

Supplementary information for the paper entitled: „ **Extraordinary optical absorption in Y₃Al₅O₁₂:Eu ceramics and the role of stable Eu²⁺ in the energy transfer processes**“

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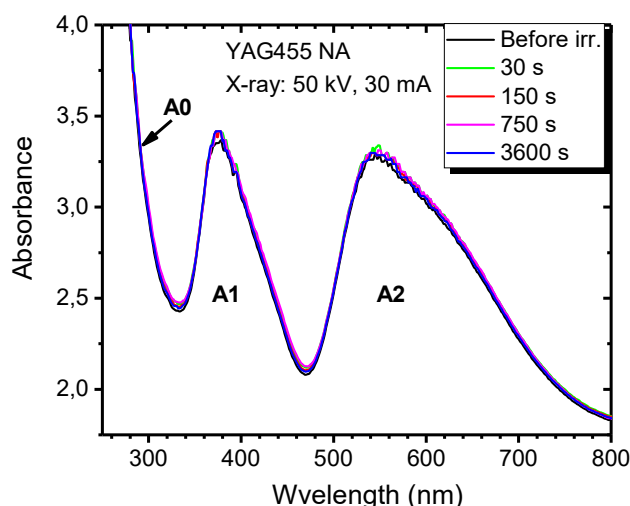


Fig. S1. RT absorption spectra of YAG455 NA treated under different irradiation conditions, see the text. The two bands, A1 and A2 are clearly visible, whereas the A0 one is strongly overlapped with the absorption edge.

Octahedral and tetrahedral Fe³⁺ EPR spectra were simulated by using the following spin-Hamiltonians

$$\hat{H} = \beta_e g \mathbf{H} \hat{S} + \frac{D}{3} O_2^0 + B_4^0 O_4^0 + B_4^4 O_4^4 + B_4^{-4} O_4^{-4}, \text{ tetrahedral, } B_4^0 = \frac{a + \frac{2}{3}F}{120}, B_4^{\pm 4} = \pm \frac{a}{24} \cos(\sin) 4\beta, \quad (\text{S1})$$
$$\hat{H} = \beta_e g \mathbf{H} \hat{S} + \frac{D}{3} O_2^0 + B_4^0 O_4^0 + B_4^3 O_4^3 + B_4^{-3} O_4^{-3}, \text{ octahedral, } B_4^0 = \frac{F - a}{180}, B_4^{\pm 3} = \pm \frac{a\sqrt{2}}{9} \cos(\sin) 3\alpha,$$

the cosine function is used for “+” whereas the sine for “-”.

where β_e is the Bohr magneton, \hat{S} is an electron spin operator of the $S = 5/2$ spin, D , B_k^q , and O_k^q are zero field splitting (ZFS) parameters and Stevens operators, respectively [S1]. The ZFS parameters for

the spectra simulation (Fig. 13II in the main article text) were calculated from the a and F ZFS parameters and angles $\alpha = 27.5^\circ$, $\beta = 16^\circ$, reported in [S2], corresponding to the rotation of the Al tetrahedron, and octahedron around [111], and [001] directions, respectively.

The following spin-Hamiltonian has been used for the Cr^{3+} EPR powder spectrum usual for YAG lattice [S3] and two a bit different (perturbed), Cr_1^{3+} and Cr_2^{3+} , EPR powder spectra simulation (the parameters are listed in Table 2 in the main article text).

$$\hat{H} = \beta_e g \mathbf{H} \hat{\mathbf{S}} + \frac{D}{3} O_2^0. \quad (\text{S2})$$

The following spin-Hamiltonian was used to simulate the Gd^{3+} powder EPR spectrum:

$$\hat{H} = \beta_e g \mathbf{H} \hat{\mathbf{S}} + b_2^0 O_2^0 + b_2^2 O_2^2 + b_4^0 O_4^0 + b_4^4 O_4^4 + b_6^0 O_6^0 + b_6^4 O_6^4, \quad (\text{S3})$$

$\hat{\mathbf{S}}$ is an electron spin operator with $S = 7/2$ eigenvalue, b_k^q are the ZFS parameters directly proportional to the B_k^q in Eq. 1 [S1]. Spin-Hamiltonian parameters were taken from [S4].

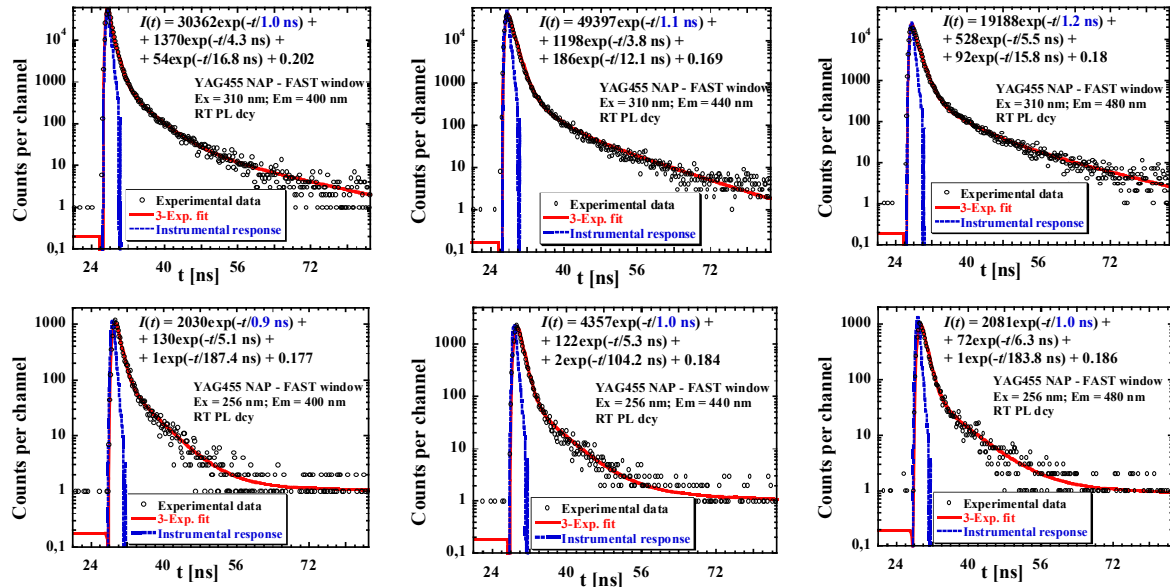


Fig. S2. Decay curves measured in the powdered YAG455 NA sample (YAG455 NAP) for three emission maxima: 400, 440 and 480 nm. Three upper graphs correspond to the 310 nm excitation wavelength whereas the lower three to the 256 nm.

References

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