# Beyond The Quasiharmonic Approximation: Local Structure of Perovskites with Negative Thermal Expansion

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The interest towards $ReO_3$-type perovskites has been recently renewed by the discovery of large negative thermal expansion (NTE) in cubic $ScF_3$ structure in a wide temperature range [1], to be compared with a much less intense effect measured for the cubic $ReO_3$ [2]. At present, the great difference between the isostructural compounds is not yet explained, but it is found that the materials correspond to cases of strong anharmonic effects.

Anharmonicity is of general importance in condensed matter in relation to thermal expansion, structural phase transitions, soft modes in ferroelectrics, melting and related phenomena. Usually anharmonicity in crystals is weak enough and thus so called *implicit* anharmonisity can be described in the framework of Quasiharmonic approximation (QHA) as variations of the phonon frequency due to the change in volume with temperature or pressure. However, this might be not the case for strongly *explicit* anharmonic systems, like perovskites with NTE. The explicit anharmonic effect links the phonon frequencies to the amplitude of the atomic vibrations.

Synchrotron radiation EXAFS studies of local structure with femtometer accuracy [3] offer the possibility to study implicit and explicit anharmonic effects for perovskites with NTE. The temperature dependent EXAFS measurements include both anharmonic effects. The relative contributions of these two effects can be estimated by the extent to which quasiharmonic calculations of amplitude of the atomic vibrations reproduce the experimental EXAFS data. In my talk a description will be made of the most important achievements.

References

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