A multiscale stochastic approach for the nucleation, growth and coalescence process

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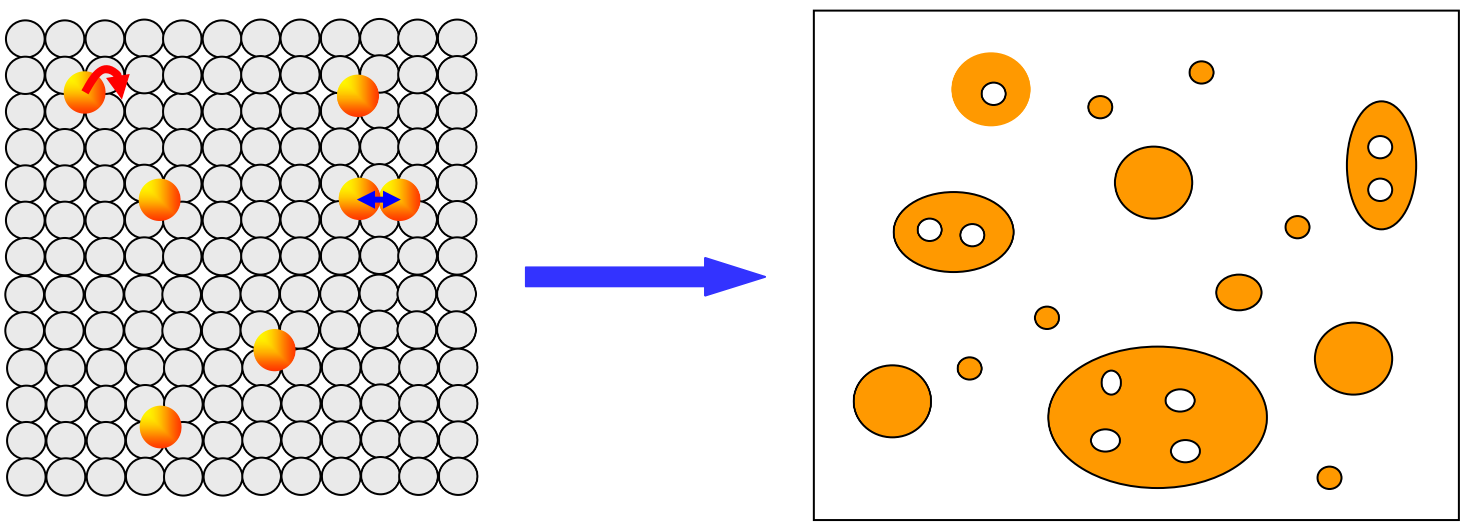
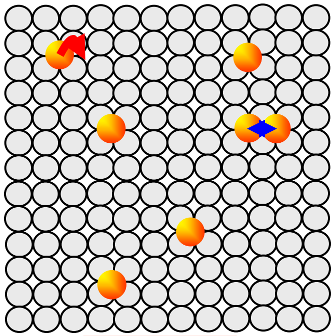
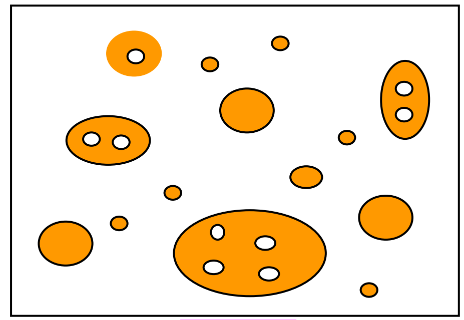


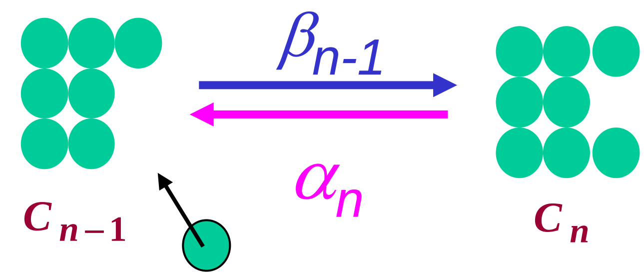
Monte Carlo Kinetics / Cluster Dynamics



KMC



CD



$$\frac{dC_n}{dt} = \beta_{n-1}C_{n-1} - (\alpha_n + \beta_n)C_n + \alpha_{n+1}C_{n+1}$$

