AMDG

University of Twente

Onset of unimodal to bimodal random packings

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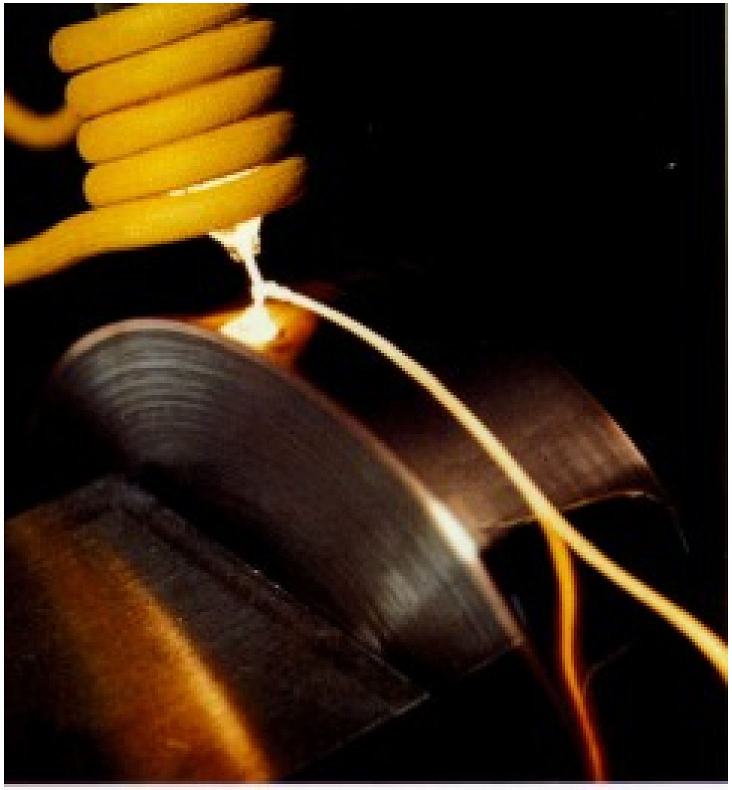
Onset of unimodal to bimodal random packings; with application to

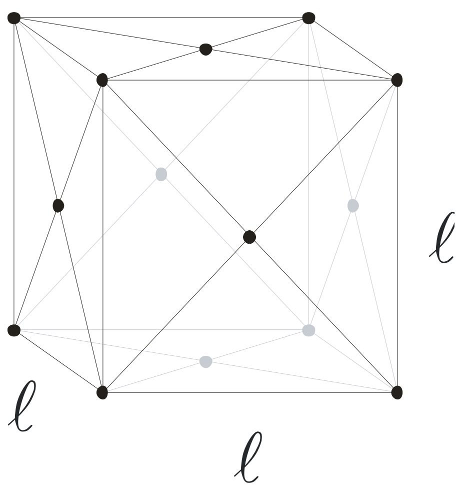
1. Polydisperse geometric packing
    1. Bimodal discrete random
    2. Polydisperse discrete random
    3. Continuous random
2. Amorphisation
    1. Bimodal discrete random
    2. Bimodal discrete crystalline
    3. Cross-over

Concrete: granular mix with size range nm to mm

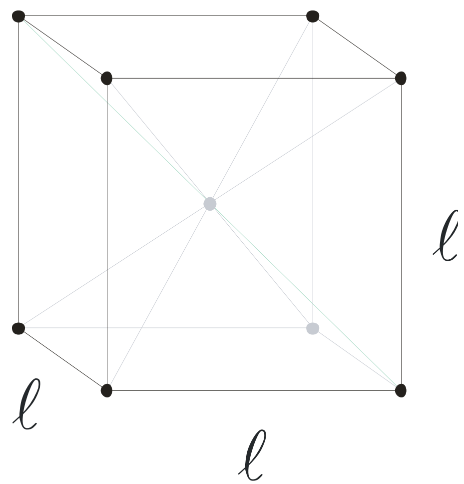
Amorphous (glassy) metal alloys



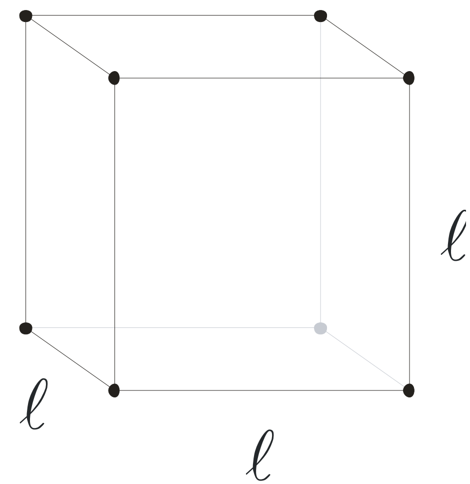
Bravais lattices crystalline (cubic) system



