Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Predicting Plasma Conditions Necessary for Crystallization of γ-Al_2O_3 Nanocrystals

A.J. Cendejas[†], He Sun[‡,§], Sophia E. Hayes[‡,§], Uwe Kortshagen[‖], Elijah Thimsen[†,§*]

[†] Department of Energy, Environmental and Chemical Engineering, Washington University in Saint Louis, Saint Louis, Missouri

[‡] Department of Chemistry, Washington University in Saint Louis, Saint Louis, Missouri

[§] Institute of Materials Science and Engineering, Washington University in Saint Louis, Saint Louis, Missouri

[‖] Department of Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota

*Author to whom correspondence should be addressed: elijah.thimsen@wustl.edu

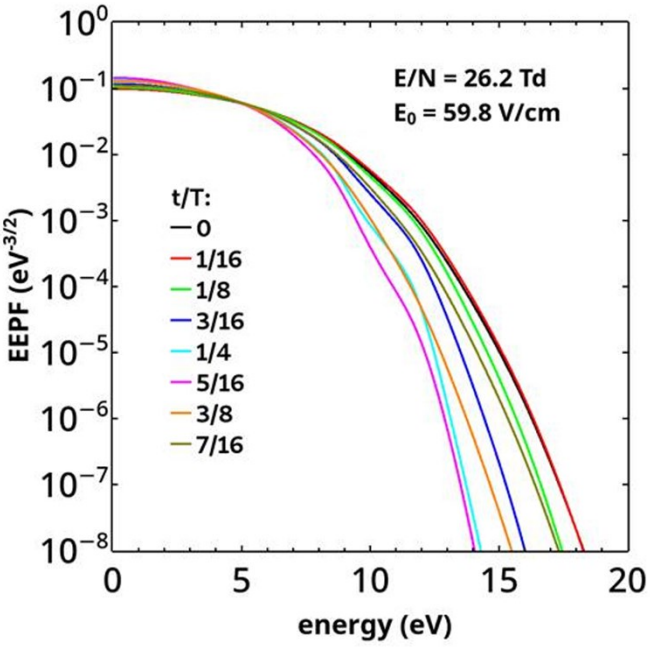

FIG. S1. Time dependent electron energy distribution function at different stages throughout the RF period.

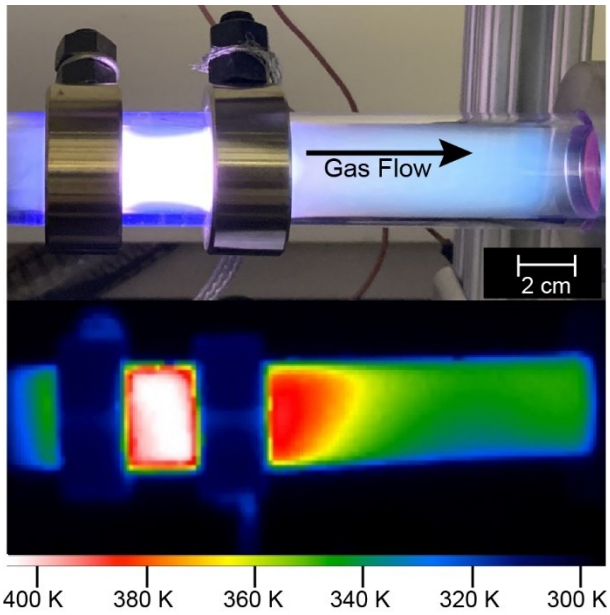

FIG. S2. Digital image and IR thermal image of Al_2O_3 synthesis reactor during operation at 100 W. Background gas temperatures at each power were estimated at the position between the two electrodes.

Solid State NMR – Czjzek Model Fitting

The experimental NMR data were processed by the GSim program using the Baseline Corrector application[1] to generate the frequency domain spectra. Preliminary fitting of the ^{27}Al line shapes corresponding to the central transitions were fit from the 1-dimensional spectra using Dmfit[2] using the CzjzekSimple model. The contributions to the central transition intensity from satellite transitions were included by fitting the spinning sidebands (of those satellite transitions) underlying the central transitions. In Figure S3, the 100 W Al_2O_3 nanocrystal sample deconvolution is shown. The model extracts both the isotropic chemical shift (δ_{iso}) and quadrupolar coupling constant (C_Q) values for 4-, 5- and 6-coordinate aluminum sites. The values are shown in Table S1 below.

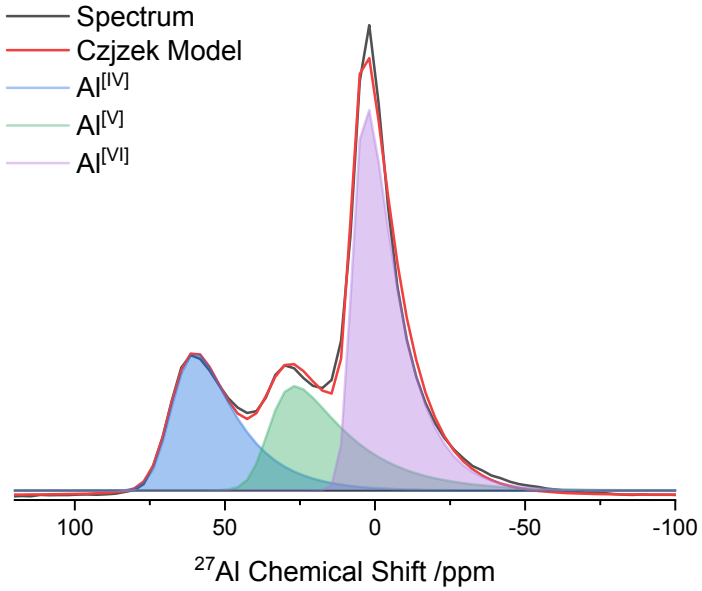

FIG. S3. ^{27}Al SSNMR (with MAS) spectrum for Al_2O_3 nanocrystals synthesized at 100 W, deconvoluted into separate resonances using DMfit. The Czjzek peak fitting for the 4- (blue), 5- (green), and 6-coordinate (purple) aluminum sites is shown. The small resonances with very low intensity are spinning sidebands from the satellite transitions.

TABLE S1. Parameters extracted from the preliminary Czjzek fitting of the ^{27}Al resonances for the "100 W" synthesized sample of Al_2O_3 nanoclusters. (Note: the isotropic resonance values, δ_{iso}, extracted for the Czjzek-broadened lineshapes differ from the appearance of the most intense peaks in the 1-dimensional spectrum.)

	$^{[4]}Al$	$^{[5]}Al$	$^{[6]}Al$
δ_{iso}	67.3 ppm	32.3 ppm	8.8 ppm
C_Q	6.9 MHz	5.4 MHz	6.5 MHz

References

(1) Yon, M.; Fayon, F.; Massiot, D.; Sarou-Kanian, V. Iterative Baseline Correction Algorithm for Dead Time Truncated One-Dimensional Solid-State MAS NMR Spectra. *Solid State Nuclear Magnetic Resonance* **2020**, *110*, 101699.

(2) Massiot, D.; Fayon, F.; Capron, M.; King, I.; Calvé, S. L.; Alonso, B.; Durand, J.-O.; Bujoli, B.; Gan, Z.; Hoatson, G. Modelling One- and Two-Dimensional Solid-State NMR Spectra. *Magnetic Resonance in Chemistry* **2002**, *40* (1), 70–76.