Stochastic simulation of growth tessellation models based on limited microstructure data

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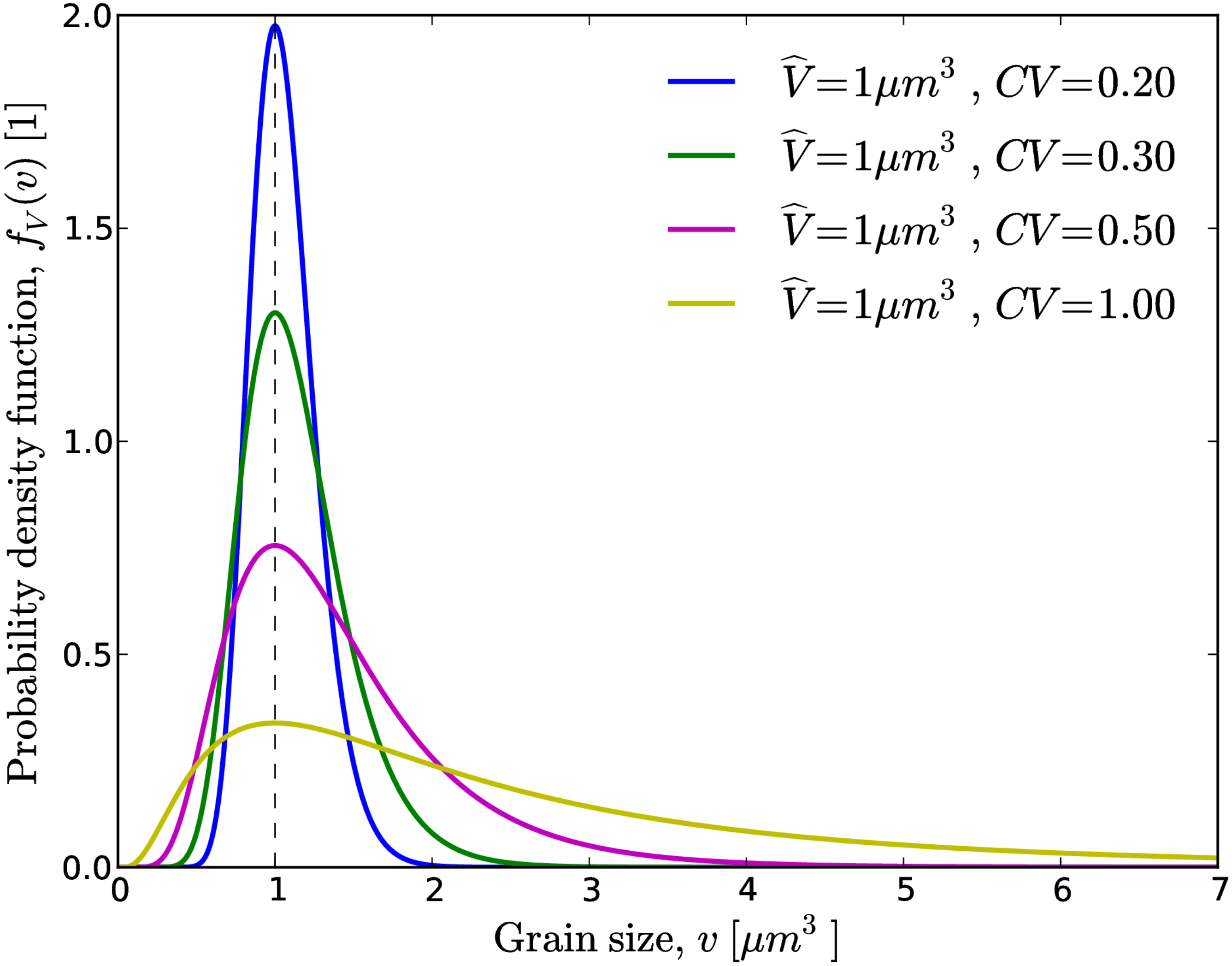
Simulation of **SGT** models
based on **grain size distributions**
with a **single mode**

Target distributions #1



Method #1: Poisson Process & Independent Simulation of Volume Equivalent Spherical Grain Radii

- A point pattern is simulated by a Poisson process with intensity λ obtained from the average of the grain size distribution, i.e. $\lambda = 1/\mathbb{E}[V]$.

- Let M be the random growth velocity independent of grain locations. Then, volume equivalent spherical grain radii are simulated after a marginal distribution obtained from the grain size distribution by assuming $V = 4\pi(M\Delta t)^3/3$ where Δt is the time required to fully grow the SGT model.

Simulation of unmarked point patterns

- Intensity: $\lambda = 1/\mathbb{E}[V]$
- Volume of the domain: $20 \times 20 \times 20 \ \mu m^3$
- Number of realizations: 3

$\widehat{\text{V}}$ $[\mu m^3]$	CV	λ $[\mu m^{-3}]$	Ngrain #1	Ngrain #2	Ngrain #3
1.0	0.20	0.9429	7638 (7632)	7509 (7506)	7576 (7575)
1.0	0.30	0.8787	6999 (6995)	7035 (7027)	7285 (7280)
1.0	0.50	0.7155	5673 (5647)	5748 (5734)	5628 (5598)
1.0	1.00	0.3536	2891(2847)	2829 (2773)	2906 (2856)

NB: The number of grains in parentheses are obtained after removal of "bad grains" from the SGT models computed with 100x100x100 voxels.

Simulation of volume equivalent spherical grain radii

- Relation between the volume and grain growth velocity, M:

$$V = 4\pi(M\Delta t)^3/3 \longrightarrow \mathrm{d}v = 4\pi(m\Delta t)^2 \mathrm{d}m\Delta t$$

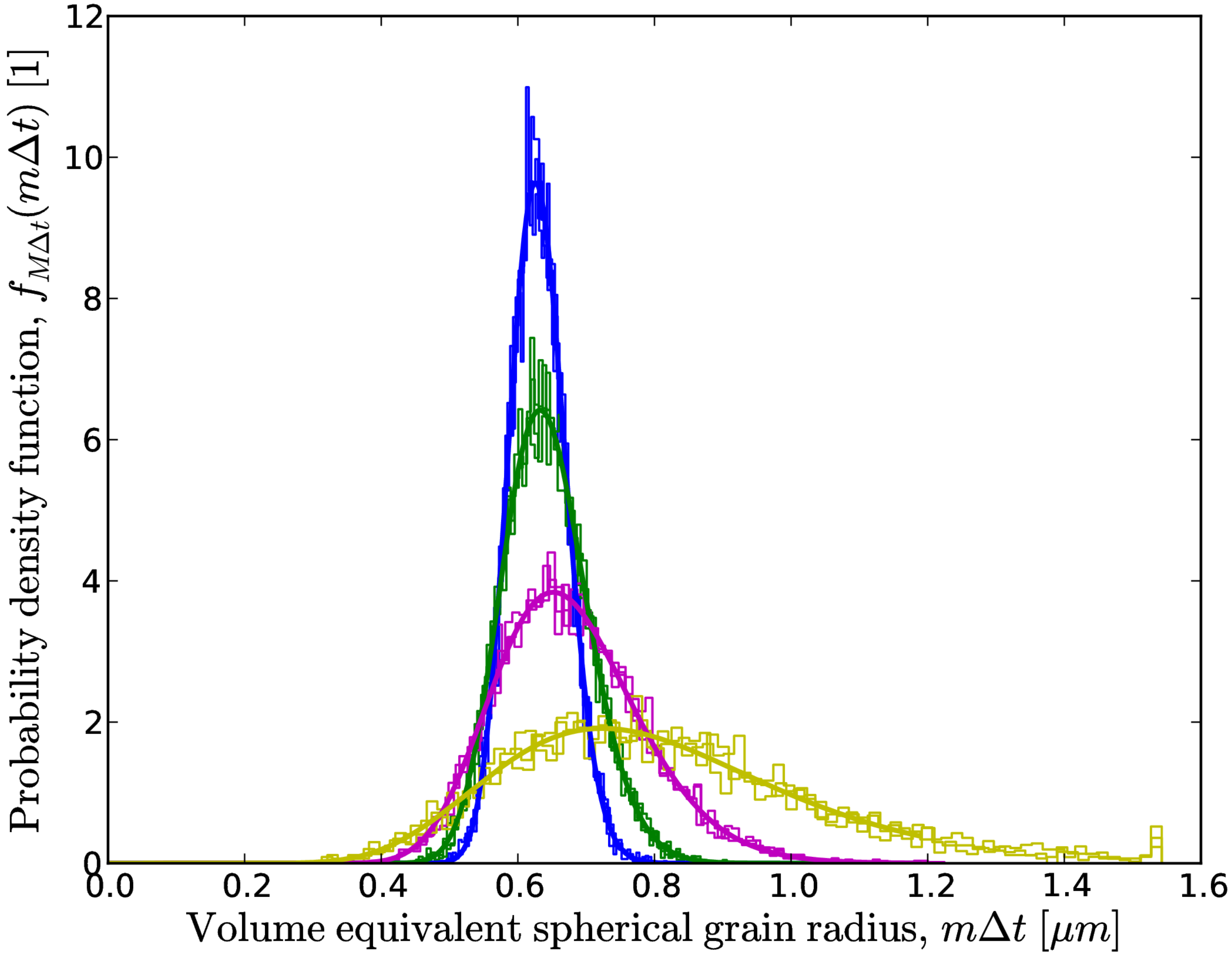
- Marginal distribution, $f_{M\Delta t}(m\Delta t)$

$$\int_{-\infty}^{\infty} f_V(v)\mathrm{d}v = \int_{-\infty}^{\infty} f_V(v(m\Delta t))4\pi(m\Delta t)^2 \mathrm{d}m\Delta t = \int_{-\infty}^{\infty} f_{M\Delta t}(m\Delta t)\mathrm{d}m\Delta t = 1$$