fcc
A1, α



bcc
A2, β

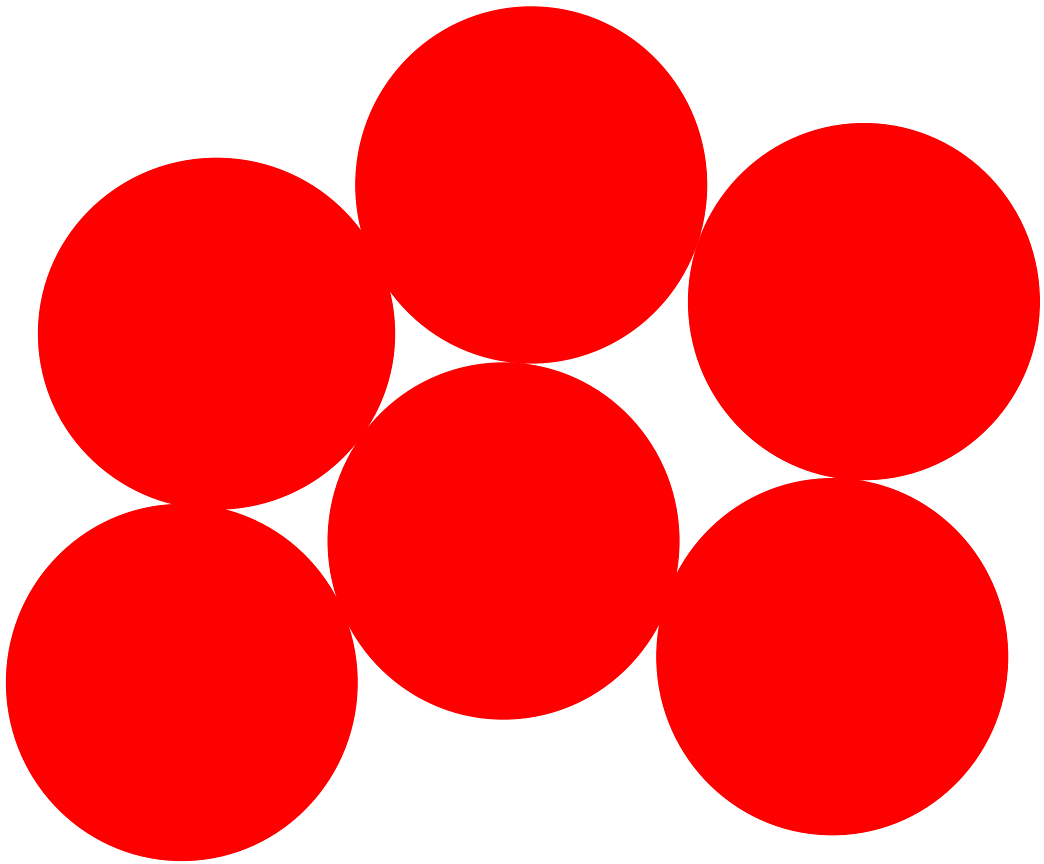


sc

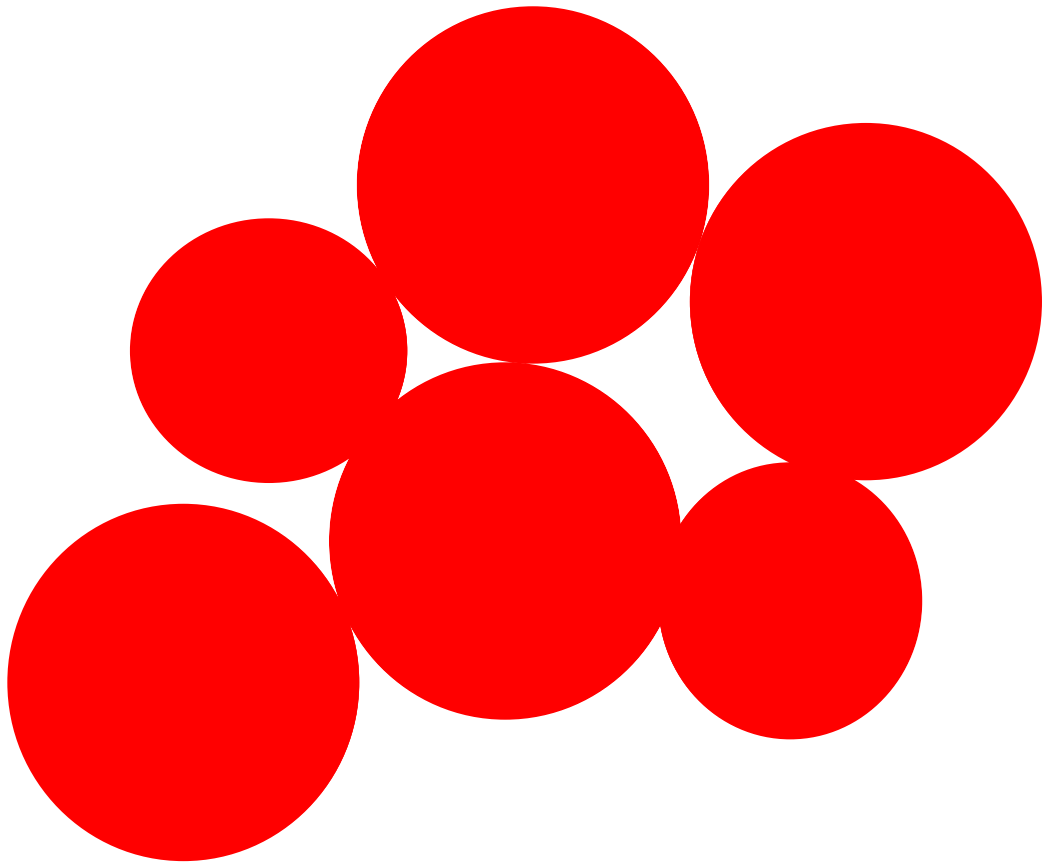
Disordered closed packing monosized spheres

RCP: $f_{rcp} = 0.64$;