monomers are the only diffusing species

kinetic controlled by diffusion

$$\beta_n = m_n C_1 / C_1^{eq} \approx m_n\left(1 + \frac{2\tilde{\sigma}}{\sqrt{n^*}}\right)$$

$$\alpha_n \approx m_n\left(1 + \frac{2\tilde{\sigma}}{\sqrt{n}}\right)$$

$$m_n = f\left(D, n, d, C_1^{eq}\right)$$

$$\tilde{\sigma} = \sigma / kT$$

critical size ≡ driving force

Model of nucleation-growth-coarsening (MNGC)

$$v_n = \frac{dn}{dt} = \beta_n - \alpha_n \approx m_n \tilde{\sigma}\left(\frac{2}{\sqrt{n^*}} - \frac{2}{\sqrt{n}}\right)$$

Ensures the coherence between CD and MNGC

CNT $\begin{cases} n^*(t) \\ n(t) \\ J(t) \end{cases}$

$n(t+\Delta t)$

$$\theta_{PP}(t+\Delta T) = \sum_{n \in PP} nC_n(t+\Delta T)$$

PP : Precipitate Phase

Iterative loop

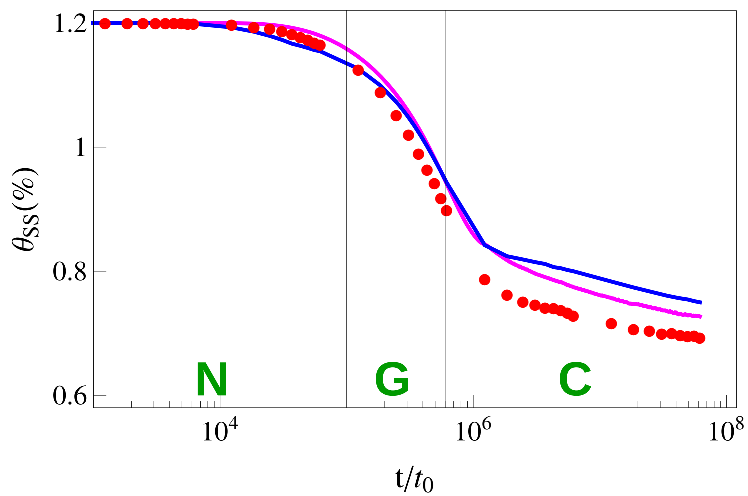
$$\theta_{SS}(t+\Delta t) = \theta - \theta_{PP}(t+\Delta T)$$

SS : Solid Solution

$$n^*(t+\Delta t) \Big| \sum_{n<n^*} nC_n^{eq} \, exp\left(\frac{2n\sigma}{kT\sqrt{n^*}}\right) = \theta_{SS}$$

