Enhanced transparency through second phase crystallization in BaAl₄O₇ scintillating ceramics

Marina Boyer^{*,a}, Salaheddine Alahraché^a, Cécile Genevois^a, Marina Licheron^a, François-Xavier Lefevre^b, Célia Castro ^c, Guillaume Bonnefont^d, Gaël Patton^e, Federico Moretti^e, Christophe Dujardin^e, Guy Matzen^a and Mathieu Allix^{*,a}

SUPPLEMENTARY INFORMATIONS

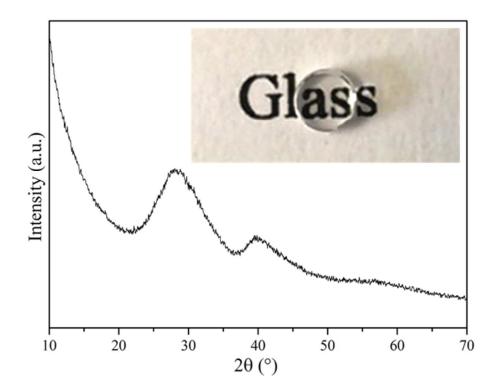


Figure SI1: XRD pattern of the $35BaO-65Al_2O_3$ glass confirming its amorphousness. The photography of the corresponding glass is in inset.

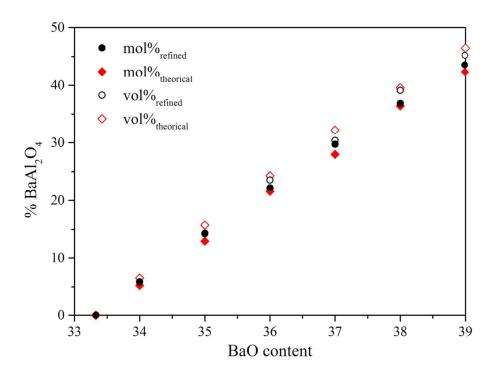


Figure SI2: Quantification of the $BaAl_2O_4$ contents in the studied biphasic $BaAl_4O_7$ - $BaAl_2O_4$ transparent polycrystalline ceramics. Both molar and volume fractions are represented. The values are obtained from Rietveld refinements performed on powder X-ray diffraction data and compared to the theoretical values deduced from nominal compositions.

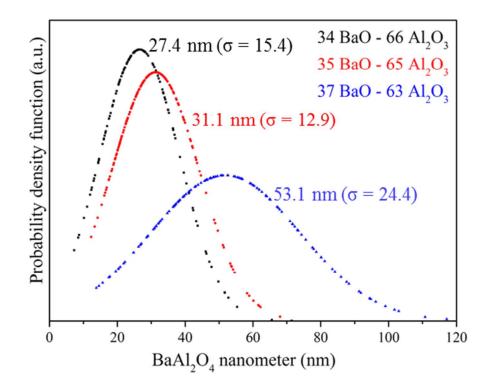


Figure SI3: Normal distribution of BaAl₂O₄ nanoparticles sizes, for the 34BaO-66Al₂O₃, 35BaO-65Al₂O₃, and 37BaO-63Al₂O₃ polycrystalline ceramic compositions. The diameters were determined from TEM patterns.

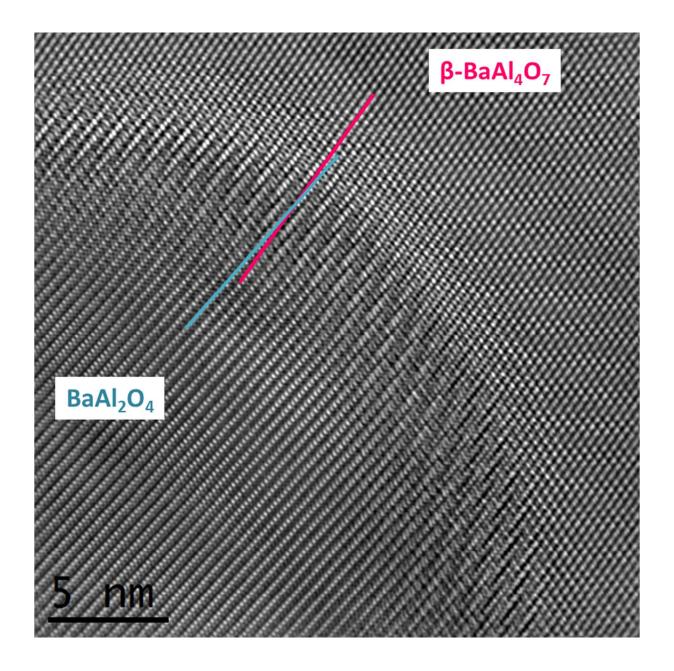


Figure SI4: Filtered HRTEM image of a $BaAl_2O_4$ nanoparticle into a $BaAl_4O_7$ grain, with a 6° misfit between the two crystallographic orientations.

$$n_x = -3.79 \times 10^{-12} \lambda^2 + 1.5866 + \frac{8934.6}{\lambda^2} + \frac{2.72 \times 10^8}{\lambda^4}$$
$$n_y = -2.97 \times 10^{-12} \lambda^2 + 1.5960 + \frac{8939.5}{\lambda^2} + \frac{2.46 \times 10^8}{\lambda^4}$$
$$n_z = -9.02 \times 10^{-12} \lambda^2 + 1.5871 + \frac{9090.2}{\lambda^2} + \frac{3.71 \times 10^8}{\lambda^4}.$$

Figure SI5: Expression of the refractive index components of β -BaAl₄O₇ along the three crystallographic orientations in the 500 – 4000 nm range. These values were obtained from DFT calculations.²⁸

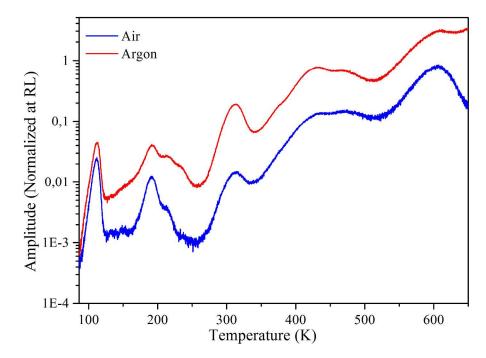


Figure SI6: Comparison of TSL from 90 to 670 K for the 34BaAl-66Al₂O₃ sample grown in air and in argon.