$\varphi_1 = 0.36$



Disordered packing bimodal spheres with small size ratio u



Onset of unimodal to bimodal random packings; with application to

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Bimodal discrete

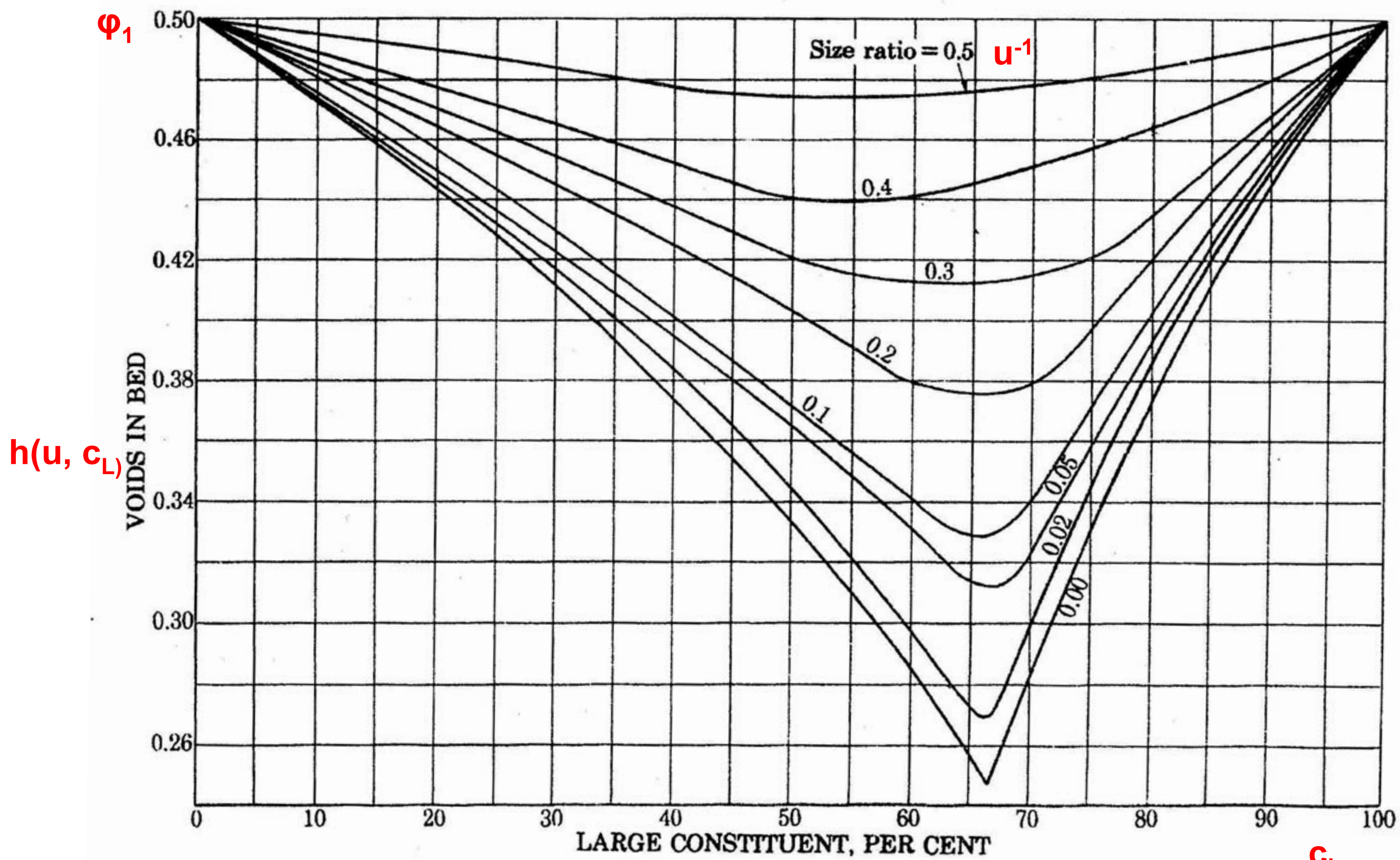
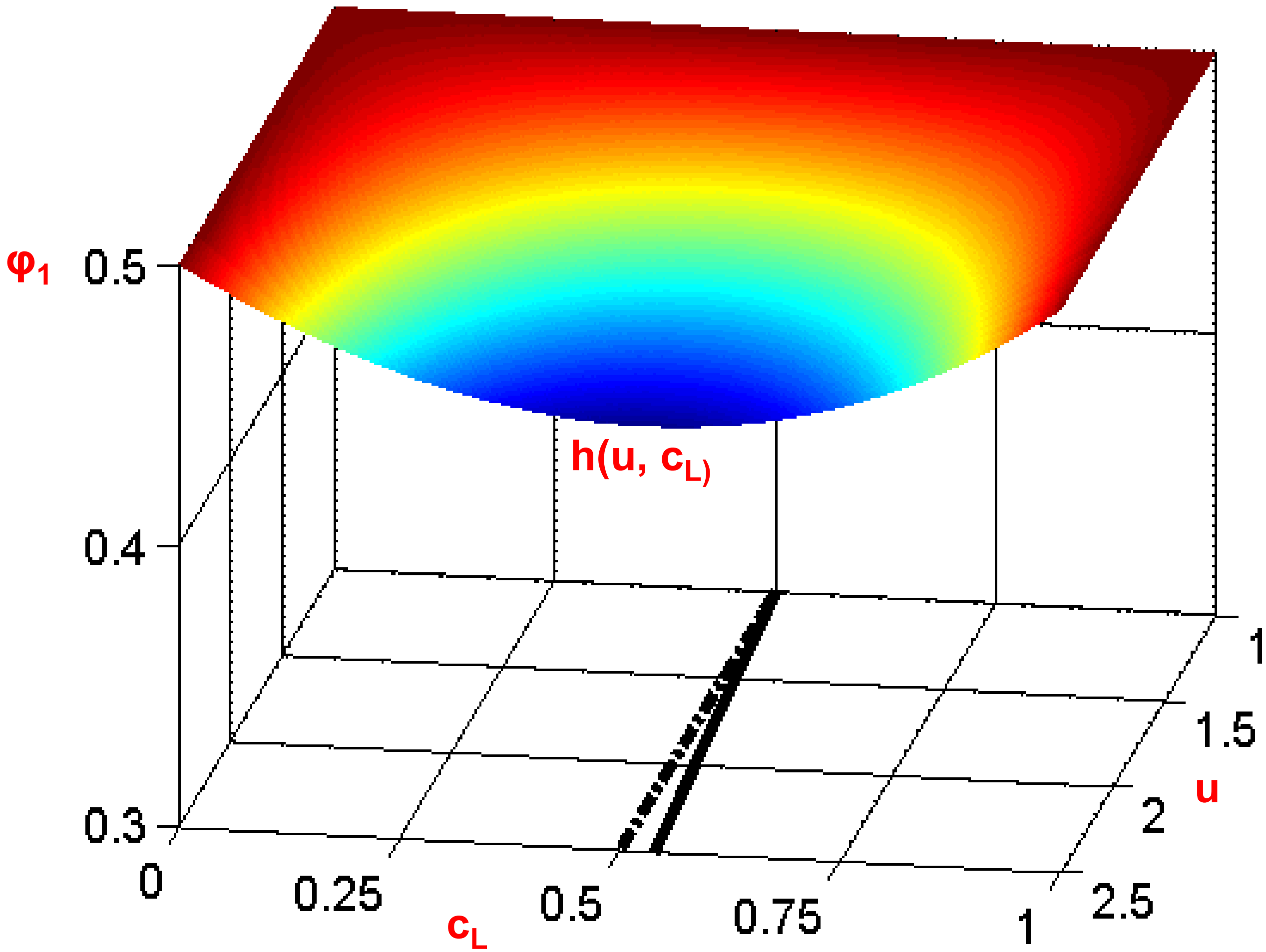