constrained equilibrium

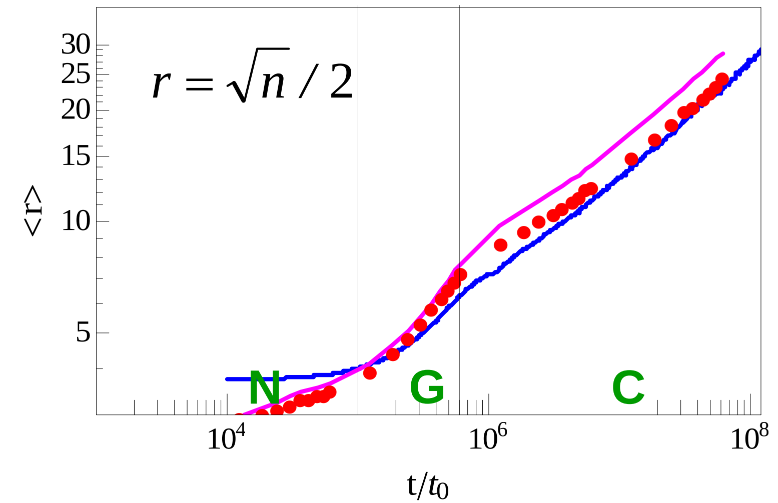
KMC / CD / MNGC / LSW

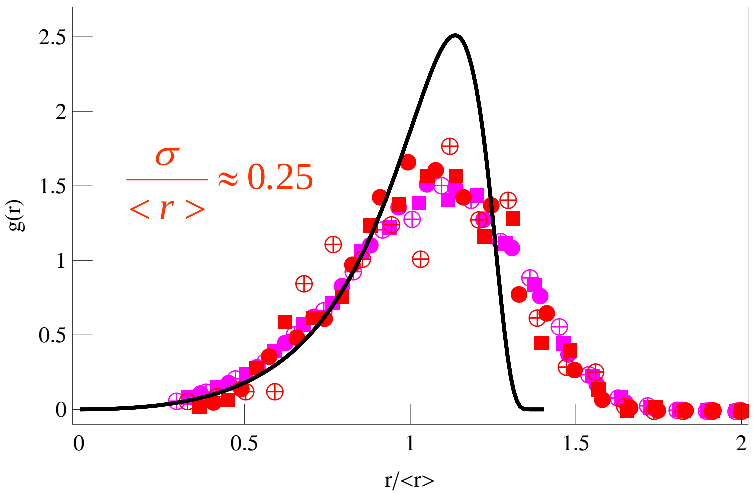


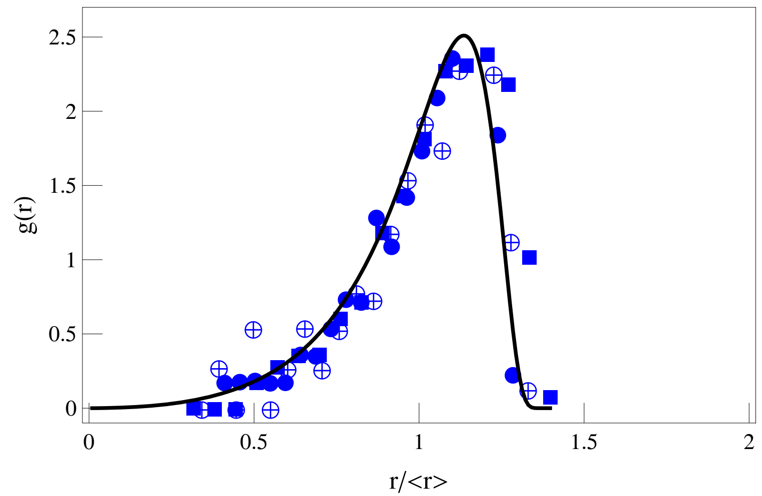
Ag / Cu (100)