$$\downarrow$$

$$f_{M\Delta t}(m\Delta t) = 4\pi f_V(4\pi(m\Delta t)^3/3)$$

Simulation of the volume equivalent spherical grain radii

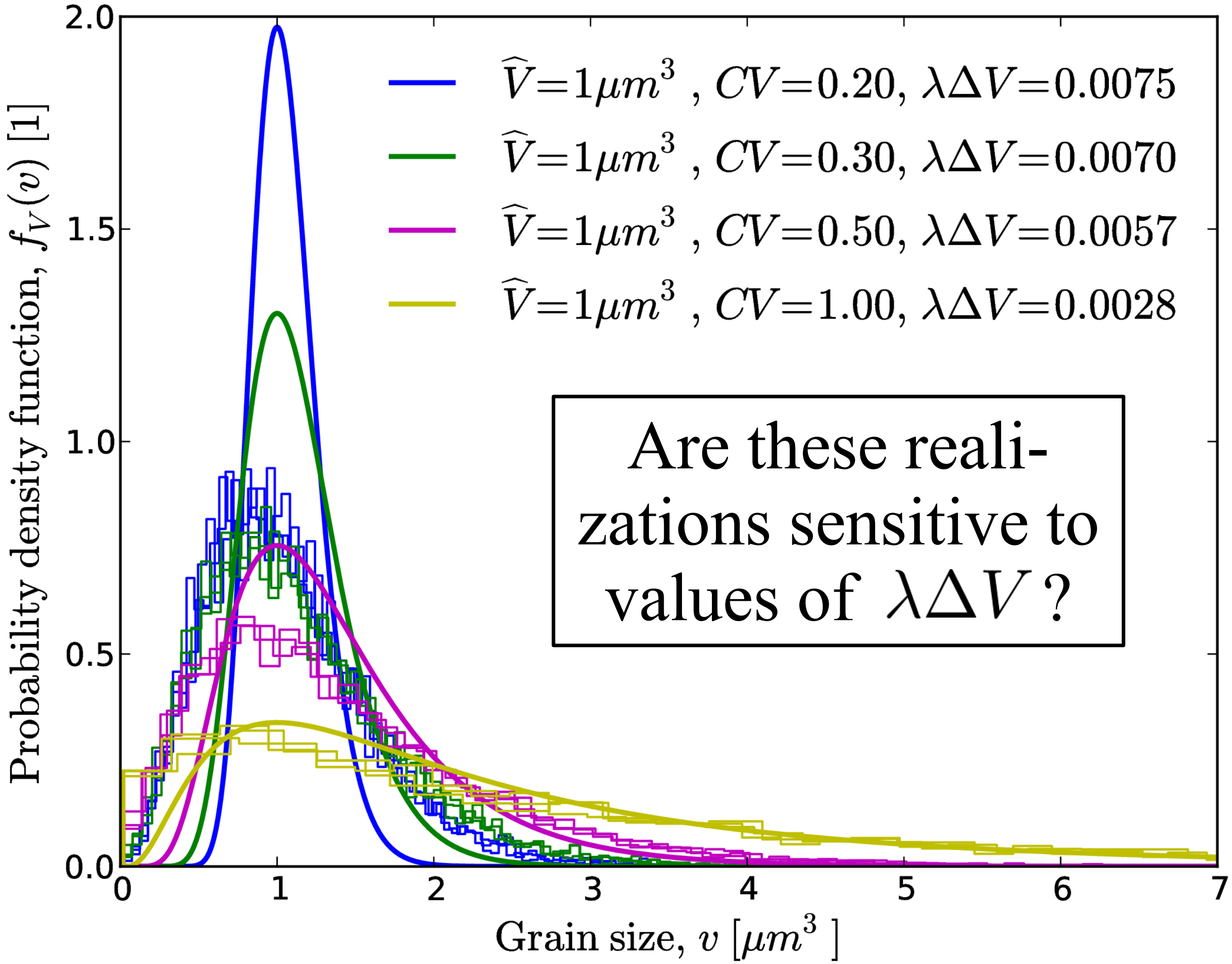


Grain size distribution of SGT models

- Size of the simulation domain: $8000\ \mu m^3$
- Voxel size, ΔV: $0.008\ \mu m^3$

- Tesselation rule: Every voxel belongs to the simply connected grain it is reached by the quickest. Grains embedded within other grains are removed and their voxels are attributed to the surrounding grain.

Grain size distributions of simulated SGT models



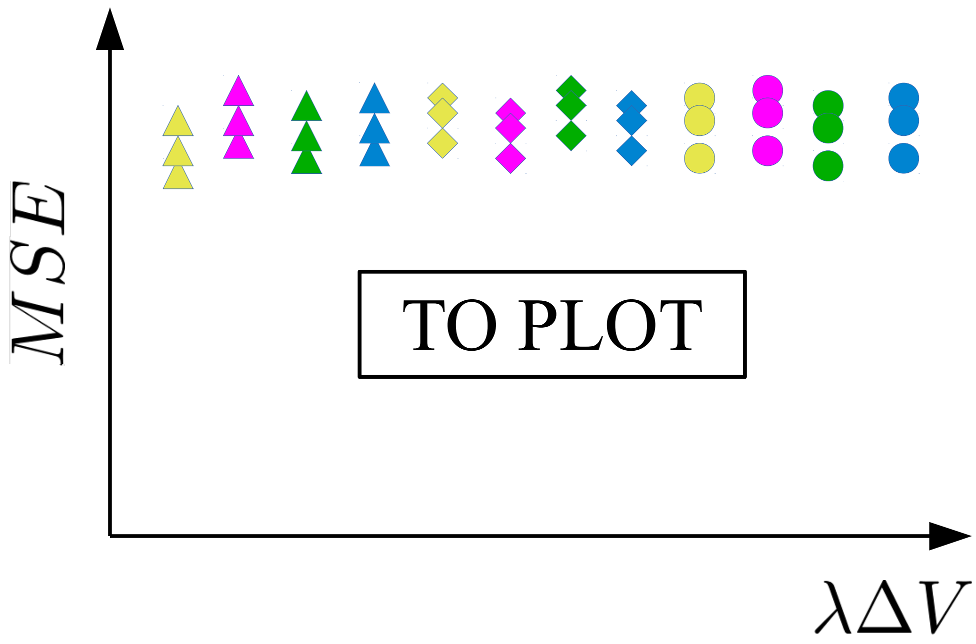
Different discretizations of the simulation domain

$\widehat{V}$ $[\mu m^3]$	CV	Number of voxels	ΔV $[\mu m^3]$	$\lambda \Delta V$ [1]
		100x100x100	0.0080	0.0075
1.0	0.20	150x150x150	0.0024	0.0023
		200x200x200	0.0010	0.0009
		100x100x100	0.0080	0.0070
1.0	0.30	150x150x150	0.0024	0.0021
		200x200x200	0.0010	0.0009
		100x100x100	0.0080	0.0057
1.0	0.50	150x150x150	0.0024	0.0017
		200x200x200	0.0010	0.0007
		100x100x100	0.0080	0.0028
1.0	0.50	150x150x150	0.0024	0.0008
		200x200x200	0.0010	0.0004

Effect of discretization of the domain

$$MSE = \left\{ \frac{1}{V_{max} - V_{min}} \int_{v=0}^{\infty} \left[f_V(v) - \hat{f}_V(v) \right]^2 \mathrm{d}v \right\}^{1/2}$$

where $\hat{f}_V(v)$ is the grain size distribution of the SGT model.

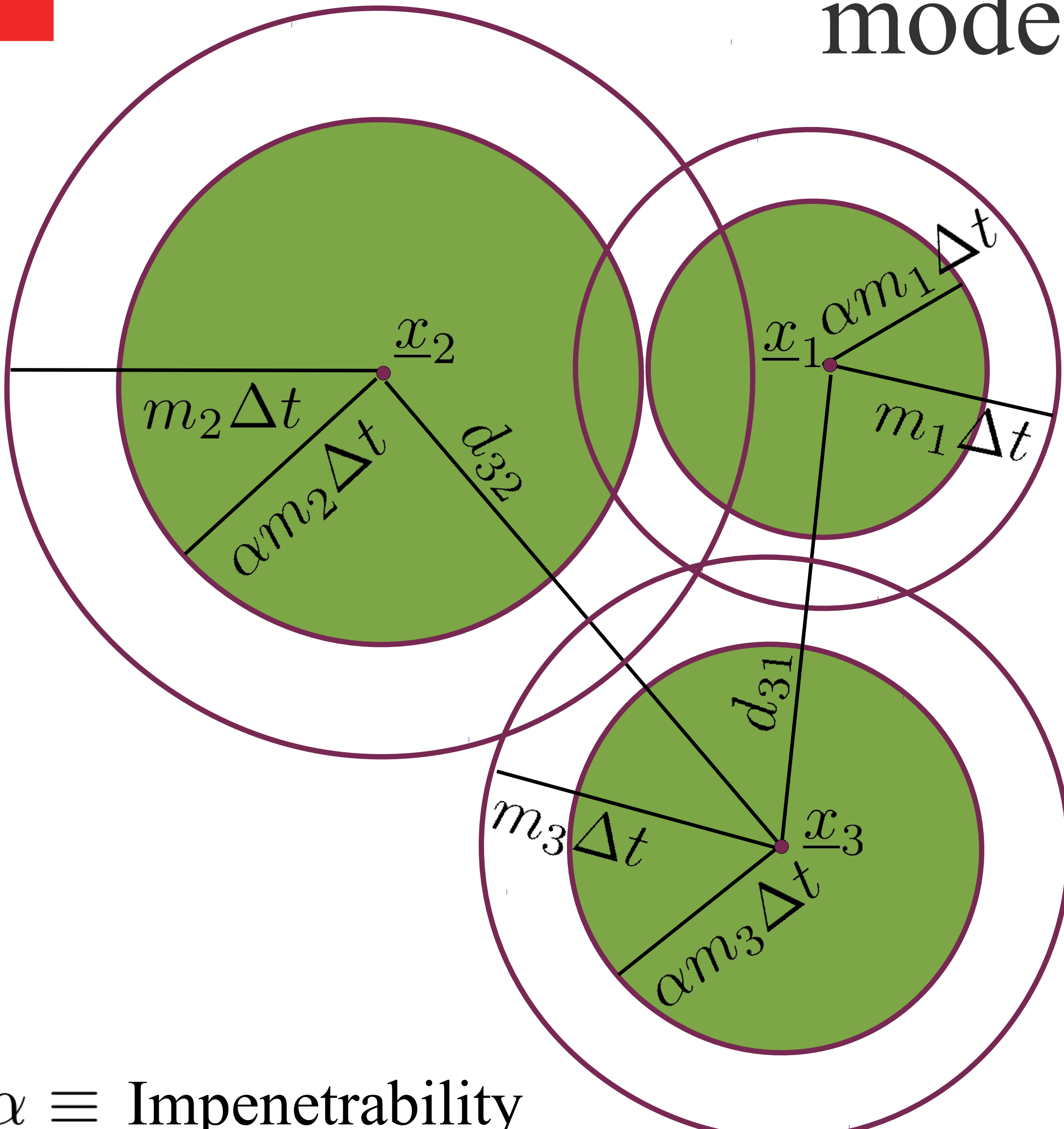


Observations

- The simulated grain size distributions have:
  - **Over-estimated variability**, especially for sharp distributions,
  - **Over-estimated fractions of small grains**.