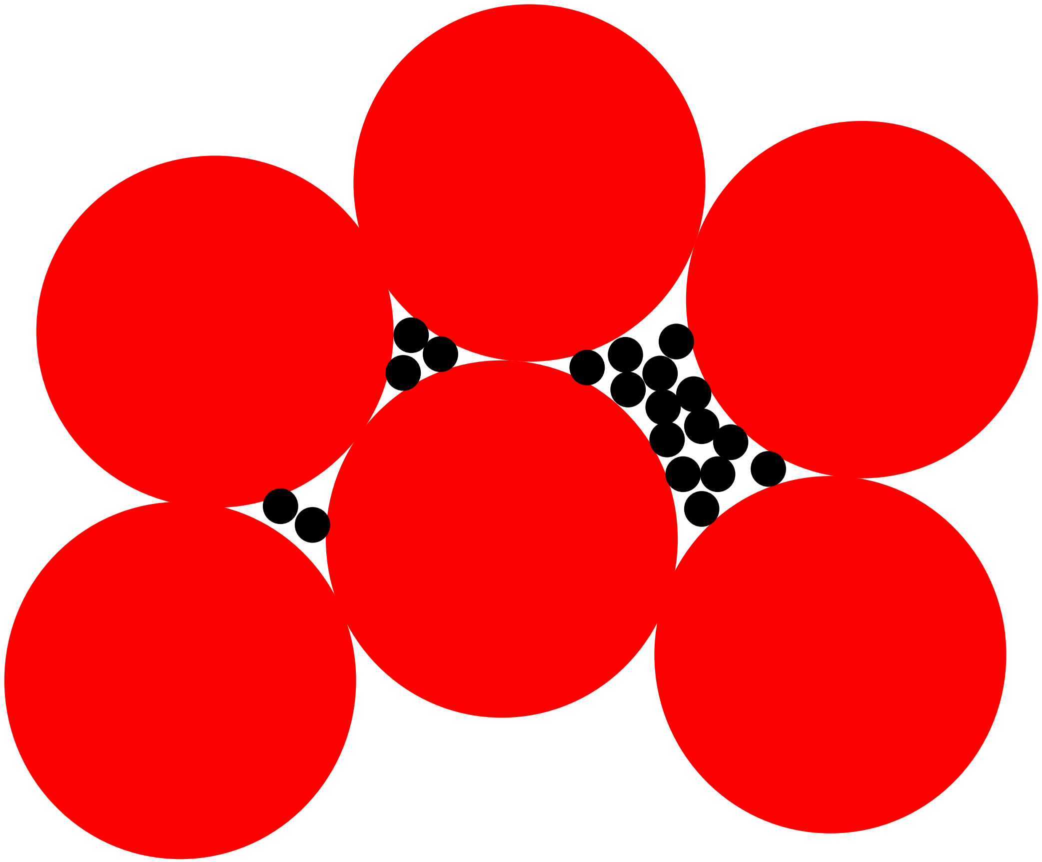
Figure 3.- Relation between voids and size composition in two-component systems of broken solids, when voids of mixed components = 0.50

Furnas (1928, 1929)

Bimodal discrete



Bimodal discrete (saturated)



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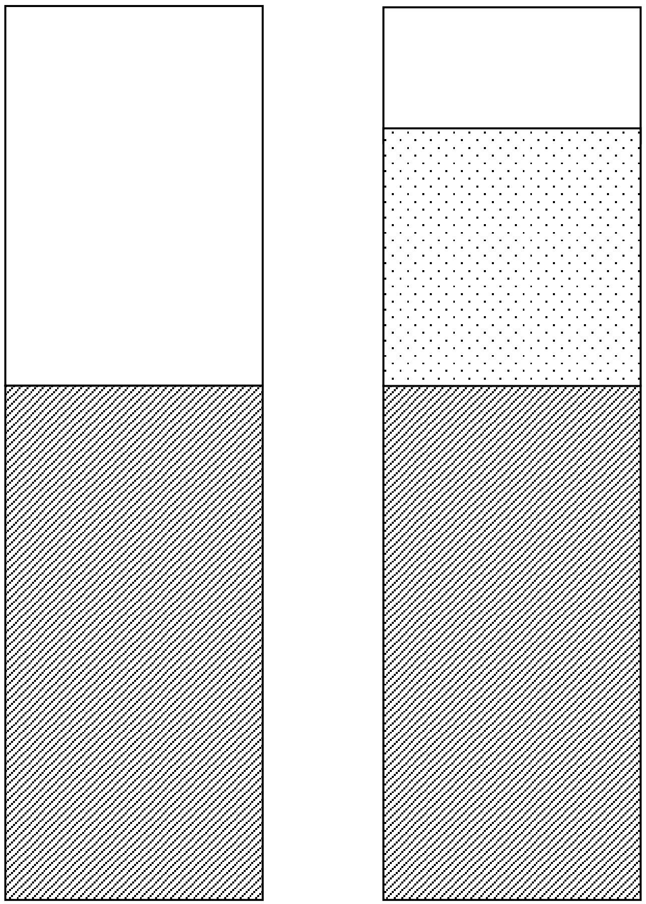