$$\theta = 0.012$$

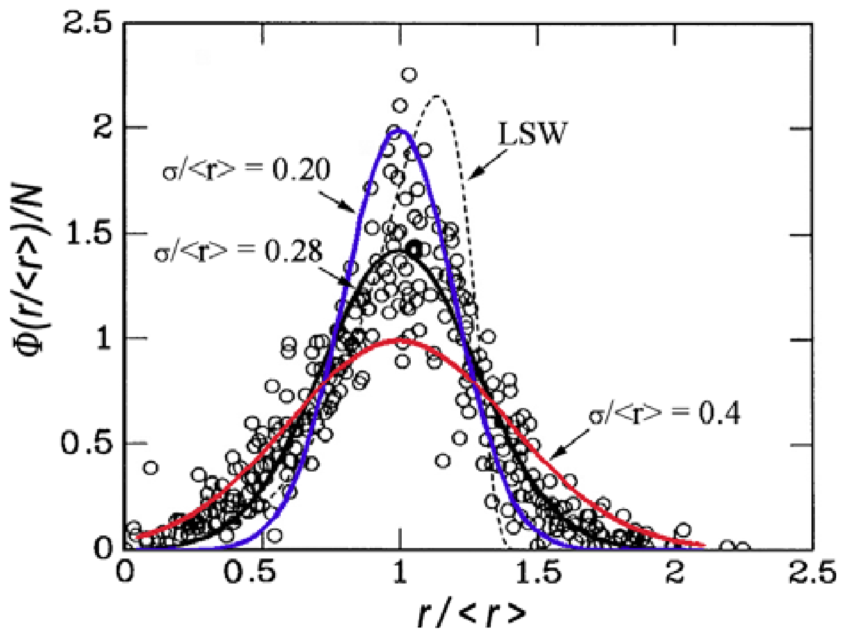
$$T / T_c = 0.66$$







KMC / CD / MNGC / LSW



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KMC

$$\Gamma_{i\to f} = \nu \exp\left(-\frac{Q}{kT}\right)\exp\left(-\frac{E_f - E_i}{2kT}\right)$$

CD

$$\frac{dC_n}{dt} = \beta_{n-1}C_{n-1} - (\alpha_n + \beta_n)C_n + \alpha_{n+1}C_{n+1}$$

LSW

$$v_r = \frac{K}{r}\left(\frac{1}{r^*} - \frac{1}{r}\right)$$

$$< r > \propto t^{1/3}$$

MNGC

$$v_r = \frac{K}{r}\left(\frac{1}{r^*} - \frac{1}{r}\right)$$

$$K = m\tilde{\sigma}/8$$

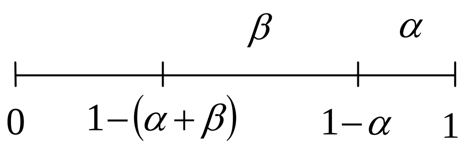
$$v_r = \frac{dr}{dt} = \frac{K}{r^2}\left(\frac{r}{r^*} - 1\right) + g(r,t)\varepsilon$$

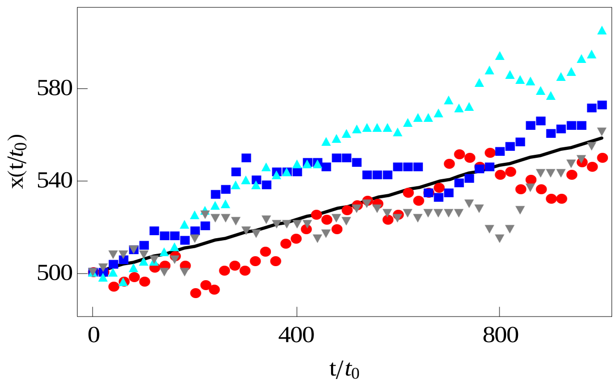
????

