High temperature thermoelastic properties of Mg-cordierite: experimental studies and atomistic simulations

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The temperature dependence of the elastic constants of natural, ordered, orthorhombic Mg-cordierite was studied between 295 K and 1573 K using resonant ultrasound spectroscopy (RUS).

The measurements clearly showed a continuous decrease of all c_{ij} on increasing temperature and consequently a softening of the bulk modulus from about 129 (2) GPa at 295K to 110 (2) GPa at 1473 K. This behaviour seems to be in contradiction to the Landau-theory based prediction by Salje (1987).

In order to link the macroscopic observation to the interatomic interactions, force-field and quantum mechanical calculations were performed to investigate the influence of Al/Si disorder on the elastic properties during heating.

The calculated coefficients of thermal expansion (CTE) were in good agreement with those obtained experimentally in the range 95 K to 1473 K using dilatometry. In particular, the contraction of the c-axis was reproduced very well. While the agreements of the CTEs were satisfactory, the models predicted a much smaller elastic softening in the temperature range studied. Hence, we currently conclude that neither the thermal expansion nor the Al/Si order/disorder, both of which were well described in the model, are responsible for the elastic behaviour at high temperature.

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References

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