φ_1

f_1

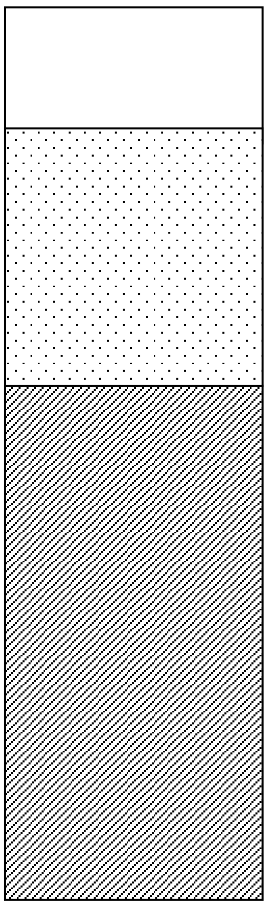
$\varphi_2 = \varphi_1^2$

$\varphi_1 f_1 = (1 - f_1)\, f_1$

$f_2 = (2 - f_1)\, f_1$

f_1

Bimodal discrete (saturated)



$\varphi_2 = \varphi_1^2$ $\quad \varphi_1 = 0.5 \rightarrow \varphi_2 = 0.25$

$f_1 = 0.5$

$\varphi_1 f_1 = (1 - f_1)\, f_1$

$f_2 = (2 - f_1)\, f_1$

$f_2 = 0.75$

f_1

$$c_S = \frac{(1-f_1)f_1}{(2-f_1)f_1} = \frac{\varphi_1}{1+\varphi_1}$$

$c_S = 1/3$

$$c_L = \frac{f_1}{(2-f_1)f_1} = \frac{1}{1+\varphi_1}$$

$c_L = 2/3$

$r = 1/\varphi_1 = c_L/c_S = 2$

Bimodal discrete (saturated)

