

## XRS study of medium range order in crystalline alkali borates

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The alkali borate binary system is peculiar as the short-range order around the network former element can be modified with alkali content. When adding alkali ion into vitreous B<sub>2</sub>O<sub>3</sub>, a <sup>[3]</sup>B to <sup>[4]</sup>B coordination change occurs, ensuring the charge neutrality of the system with the formation of negatively charged BO<sub>4</sub><sup>-</sup> tetrahedra. Above 40-50wt.% of alkali ion, the borate network experiences a progressive depolymerization of the borate network pairing with appearance of non-bridging oxygens (NBO). NBOs are defined as atoms bound to only one network former and bearing a negative charge, whereas bridging oxygens (BO) are bound to two network former cations. The structure of alkali borates is peculiar since it presents a short-range order (<sup>[3]</sup>B, <sup>[4]</sup>B) but also an unusual medium range order with formation of superstructural units [1]. Those units impact both the mechanical and thermodynamical properties.

X-ray Raman Scattering coupled to theoretical calculations [2] has already proved its efficiency to study the local structure around low-Z elements such as lithium, boron and oxygen atoms. By revealing the boron coordination number and the presence of non-bridging oxygens in alkali borates, XRS is thus relevant to find spectral signatures related to superstructural units on the B and O *K*-edge spectra. Thanks to the recent implementation of XRS in Quantum Espresso [3] and the comparison with calculation of density of states, we are now able to understand the spectral features of the oxygen and boron atoms in alkali borates in terms of short- and medium-range order in crystalline structures.

### References

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- [3] - E. de Clermont Gallerande et al. *Physical Review B* **98(21)**, 214104 (2018).