Supplementary Information: Localization effect for doping

and collaborative diffusion in Er³⁺:YAG melt

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In this supplement materials, the radial distribution functions (RDF) between different atomic pairs, Al–O, Y–O, Al–Al, Y–Y, Al–Y, Al–Er, and Y–Er, in different doping concentration systems at temperature for 2000 and 2600 K have been shown, as well as the relationship between the average mean square displacement (MSD) and time for all ions in systems with doping concentrations of 3% and 5%. These are important supports for the conclusions in the main text.



Fig. S1 The RDF for the Al–O (a) and Y–O (b) pairs in YAG melt (2000 K) with different concentration (at.%) of Er^{3+} .



Fig. S2 The RDF for the Al–O (a) and Y–O (b) pairs in YAG melt (2600 K) with different concentration (at.%) of Er^{3+} .



Fig. 3S RDF between Al–Al, Y–Y and Al–Y ionic pair in the YAG (2000 K) with 0, 3, 6, 9, 12, 15, 20, 30, 40 and 50 at.% Er.



Fig. 4S RDF between Al–Al, Y–Y and Al–Y ionic pair in the YAG (2600 K) with 0, 3, 6, 9, 12, 15, 20, 30, 40 and 50 at.% Er.



Fig. S5 RDF between Al-Y and Al-Er cation pairs in the melt (2000 K) with 3, 6, 9, 12, 15,

20, 30, 40, and 50 at.% doping concentration.



Fig. S6 RDF between Al–Y and Al–Er cation pairs in the melt (2600 K) with 3, 6, 9, 12, 15, 20, 30, 40, and 50 at.% doping concentration.



Fig. S7 RDF between Y–Y and Y–Er cation pairs in the melt (2000 K) with 3, 6, 9, 12, 15, 20, 30, 40, and 50 at.% doping concentration.



Fig. S8 RDF between Y–Y and Y–Er cation pairs in the melt (2600 K) with 3, 6, 9, 12, 15, 20, 30, 40, and 50 at.% doping concentration.



Fig. S9 RDF between Y–O and Er–O cation pairs in the melt (2000 K) with 3, 6, 9, 12, 15, 20, 30, 40, and 50 at.% doping concentration.



Fig. S10 RDF between Y–O and Er–O cation pairs in the melt (2600 K) with 3, 6, 9, 12, 15, 20, 30, 40, and 50 at.% doping concentration.



Fig. S11 (a), (b) and (c) represent the detailed first peak of ErO and YO RDF in systems with 3, 20 and 50 at. % doping concentration respectively. (d) show the relationship between coordination number for Y^{3+} and Er^{3+} and temperature at these three doping concentrations.



Fig. S12 Function of mean square displacement with time for O^{2-} , Al^{3+} , Y^{3+} , and Er^{3+} , which include three different dynamic stages in Er:YAG (3 at.%) melt at different temperature.



Fig. S13 Function of mean square displacement with time for O^{2-} , Al^{3+} , Y^{3+} , and Er^{3+} , which include three different dynamic stages in Er:YAG (15 at.%) melt at different temperature.