- Remark: The number of small grains can be reduced by resorting to a hard-core process.

Method #2: Concentric shell packing model

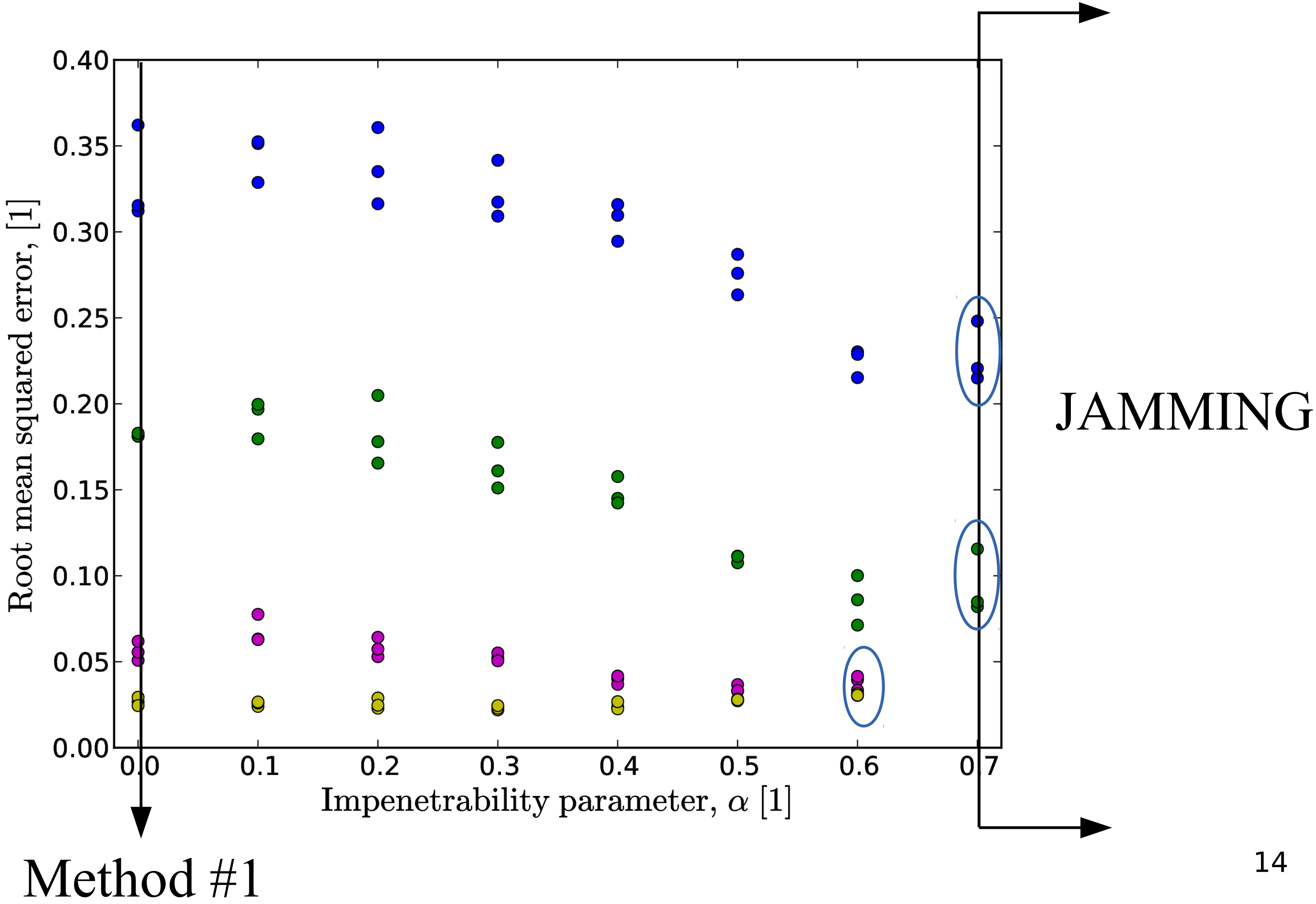


Random packing of partially penetrable spheres with random volume equivalent spherical grain radii simulated after $f_{M\Delta t}(m\Delta t)$

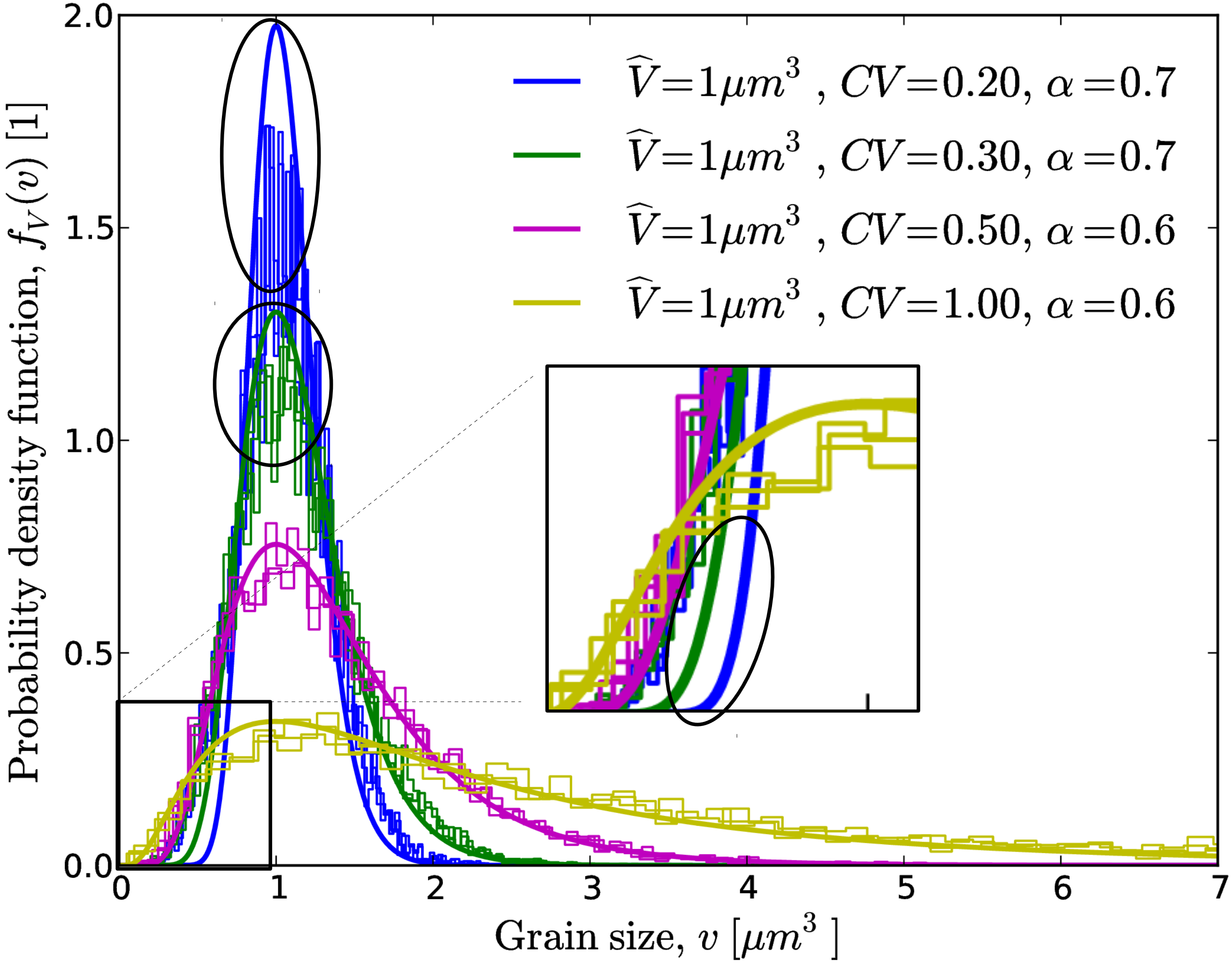
Every sphere of volume $4\pi(m\Delta t)^3/3$ has an impenetrable concentric core of volume $4\pi(\alpha m\Delta t)^3/3$.

$\alpha \equiv$ Impenetrability parameter

Effect of the impenetrability parameter



Grain size distribution of SGT models



Method #3a: Random rejection criterion

- Accept the candidate location $\underline{x}_k$ of a point ***k*** with random mark M_k after a probability p_k :

$$p_k = \prod_{i=1}^{n} p_{ik}$$

where $p_{ik} \equiv \Pr(\alpha(M_i + M_k) \leq d_{ik})$

$$= \Pr(M_i + M_k \leq d_{ik}/\alpha)$$

with $d_{ik} \equiv \|\underline{x}_k - \underline{x}_i\|$ where the point ***i*** is a nearest neighbor of the point ***k*** at the candidate location $\underline{x}_k$,

- α is the impenetrability parameter,
- n is the number of nearest neighbors considered for the computation of p_k.

