

Study of defect structure of ordered $REVO_4$ and disordered $Ca_9RE(VO_4)_7$ and $Ca_3RE_2(BO_3)_4$ (RE = rare earth metal cation) single crystals

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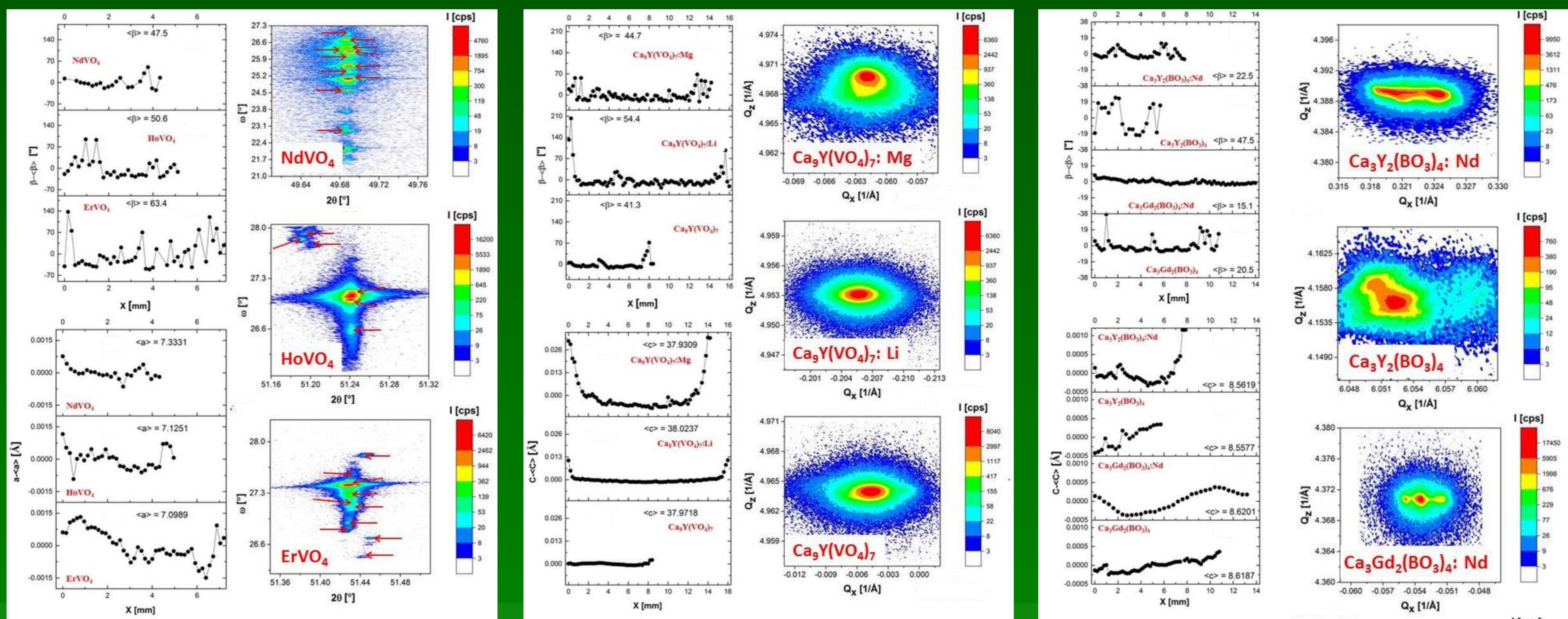
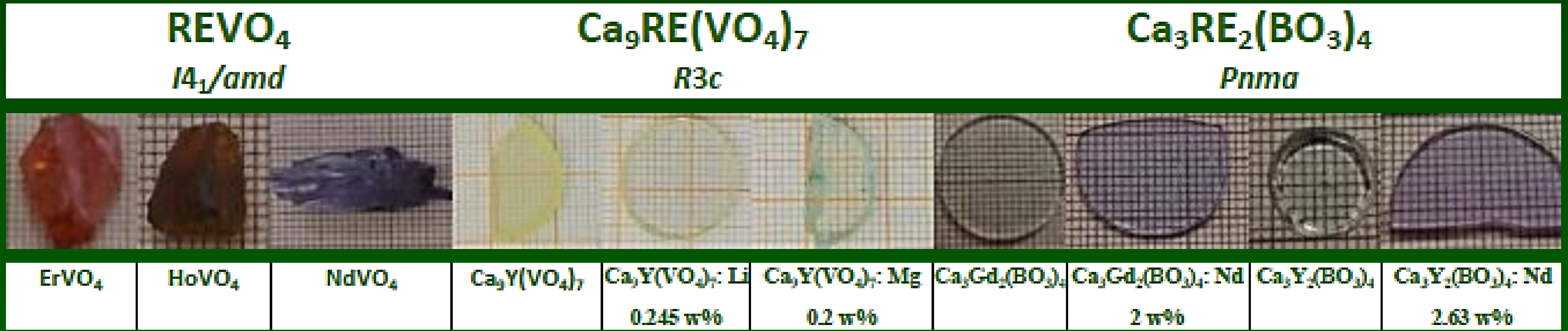


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The investigated with a high-resolution X-ray diffractometry ($\lambda = 1.5406 \text{ \AA}$) single crystals represent high-symmetrical crystallographic systems, respectively: rhombohedral, tetragonal and orthorhombic. They had been selected, because they are promising materials, dedicated especially for optoelectronics [1-3], and there were not many studies devoted to their lattice defects.



$\langle FWHM_{RC} \rangle = 64.6'' + 96.7''$ (this work)
 $\langle FWHM_{RC} \rangle = 10'' + 169''$ [4, 5]

$\langle FWHM_{RC} \rangle = 56.8'' + 76.9''$ (this work)
 $\langle FWHM_{RC} \rangle = 76'' + 158''$ [6, 7]

$\langle FWHM_{RC} \rangle = 30.2 + 144.0''$ (this work)
 $\langle FWHM_{RC} \rangle = 23 + 340''$ [8, 9]

Results

- The plots β - $\langle\beta\rangle$ vs X illustrate a diversification of ω -scan FWHM values along selected direction of the crystal surface; the series of measurements were done with an analyzer and provide an information about a spatial distribution of a micromosaics in a single-crystal
- $\langle FWHM_{RC} \rangle$ is average value of FWHM of ω -scans done with opened detector and provide an information about general crystallographic quality of the crystals: for $REVO_4$ it is $64.6'' \div 96.7''$ (for similar crystals known from literature: $10'' \div 169''$), for $Ca_9RE(VO_4)_7$ $56.8'' \div 76.9''$ (for similar crystals in literature: $76'' \div 158''$) and for $Ca_3RE_2(BO_3)_4$ $30.2'' \div 144.0''$ (for similar crystals in literature: $23'' \div 340''$).
- The plots c - $\langle c \rangle$ (or a - $\langle a \rangle$) vs X illustrate a spatial distribution of a lattice parameter values along selected direction of the crystal surface
- The reciprocal lattice point maps provide, among others, an information about a presence and number crystal blocks in the illuminated area

Summary

- The results of an assessment of general crystallographic quality of investigated samples, based on FWHM magnitude, are comparable with the literature data for the same or similar materials
- The crystals have different quality; there are detected three main types of defects in them: micromosaics (in all samples), crystal blocks (in $REVO_4$ and $Ca_3RE_2(BO_3)_4$) and inhomogeneity of chemical composition (in $REVO_4$)
- Studied single-crystals have complex crystallographic planes profiles with small bending of various coverage and signs (the most perfect profile is in $Ca_3RE_2(BO_3)_4$)

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