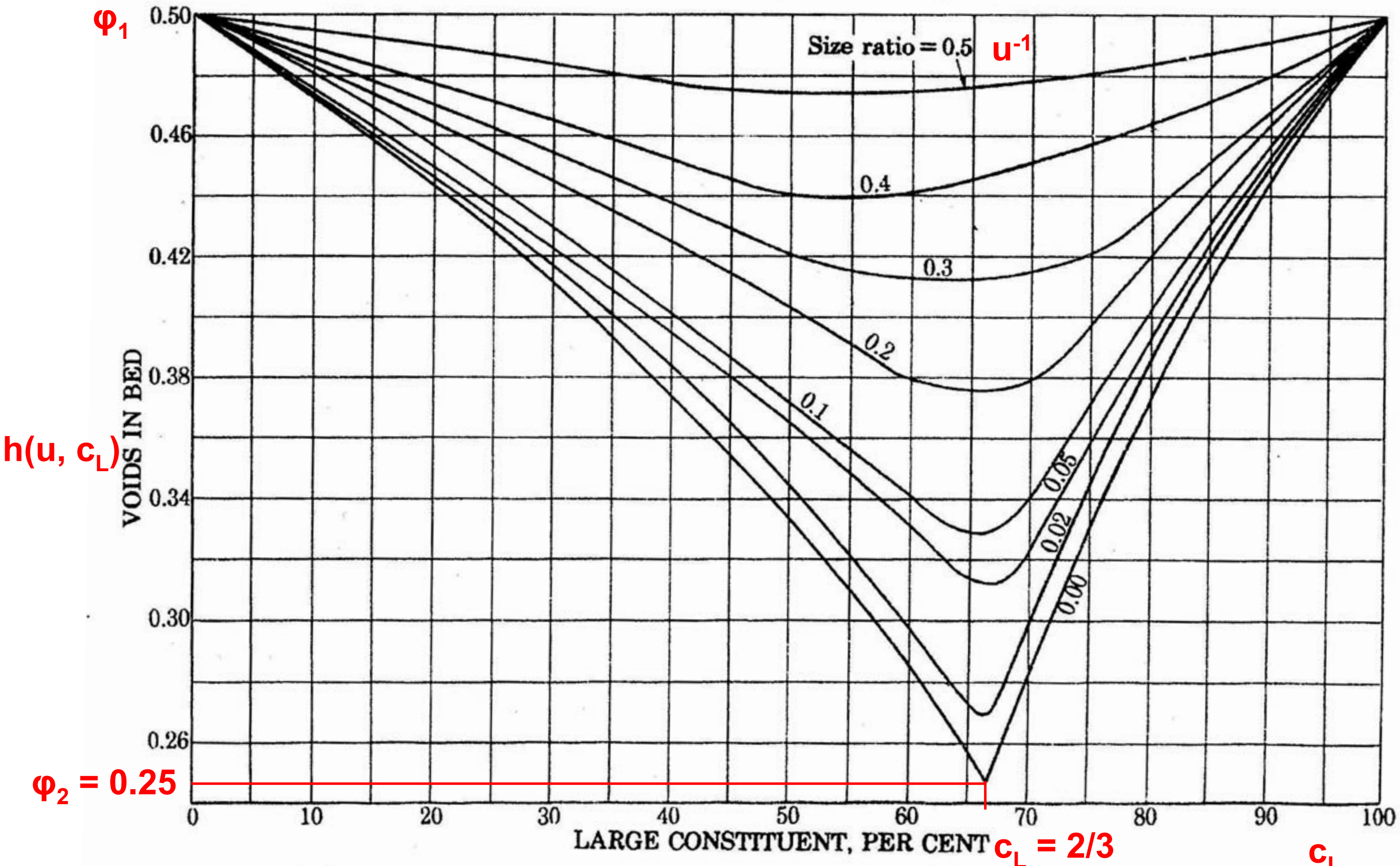
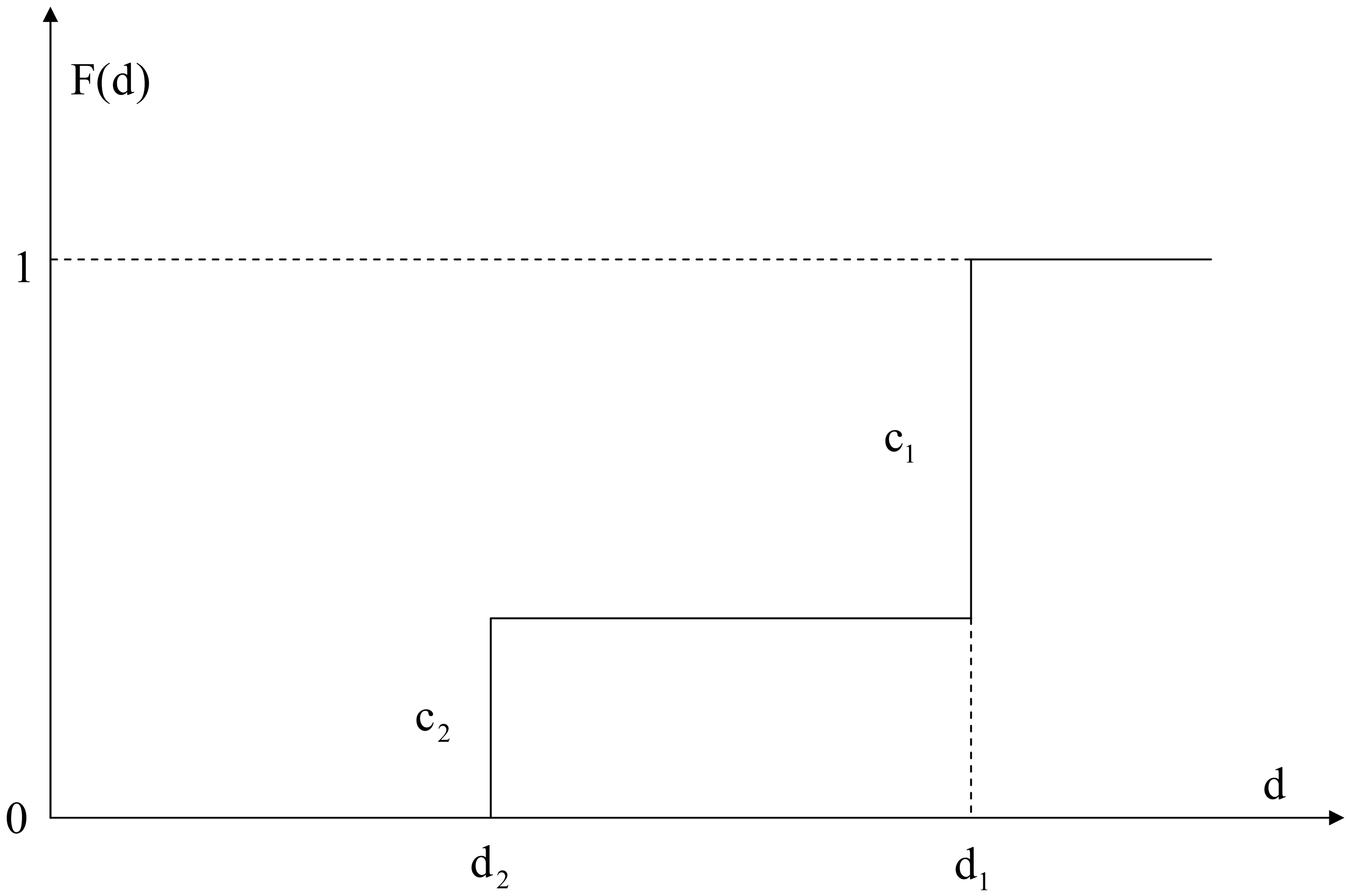


Figure 3.- Relation between voids and size composition in two-component systems of broken solids, when voids of mixed components = 0.50

Bimodal discrete (saturated)



Bimodal discrete (u → 1)