Method #3a: Random rejection criterion

- By assuming the independence of M_i and M_k, we have:

$$p_{ik} = \int_{-\infty}^{d_{ik}/\alpha} \int_{-\infty}^{\infty} f_{M_i}(m) f_{M_k}(\xi - m) \mathrm{d}m \mathrm{d}\xi$$

where $f_{M_i}(m) = f_{M_k}(m) = f_M(m)$ is taken as the radius *pdf* for grains of equivalent volumes. Thus p_{ik} is computed as follows:

$$p_{ik} = \int_{0}^{d_{ik}/\alpha} \int_{0}^{\xi} f_M(m) f_M(\xi - m) \mathrm{d}m \mathrm{d}\xi$$

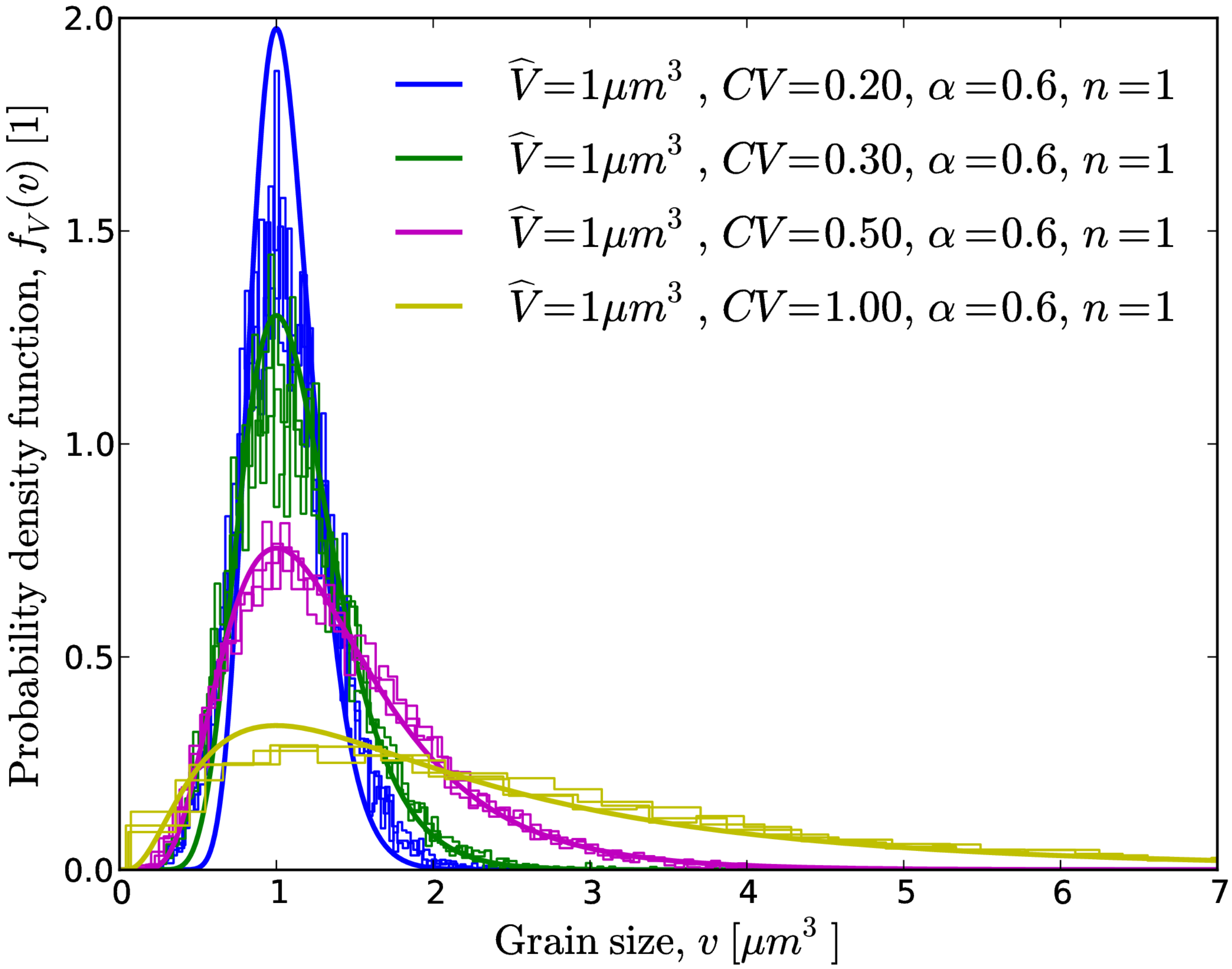
- Then the acceptance probability is given by

$$p_k \equiv \Pr(\alpha(M_1 + M_k) \leq d_{1k} \cap \alpha(M_2 + M_k) \leq d_{2k} \cap \dots)$$

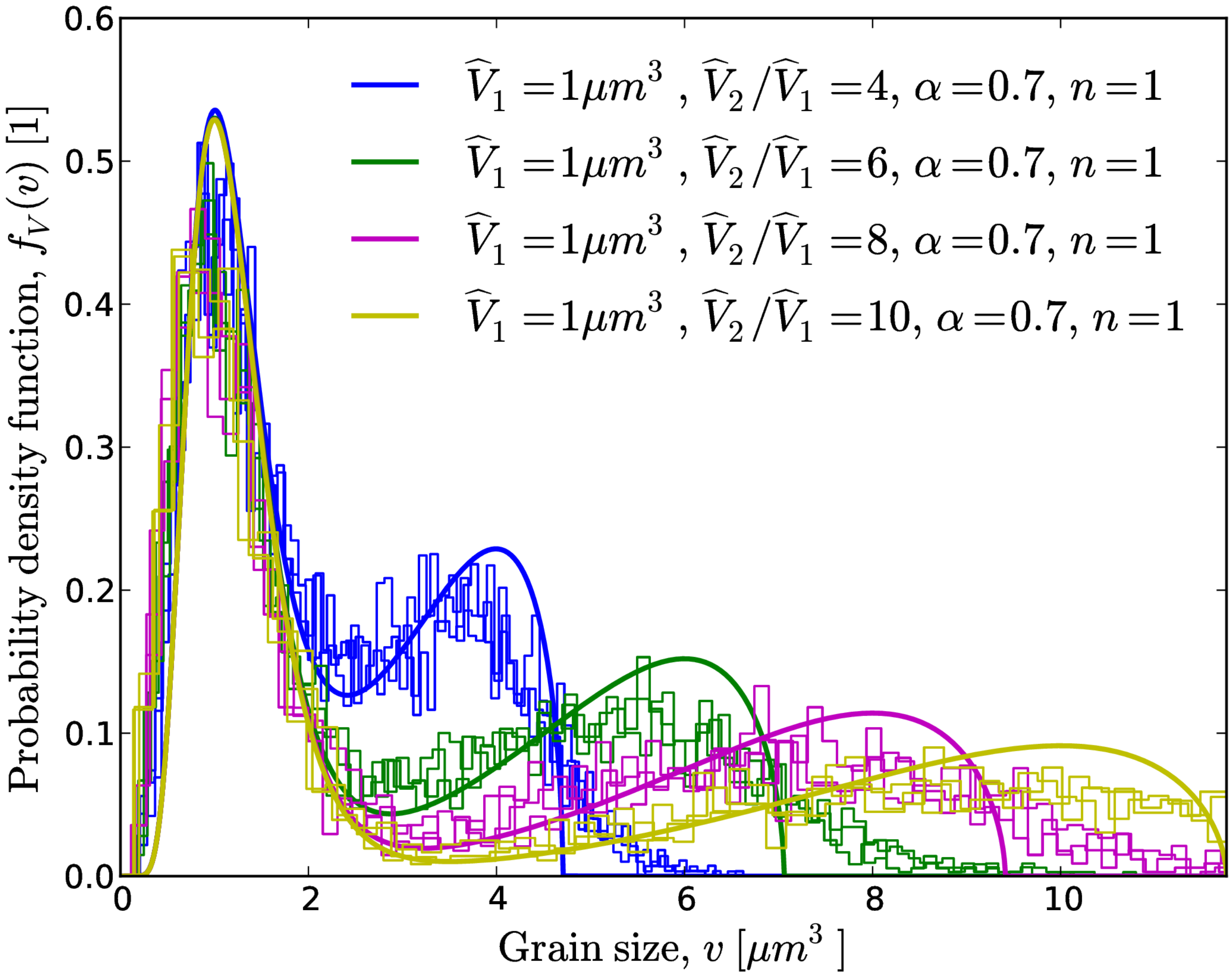
which collapses into $p_k = p_{1k} p_{2k} \dots p_{nk}$ only if $\alpha(M_1 + M_k) \leq d_{1k}$, $\alpha(M_2 + M_k) \leq d_{2k}$ and so on are mutually independent events.

- The location $\underline{x}_k$ is accepted if for an independent uniform realization, we have $u \leq p_k$. If so, the mark m_k is obtained from the same realization u as $m_k = F_M^{-1}(u)$.

