Supporting Information for the article titled:

Size Resolved High Temperature Oxidation Kinetics of Nano-Sized Titanium and Zirconium Particles

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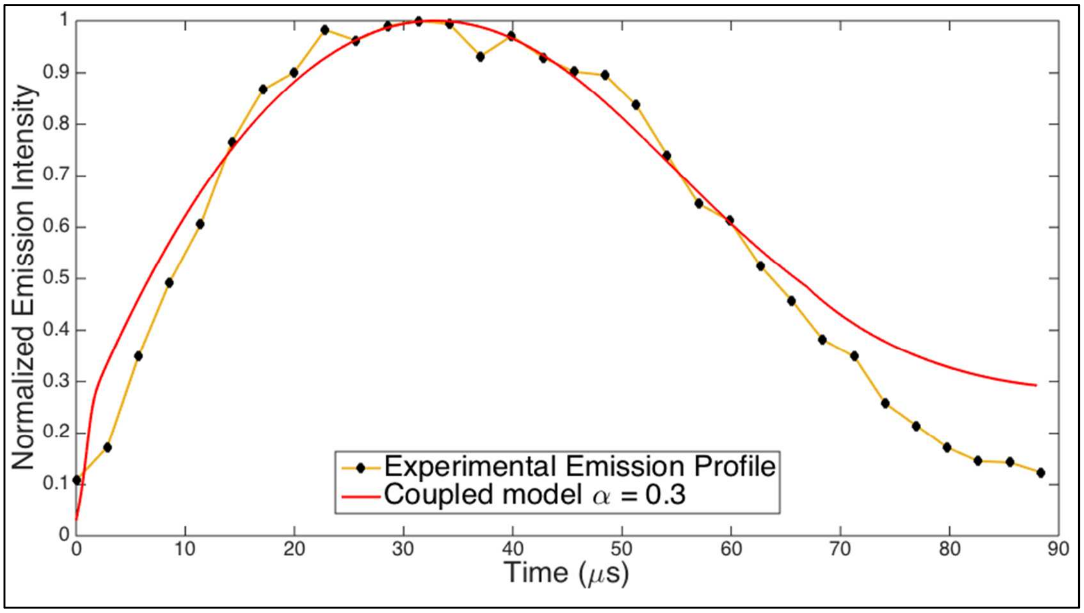

Figure S1. *Observed emission profile vs. simulated emission profile for the coupled model fit for 90 nm particle using α = 0.3.*

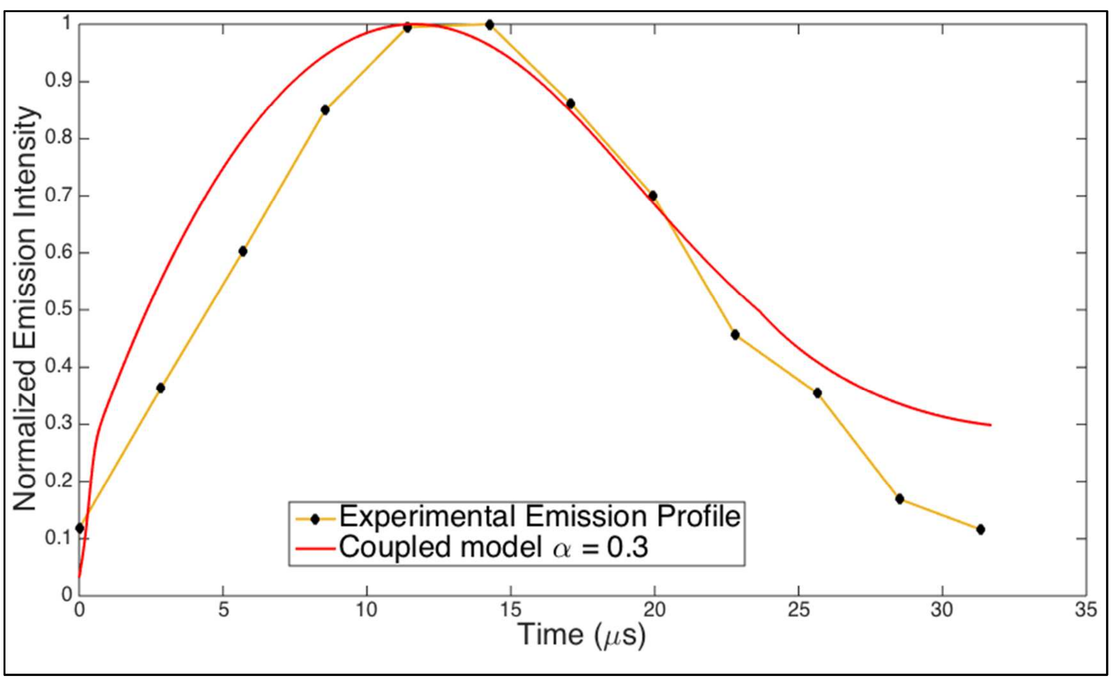

Figure S2. *Observed emission profile vs. simulated emission profile for the coupled model fit for 28 nm particle using α = 0.3.*

