and increases gradually at higher temperatures. Thus, the cation disorder in $MgGa_2O_4$ is most likely in equilibrium at high temperatures and undergoes a transition to a nonequilibrium state below 820 K, where the disorder cannot relax in laboratory timescales; a glass-like transition. This transition is likely also related to the anomalies in heat capacity[1] and thermal diffusivity[2]. The bond-valence model can qualitatively explain the relation between changing cation order and thermoelastic properties.

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