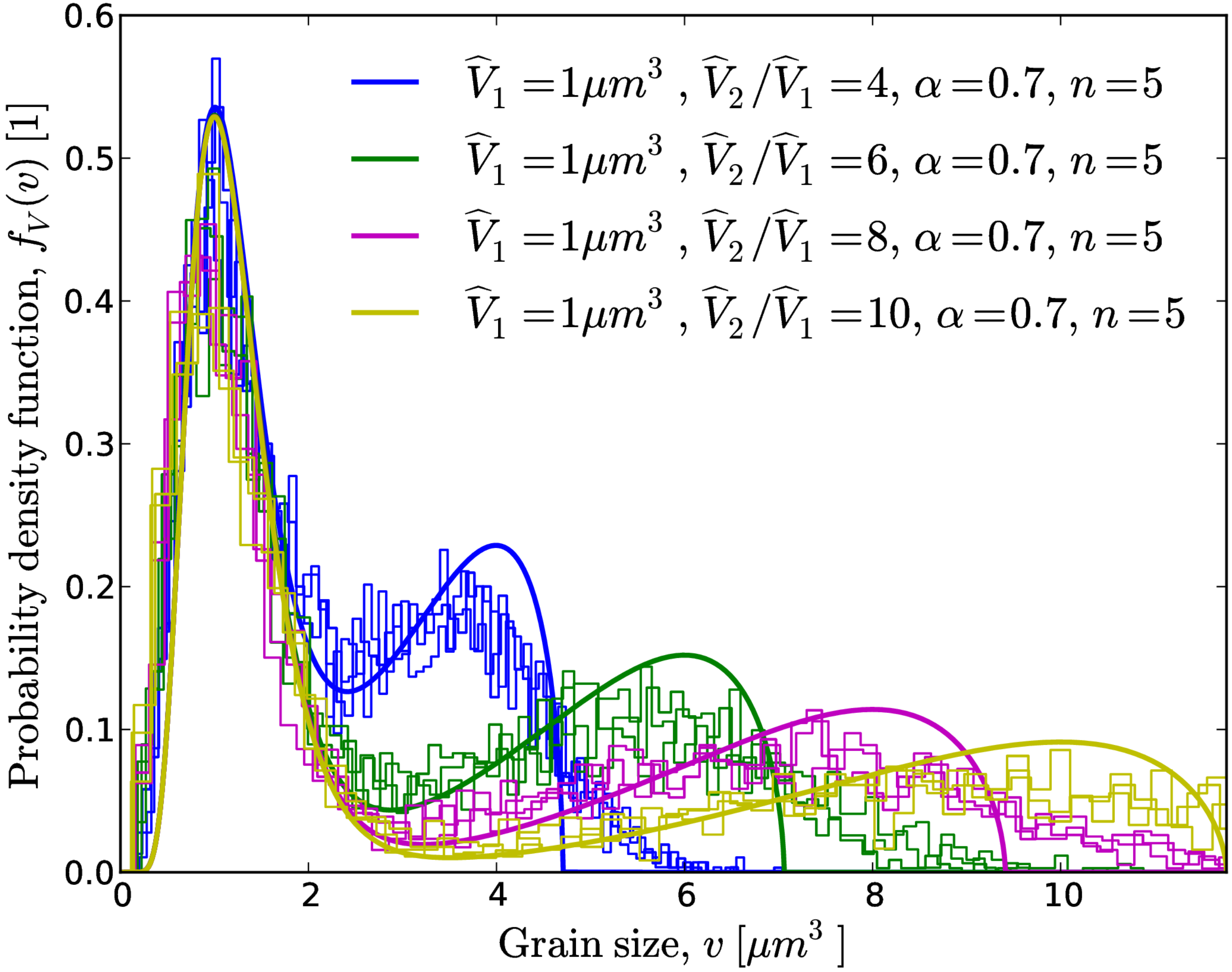
Grain size distribution of SGT models



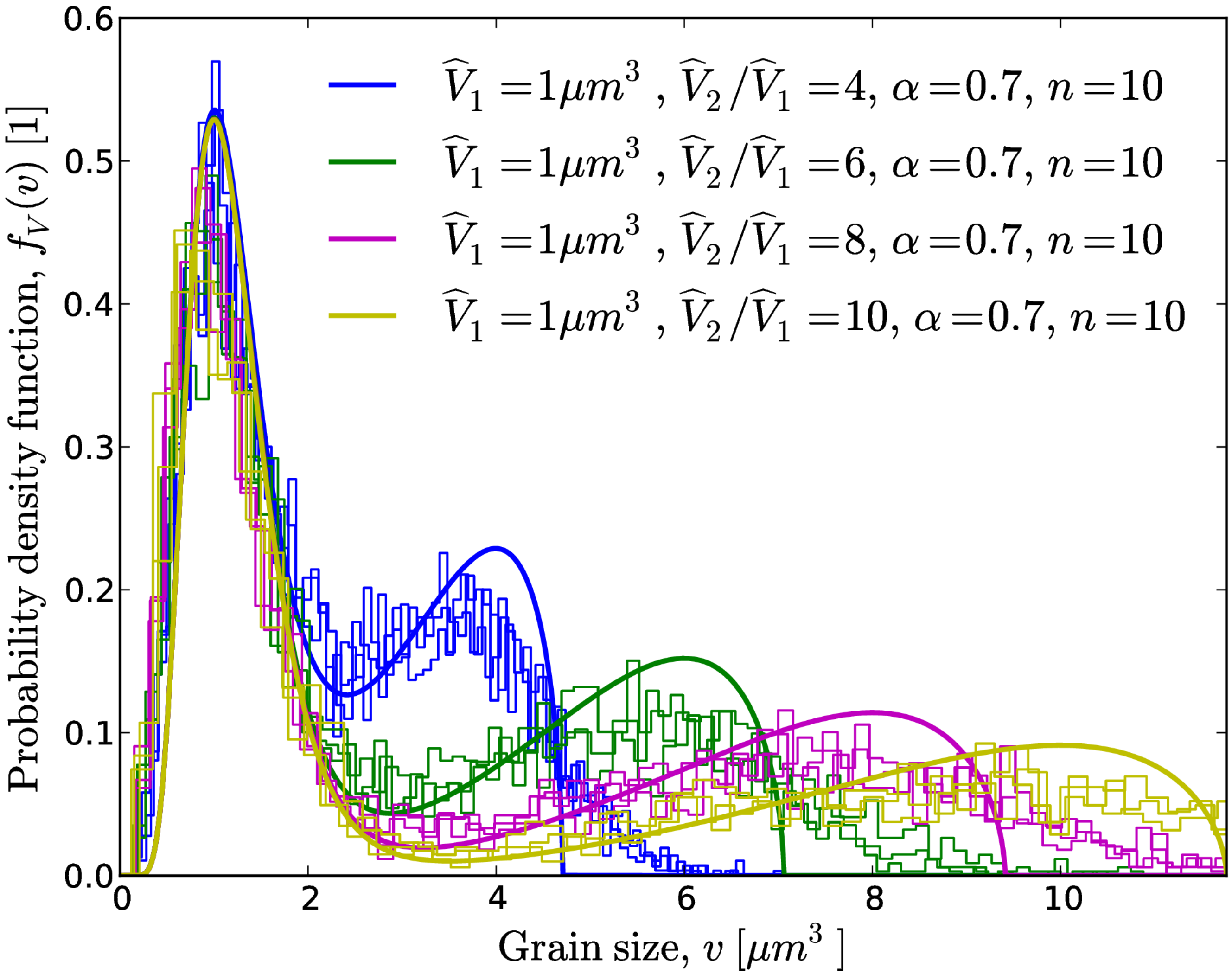
Grain size distribution of SGT models



Grain size distribution of SGT models



Grain size distribution of SGT models



Method #3b: Conditioned random rejection criterion

- Accept the candidate location $\underline{x}_k$ of a point ***k*** with random mark M_k after a probability p_k knowing the marks of the nearest neighbors:

$$p_k = \prod_{i=1}^{n} p_{ik}$$

where $p_{ik} \equiv \Pr(\alpha(M_i + M_k) \leq d_{ik} | M_i = m_i)$

$$p_{ik} = \int_0^{d_{ik}/\alpha} f_M(m_i) f_M(\xi - m_i) \mathrm{d}\xi$$

- … yields very small values of p_{ik} .

Method #4: Markov marked point process

- Prescribe a potential measure ϕ of point pair interaction:

$$\phi = \phi(\underline{x}_i - \underline{x}_k, m_i, m_k)$$

$\phi < 0 :\rightarrow$ Attraction, $\phi = 0 :\rightarrow$ No interaction, $\phi > 0 :\rightarrow$ Repulsion,

- Define the total energy of the current point pattern:

$$U(\underline{x}_1, \underline{x}_2, ...\underline{x}_n) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \phi(\underline{x}_i - \underline{x}_k, m_i, m_k)$$

