Controlling Chaos: Quantifying the Impact of Force on Chemical Reactivity in Mechanochemical Syntheses

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Theoretical Framework for Second Order reaction

We extend the closed form solution shown in equation 12 to estimate the total change in reactant concentration for a second order reaction,

$$\Delta N_{eff} = \left(\frac{\rho_o^2 k_{eff} t}{1 + \rho_o k_{eff} t} \right) DF_{set}^{2/3} \tag{1}$$

$$D = \rho_o \pi h \left(\frac{3R}{4E^*} \right)^{2/3} \tag{2}$$

As stated in the main text, the total change in reactant concentration is a function of impact force, impact time and area concertation. By using equation 1 to write the rate of change of N over number of impacts τ.

$$\frac{dN}{d\tau} = \frac{N}{N_o} \left(\frac{\rho_o^2 k_{eff} t}{1 + \rho_o k_{eff} t} \right) DF^{2/3} \tag{3}$$

By applying separation of variables and rearranging results in equation 4 for a second order reaction.

$$\frac{N}{N_o} = e^{\frac{1}{N_o} \left(\frac{\rho_o^2 k_{eff} t}{1 + \rho_o k_{eff} t} \right) DF^{2/3} \tau} \tag{4}$$
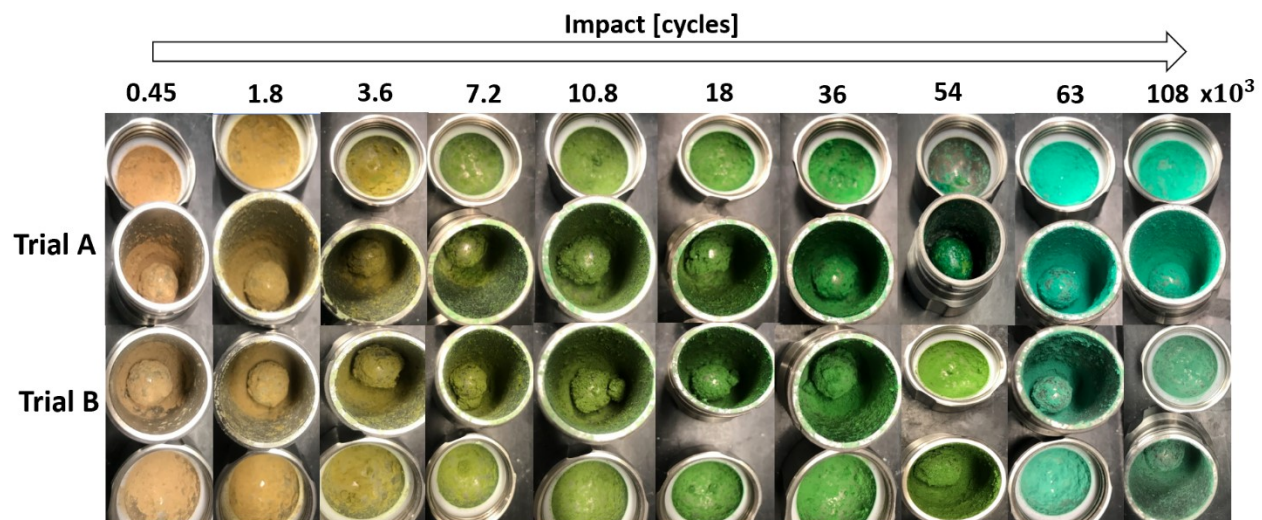
Figures