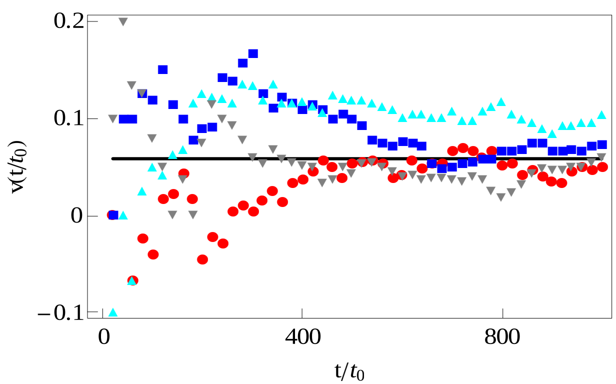
Diffusion

KMC

$$x(t)=(\beta-\alpha)\times t+x_0$$

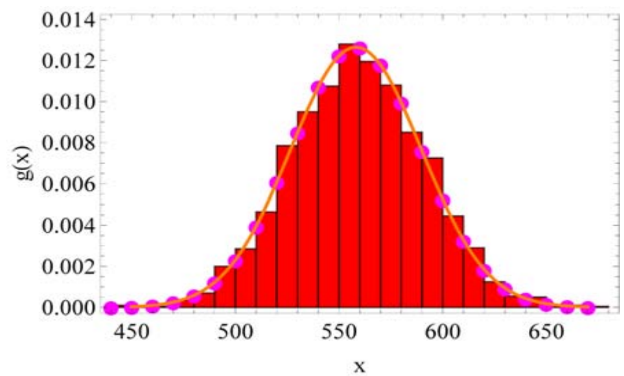






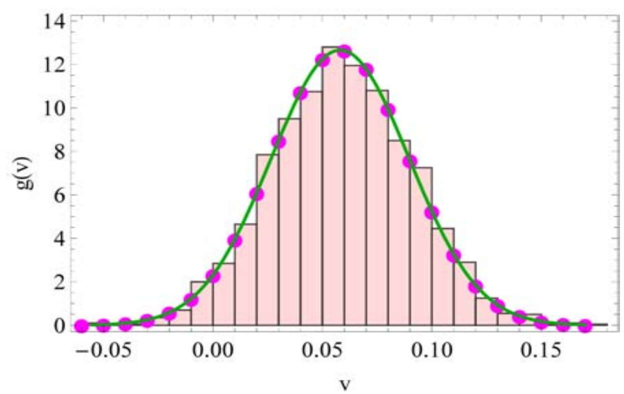
CD

$$\frac{dx_i(t)}{dt}=\beta\times x_{i-1}(t)-(\alpha+\beta)\times x_i(t)+\alpha\times x_{i+1}(t)$$



$$<x(t)>=(\beta-\alpha)t+x_0$$

$$\sigma_t^2\approx(\beta+\alpha)t$$



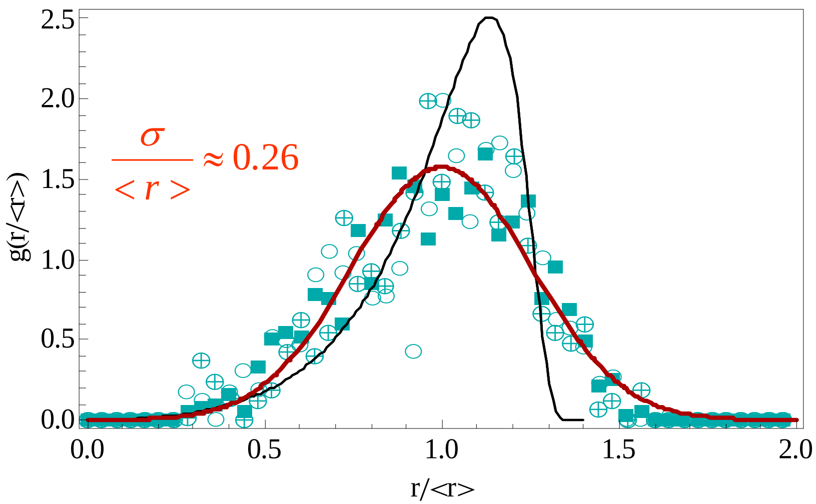
$$<v(t)>=\beta-\alpha$$

$$\sigma_{v(t)}^2\approx\frac{\beta+\alpha}{t}$$

$$v(t)=(\beta-\alpha)+\sqrt{\frac{\beta+\alpha}{t}}\varepsilon$$

Stochastic MNGC / LSW / CD

$$v_n \approx m\,\tilde{\sigma}\left(\frac{2}{\sqrt{n^*}} - \frac{2}{\sqrt{n}}\right) + \sqrt{\frac{2m}{t}}\,\varepsilon$$



SPDE

$$v_r = \frac{K}{r^2}\left(\frac{r}{r^*} - 1\right) + \frac{1}{8r}\sqrt{\frac{2m}{t}}\,\varepsilon$$

Stratonovich

Fokker- Planck Equation

$$\frac{df(r,t)}{dt} = \frac{K}{r^2}\left\{\frac{f''}{8\tilde{\sigma}} - \left[\left(\frac{r}{r^*} - 1\right) + \frac{3}{8\tilde{\sigma}r}\right] f' + \left[\left(\frac{r}{r^*} - 1\right) - 1 + \frac{3}{8\tilde{\sigma}r}\right]\frac{f}{r}\right\}$$

CD

$$\begin{cases} C_{n+1} + C_{n-1} - 2C_n = \left.\dfrac{\partial^2 C_n}{\partial n^2}\right|_n \\ C_{n+1} - C_n = C_n - C_{n-1} + \left.\dfrac{\partial^2 C_n}{\partial n^2}\right|_n \end{cases}$$