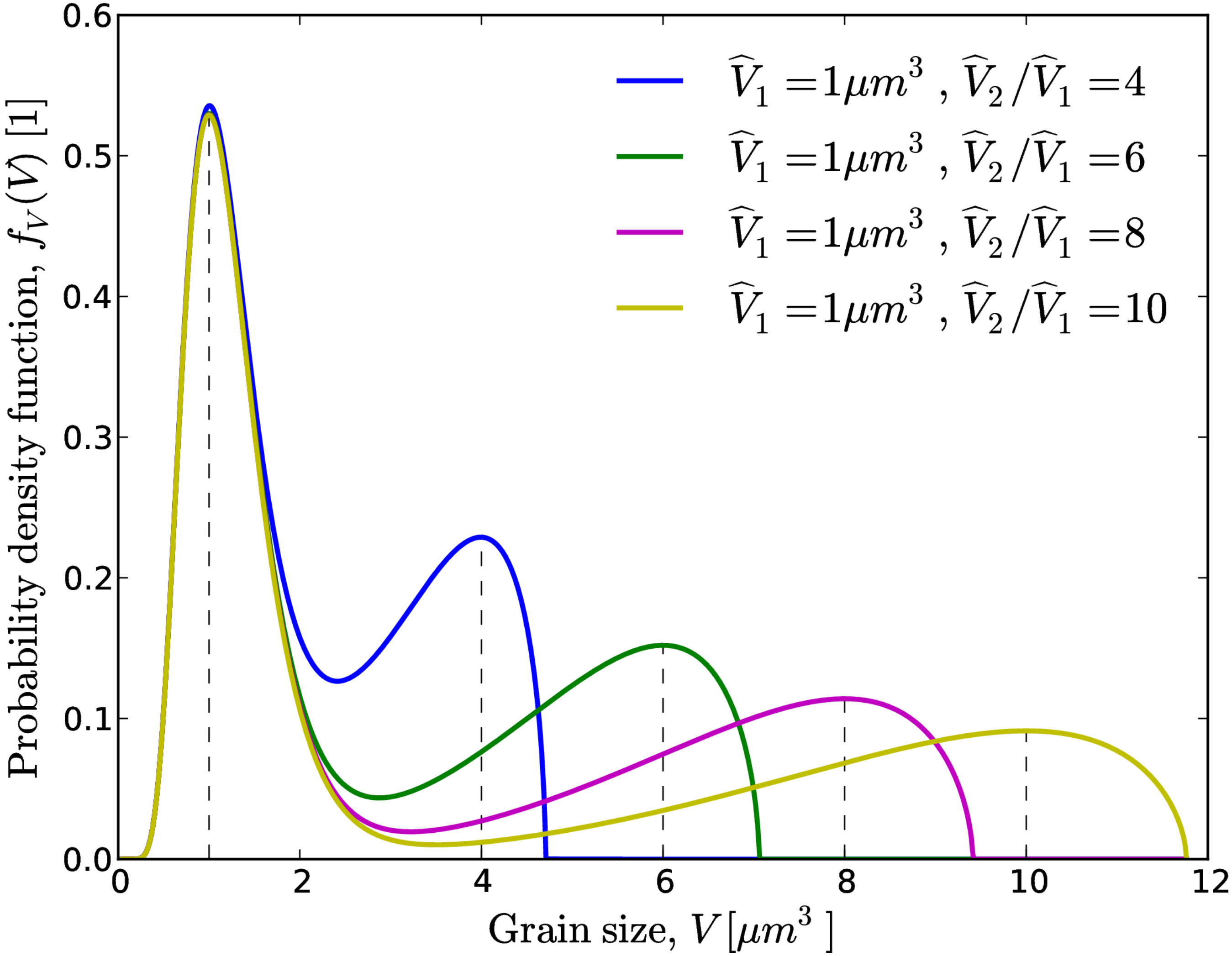
- For a fixed expectation of U, entropy is maximized for

$$f_n(\underline{x}_1, \underline{x}_2, ..., \underline{x}_n) = 1/Z_n \exp\left[-U(\underline{x}_1, \underline{x}_2, ..., \underline{x}_n)\right]$$

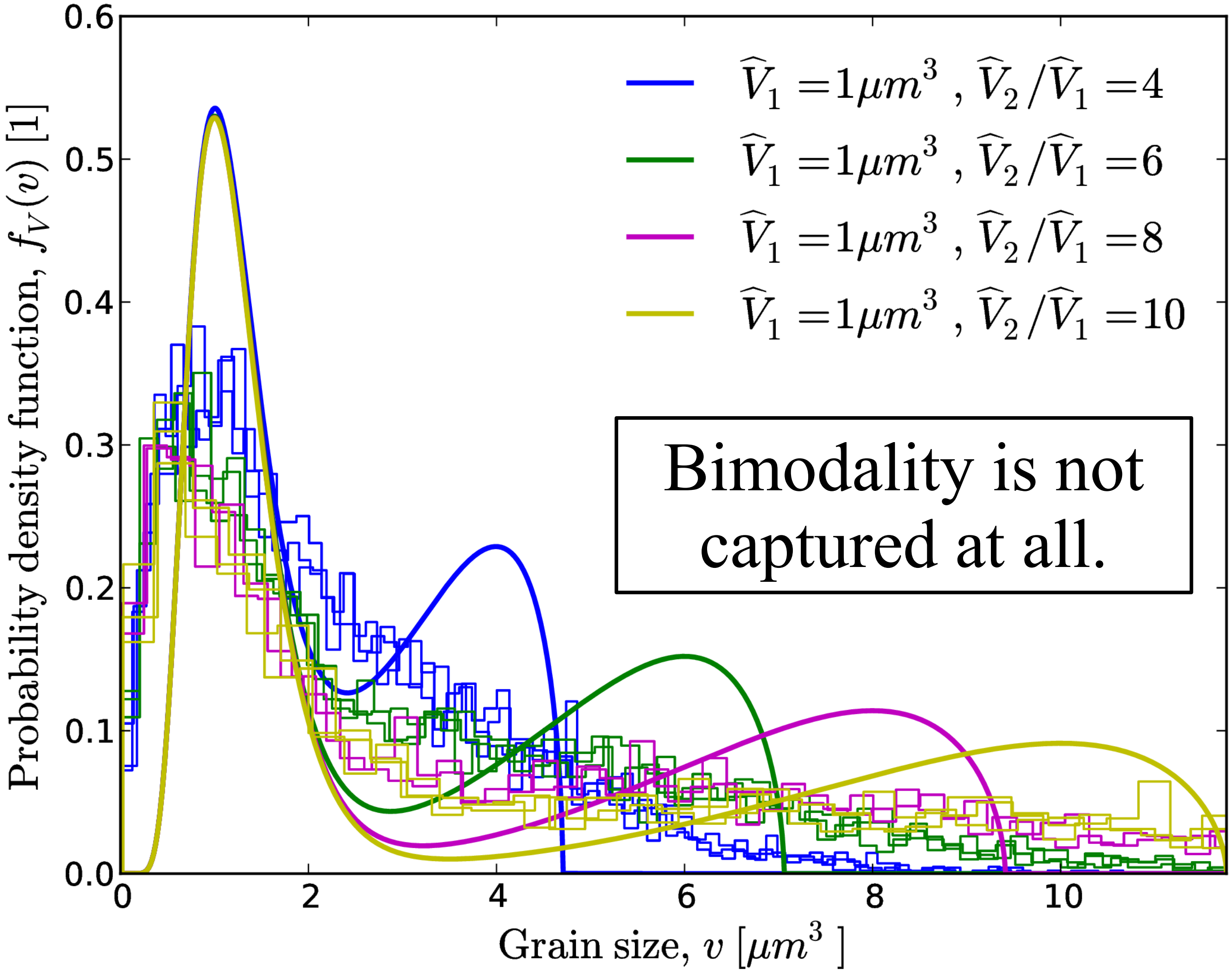
- Simulate a marked point process as a sample of f_n using a Markov chain.