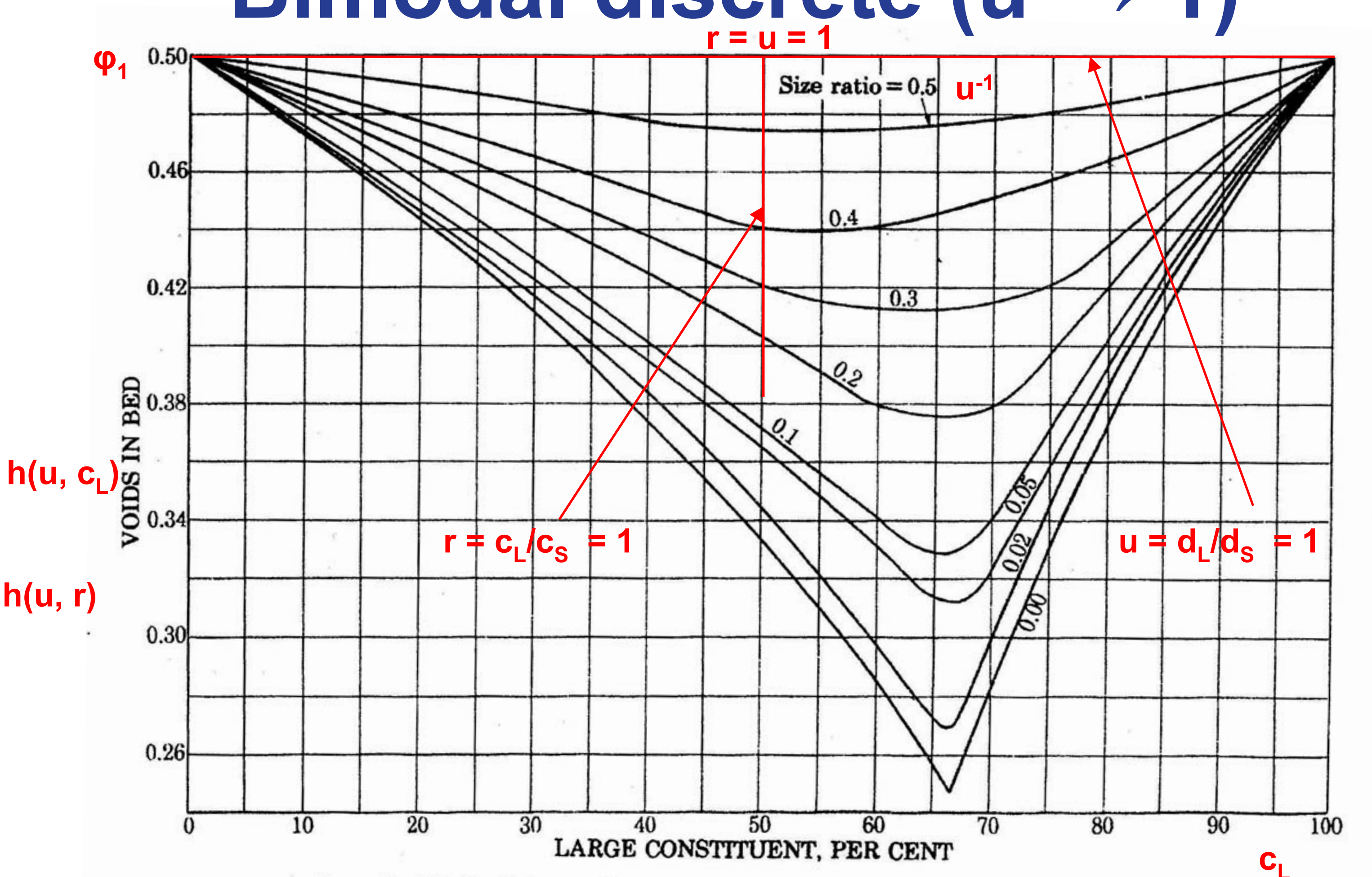


Figure 3.- Relation between voids and size composition in two-component systems of broken solids, when voids of mixed components = 0.50

Bimodal discrete (u → 1)

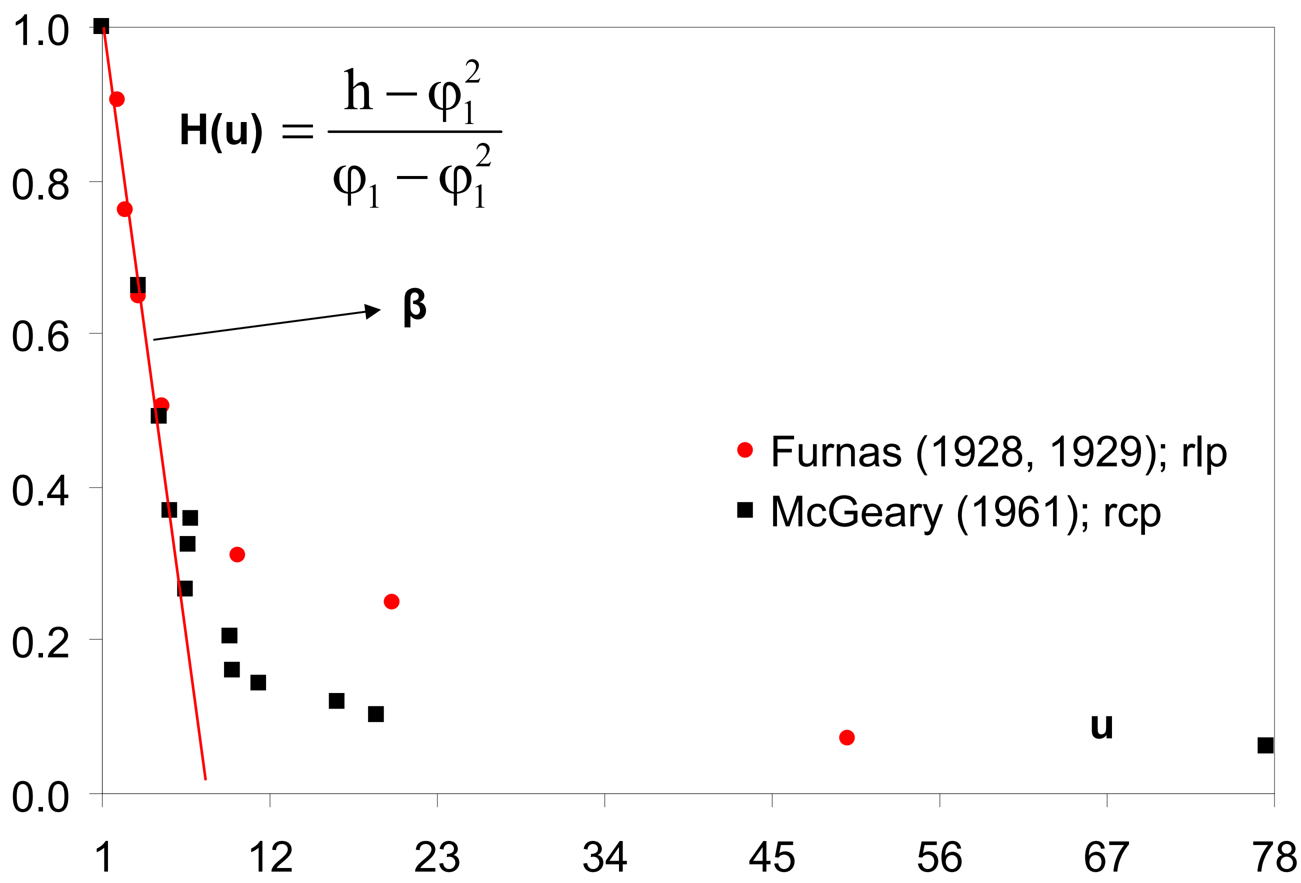
$$h(c_L, u) = \varphi_1 - 4\beta\varphi_1(1-\varphi_1)c_L(1-c_L)(u-1)$$