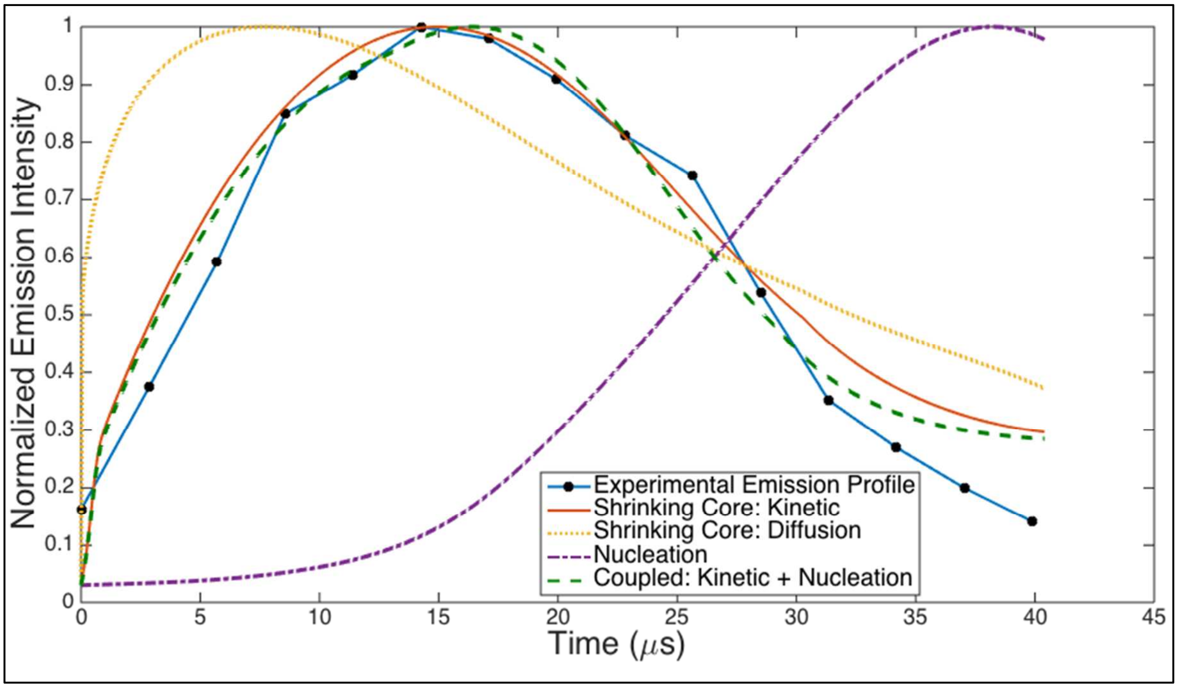

Figure S3. *Comparison of different models using α = 0.3 with the experimental emission profile for a 40 nm particle.*

Variable Definitions for Model:

X_{Ti} : Volume fraction of Titanium/ Zirconium core left

$R_{K,D,N}$: Reaction rate for Kinetic limited, Diffusion limited and Nucleation models [s^{-1}]

τ : Burn time [s]

T : Particle Temperature [K]

P_{STiO2}: Saturation Vapor pressure of Titania [N/m^2]

P_{SZrO2}: Saturation Vapor pressure of Zirconia [N/m^2]

α: Thermal accommodation Coefficient

d_p: Particle diameter

m_g: Air molecular weight ($4.8*10^{-26}$ Kg)

K: Boltzmann Constant ($1.38*10^{-23}$ m^2 Kg s^{-2} K^{-1})

P_g: Gas Pressure (1 atm)

γ: Adiabatic expansion factor (=1.3 at 1500 K)

T_g: Gas Temperature (1750 K)

σ: Stefan Boltzman constant ($5.67*10^{-8}$ W/m^2K^4)

a_p: Surface area of particle (m^2)

N_{av}: Avogadro's constant

Equations used in the Model:

Kinetic Shrinking Core:

$$\frac{dR_K}{dt} = \frac{(-3) * {X_{Ti}}^{2/3}}{\tau}$$

Diffusion Shrinking Core:

$$\frac{dR_D}{dt} = \frac{1}{2\tau(1 - {X_{Ti}}^{-\frac{1}{3}})}$$

Nucleation/ Avrami-Erofeev (A4):

$$\frac{dR_N}{dt} = \frac{(-4) * X_{Ti} * (-\log(X_{Ti}))^{0.75}}{\tau}$$

Saturation Vapor Pressure for TiO_2:

$$log_{10}P_{STiO2} = 16.2 - {}^{30361}/_{T} - 0.000492 * T$$

Saturation Vapor Pressure for ZrO_2:

$$log_{10}P_{SZrO2} = 3 * 10^{-9} * T^3 - 3 * 10^{-5} * T^2 + 0.074 * T - 74.126$$

Conduction Heat Transfer:

$$Q_C = \alpha * \pi * \left[\frac{d_p}{2}\right]^2 * \frac{P_g}{2} * \left[\frac{8KT}{\pi m_g}\right]^{0.5} * \frac{(\gamma + 1)}{(\gamma - 1)} * \frac{(T - T_g)}{T_g}$$

Radiation Heat Transfer:

$$Q_R = \varepsilon_{avg} * \sigma * \pi {d_p}^2 * (T^4 - {T_g}^4)$$

Evaporative Heat Transfer:

$$Q_V = \frac{1 * P_S a_p}{\sqrt{2 \pi KT_p}} * \frac{\Delta H_{volalization}}{N_{av}}$$

Heat generation:

$$H_{gen} = \frac{dTi_{moles}}{dt} * \Delta H_{rxn}$$

Heat transfer equation:

$$C\Delta T = H_{gen} - \Delta t * \{Q_C + Q_R + Q_V\}$$