Simulation of **SGT** models based on **bimodal grain size distributions**

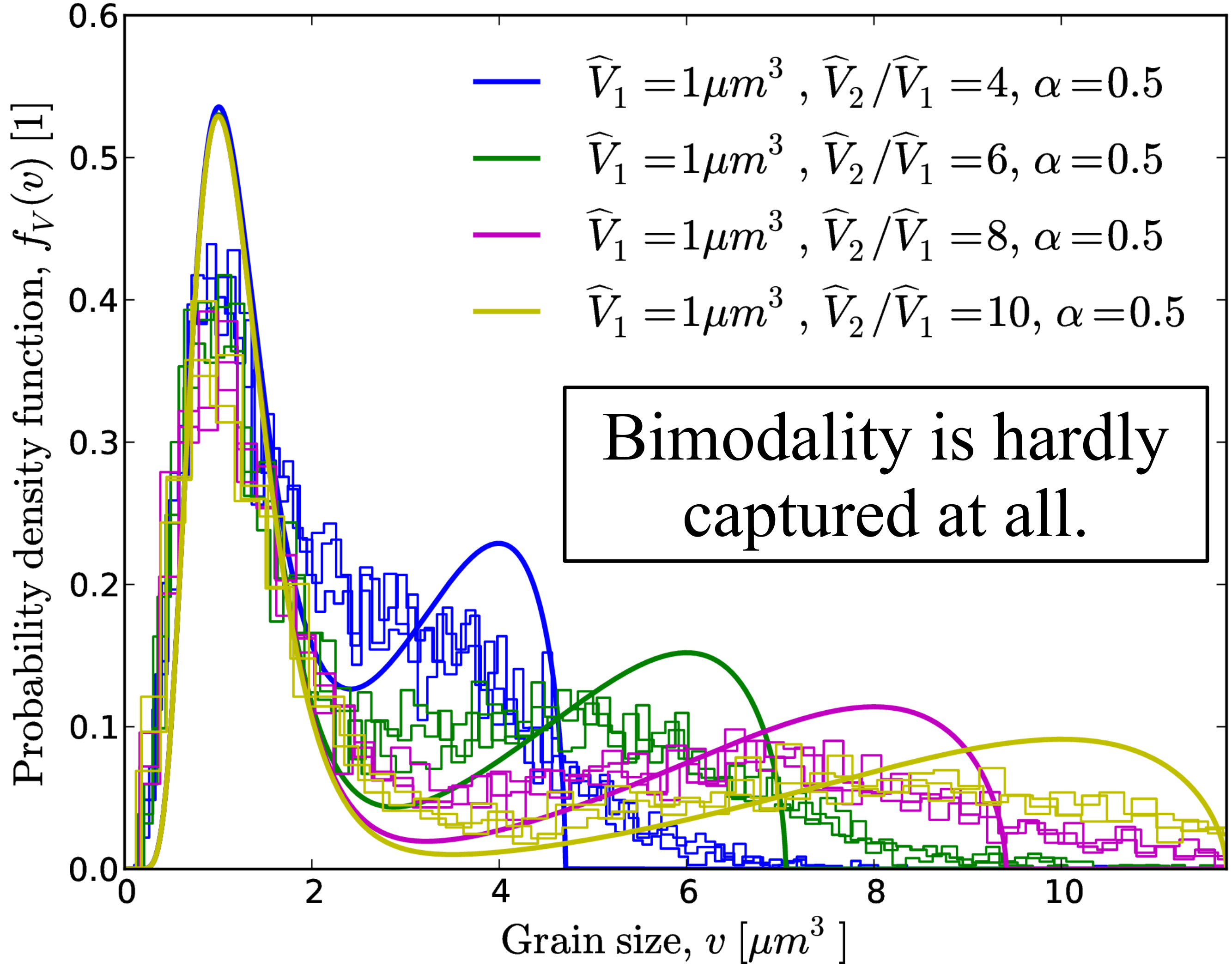
Target distributions #2



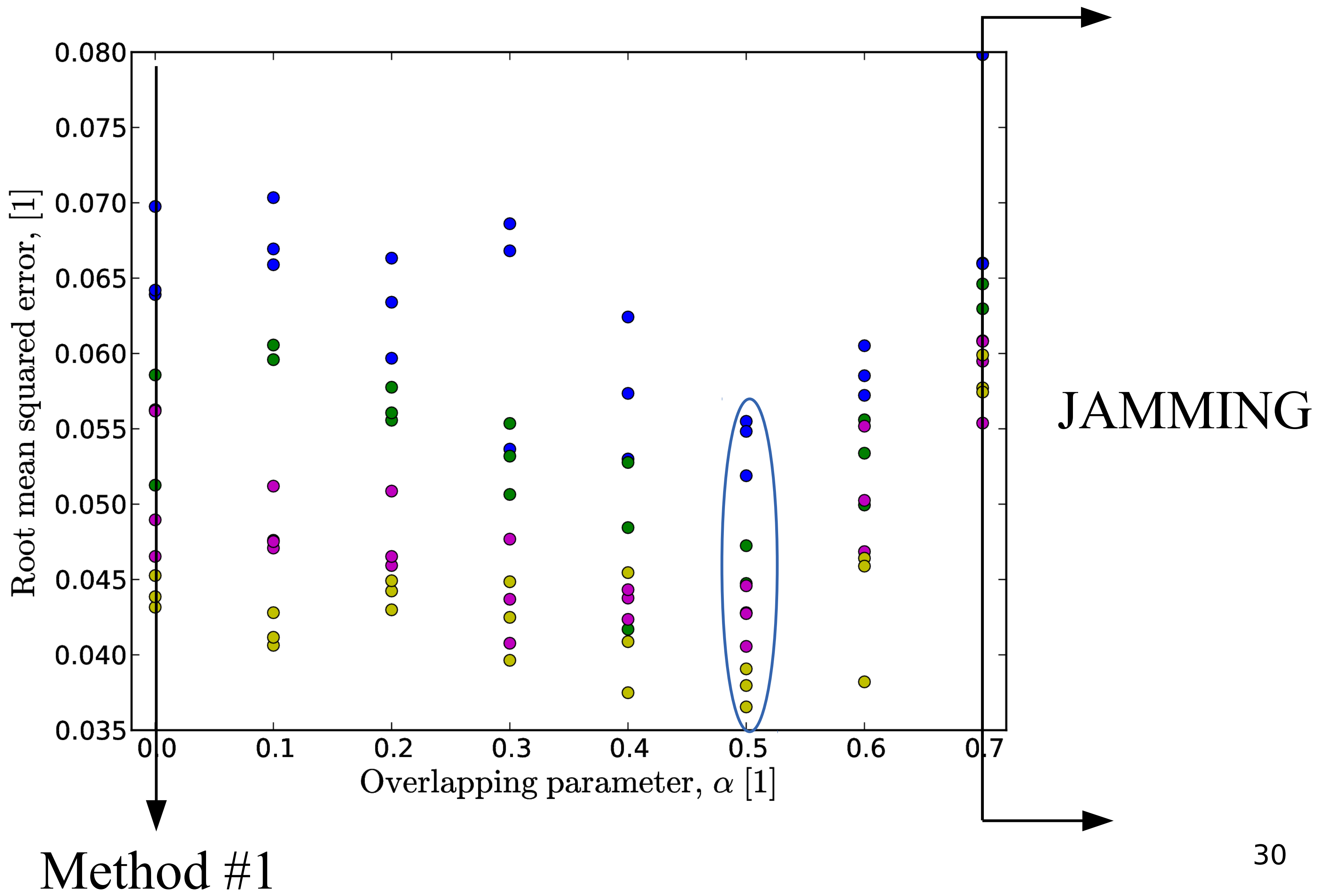
Grain size distributions simulated after Method #1



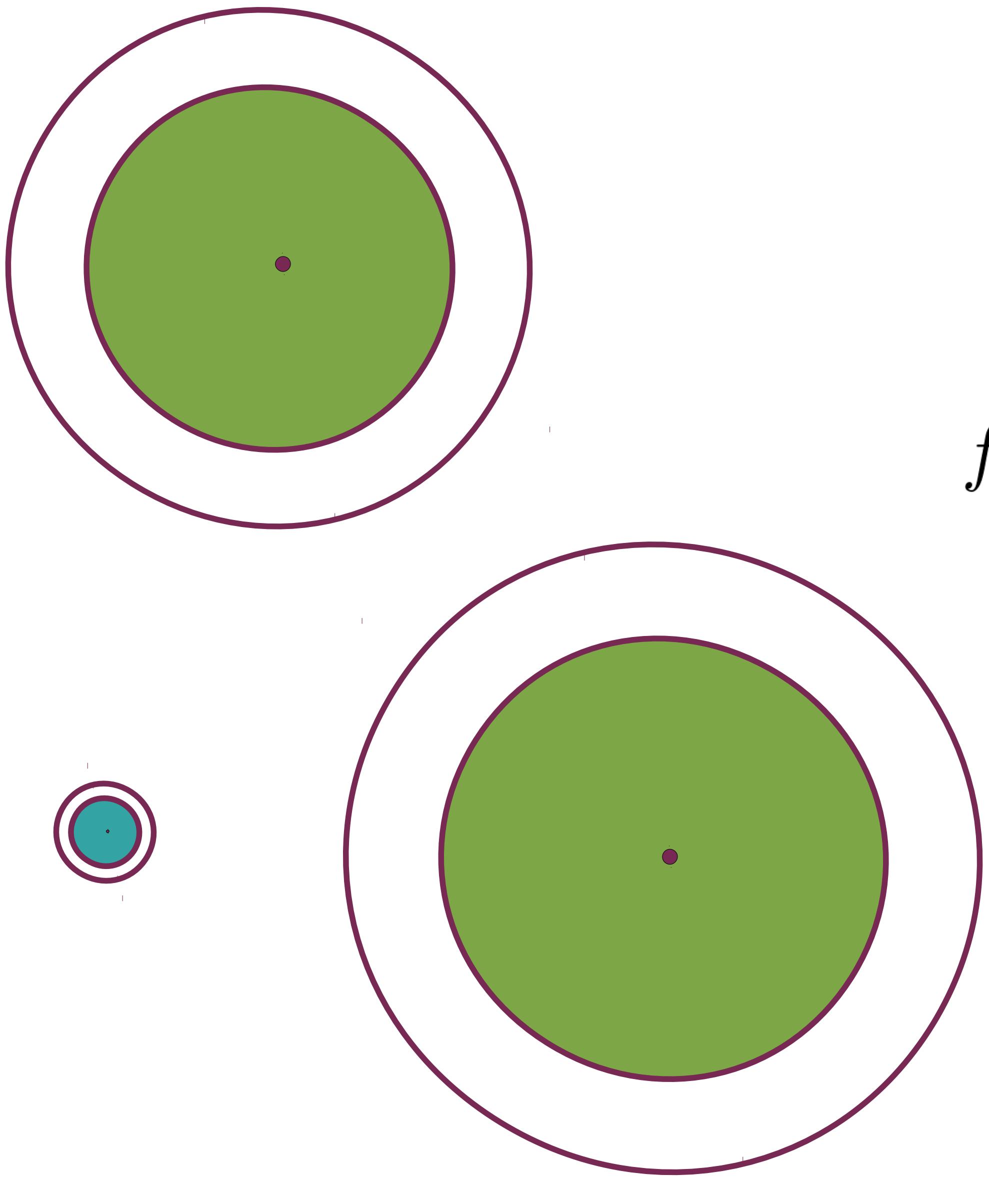
Grain size distributions simulated after Method #2