Figure S1: *Reaction of Copper (II) chloride anhydrous and 1, 10 Phenanthroline with color intensity measured at different impact cycles using the Retsch MM400 Ball Mill. 2 Trials performed at 30 Hz.*
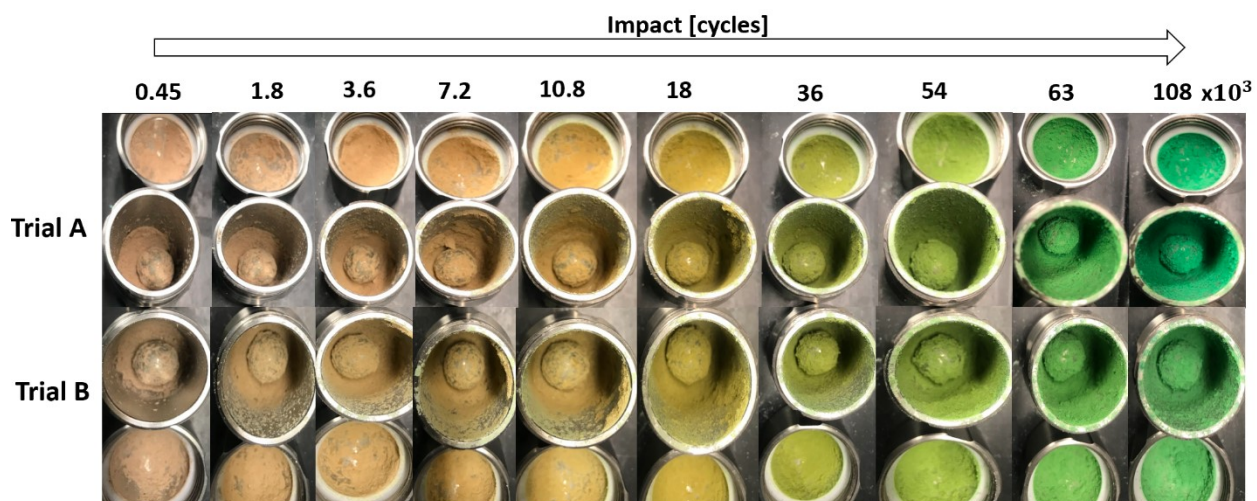

Figure S2: *Reaction of Copper (II) chloride anhydrous and 1, 10 Phenanthroline with color intensity measured at different impact cycles using the Retsch MM400 Ball Mill. 2 Trials performed at 15 Hz.*
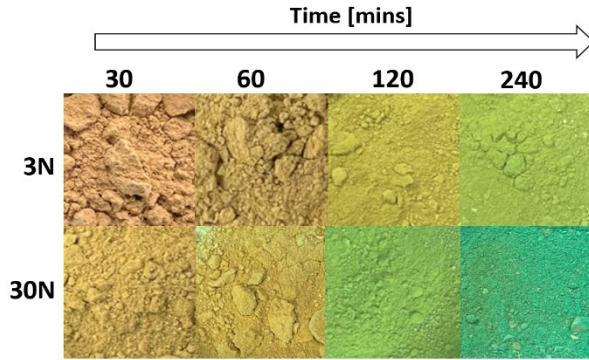
Figure S3: *Reaction of Copper (II) chloride anhydrous and 1, 10 Phenanthroline with color intensity measured at different actual impact time using the Controlled Force Reactor (CFR). Reactions was done for both 3N and 30N.*
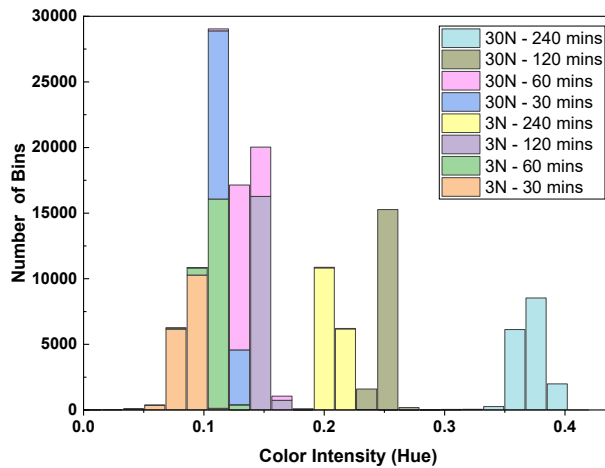

Figure 4: *Histogram of color intensity from the reaction of Copper (II) chloride anhydrous and 1, 10 Phenanthroline using the CFR for reactions at 3N and 30N.*