Effect of the impenetrability parameter



Method #3: Superposition of Concentric Shell Packing Models

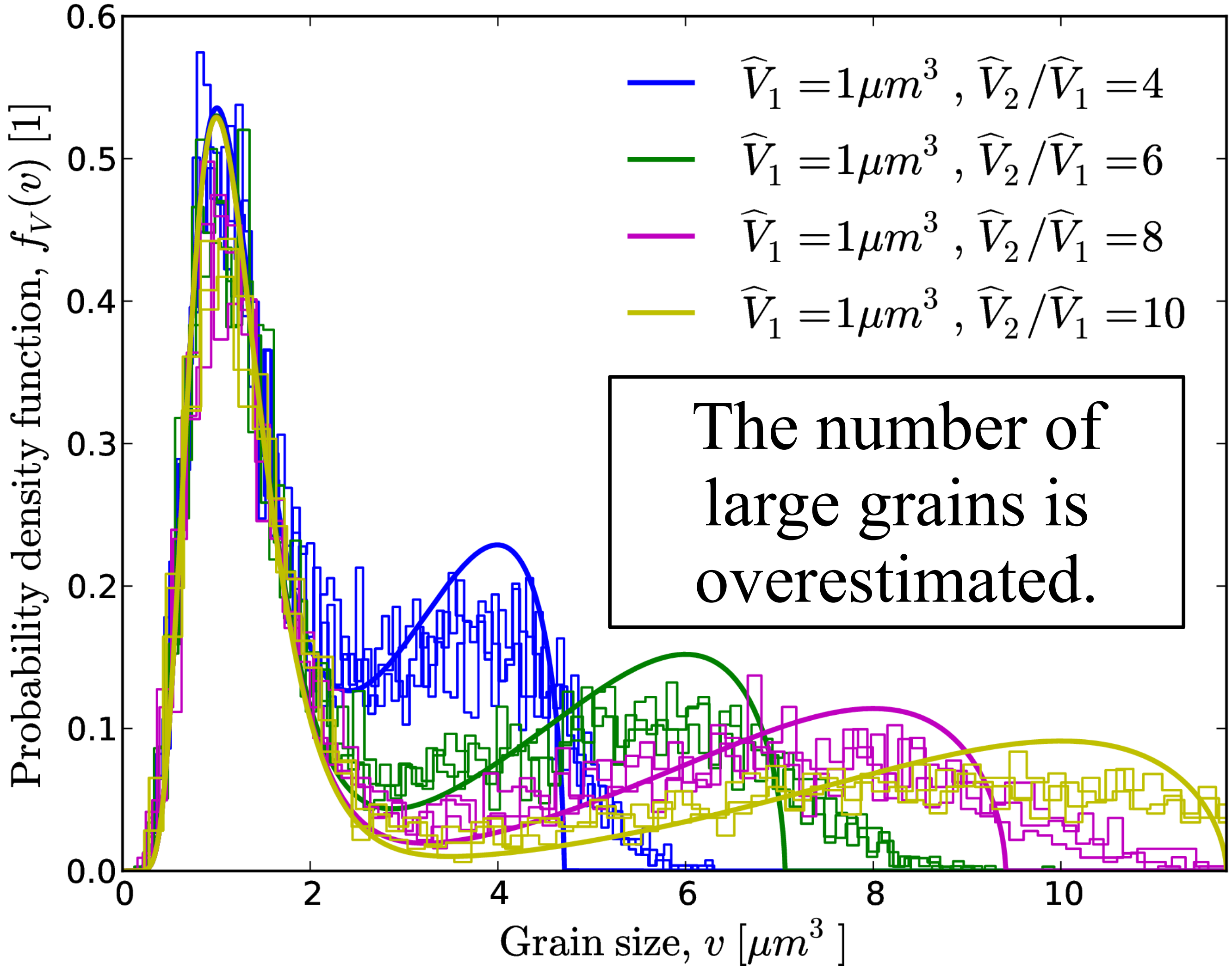


The bimodal distribution of volume equivalent spherical grain radii is deconvoluted:

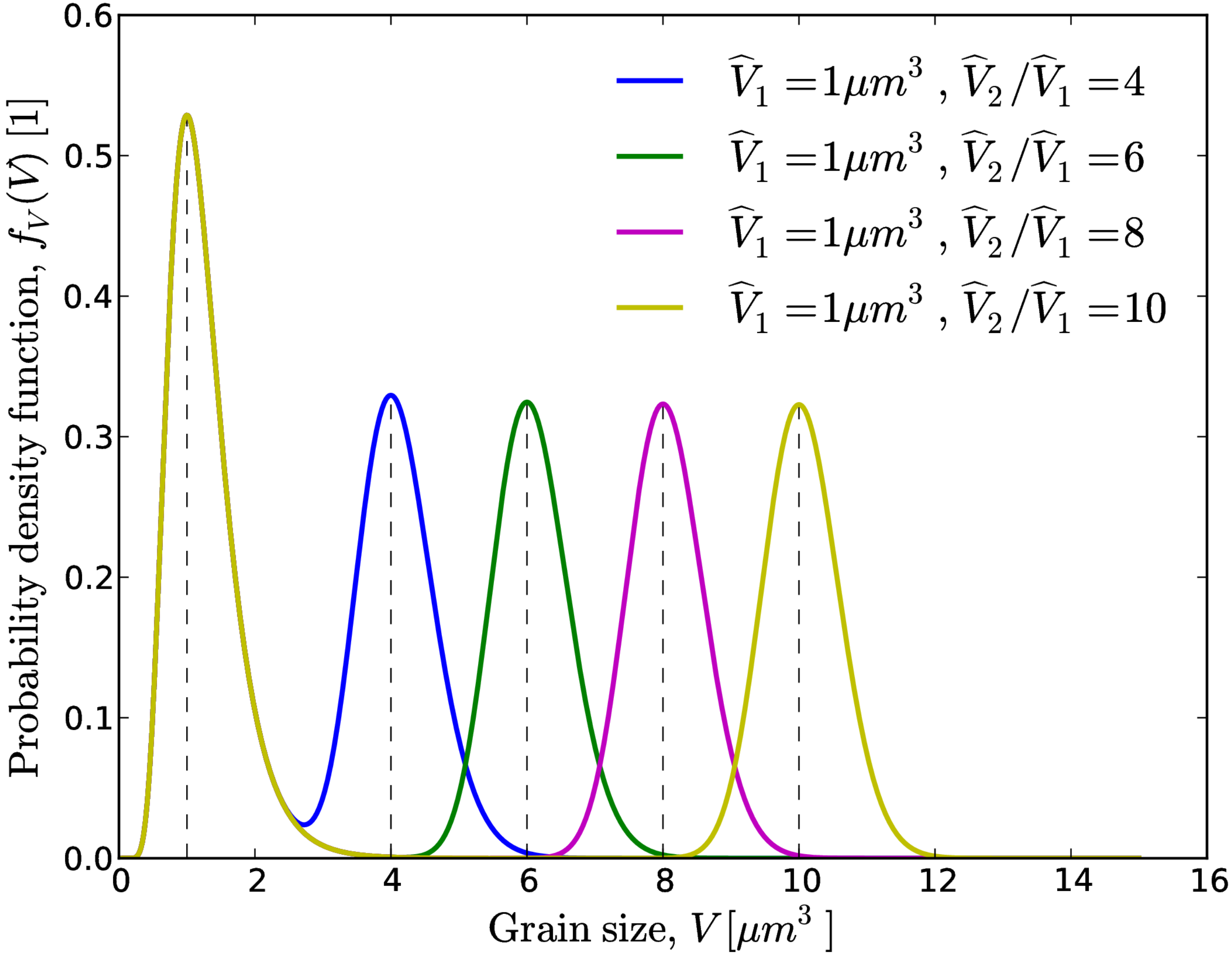
$$f_{M\Delta t}(m\Delta t) = c_1 f^{(1)}_{M\Delta t}(m\Delta t) + c_2 f^{(2)}_{M\Delta t}(m\Delta t)$$

Coarse spheres are simulated first and the fine spheres after both with the same impenetrability parameter.

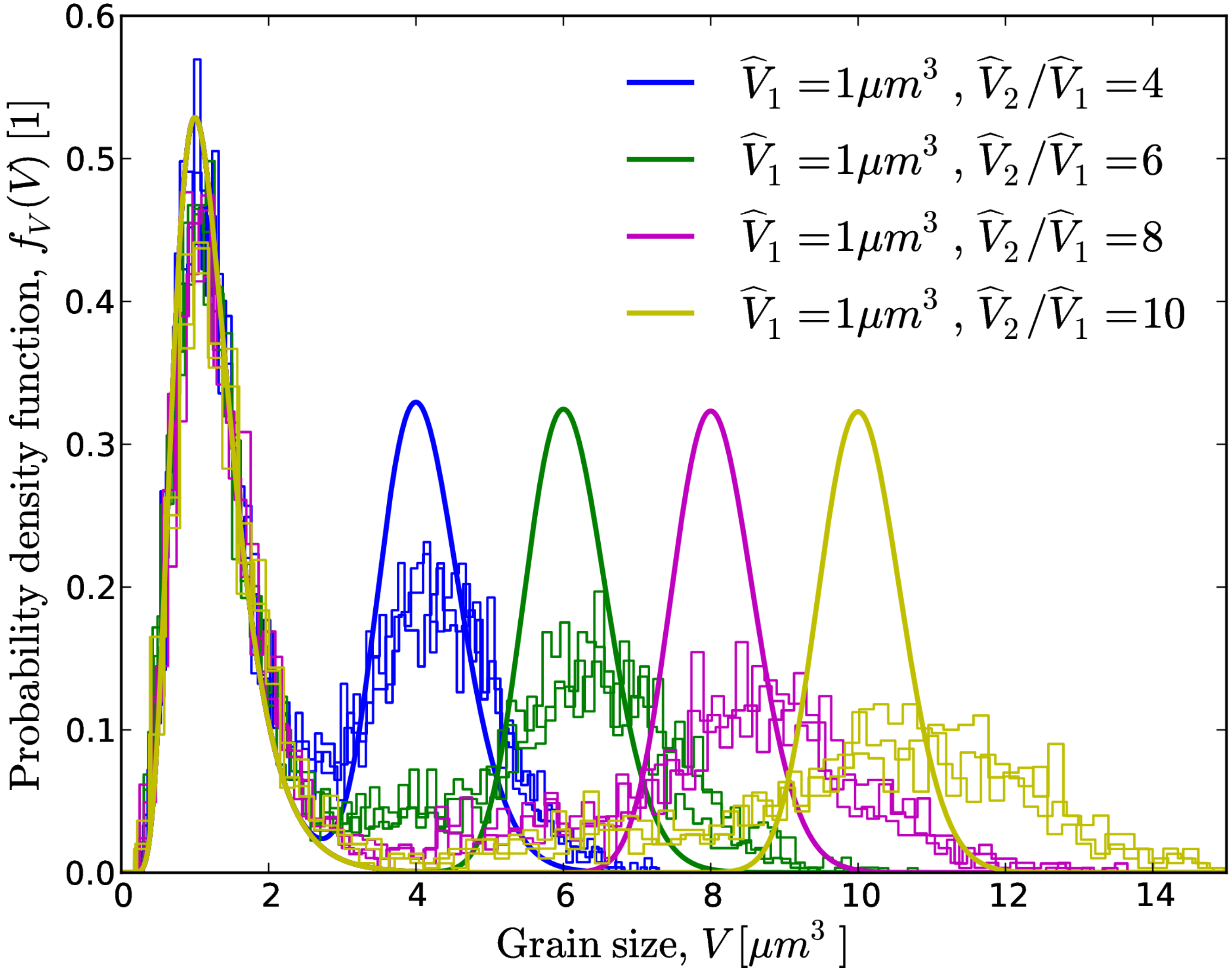
Grain size distributions simulated after Method #3



Target distributions #3



Grain size distributions simulated after Method #3



References

K. Teferra and L. Graham-Brady, Stochastic simulation of grain growth tessellation for polycrystalline microstructures. In preparation for submission to *Acta Materialla*.