$$h(c_L, u) = \varphi_1 - \tfrac{4}{3}\beta\varphi_1(1-\varphi_1)c_L(1-c_L)(u^3-1)$$

$$\beta = -\frac{1}{\varphi_1(1-\varphi_1)}\left.\frac{dh}{du}\right|_{u=1, c_L=0.5}$$

$r = c_L/c_S = 1$

1. Bimodal discrete ($u \rightarrow 1$)



Volume fraction of optimum packing

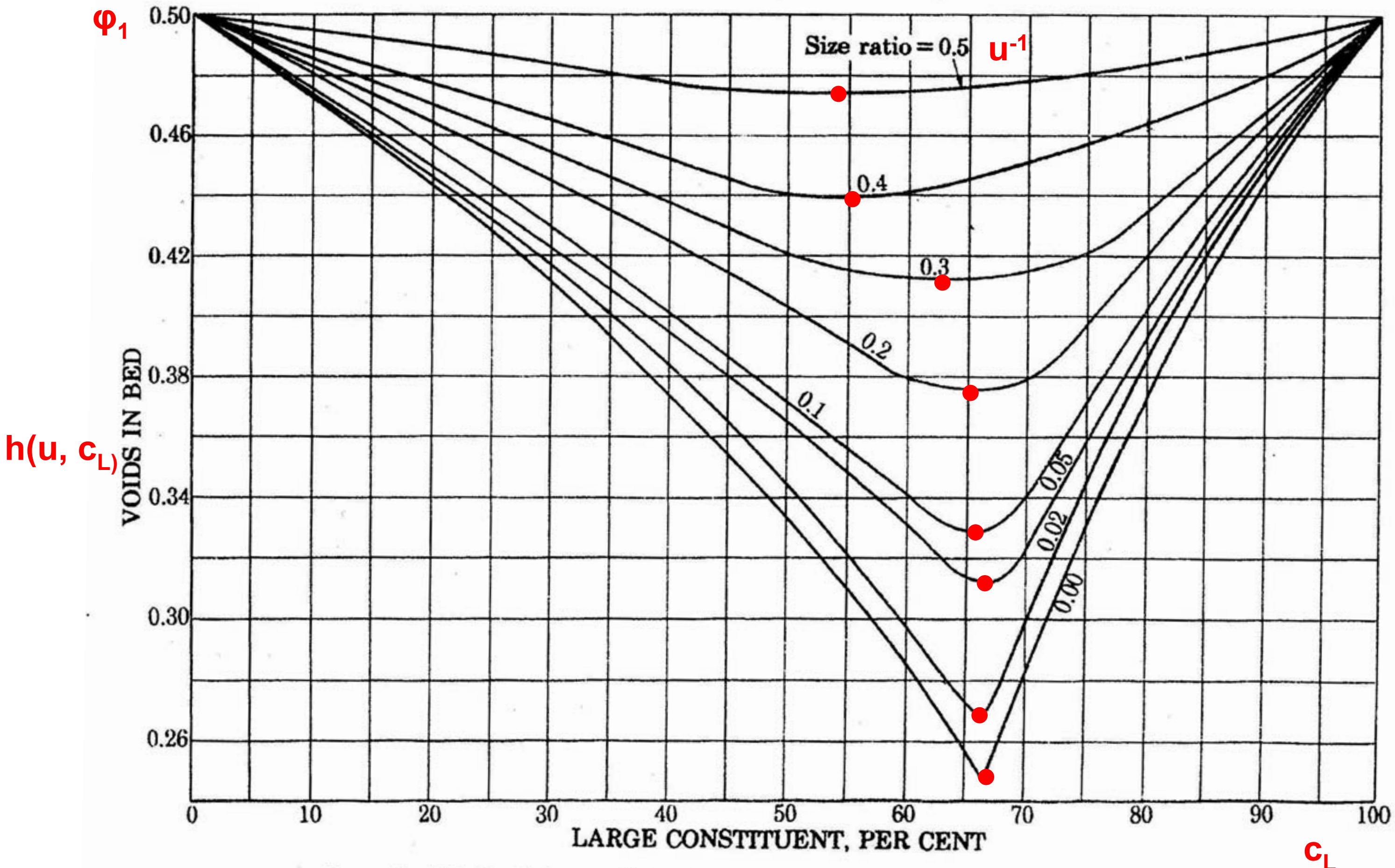
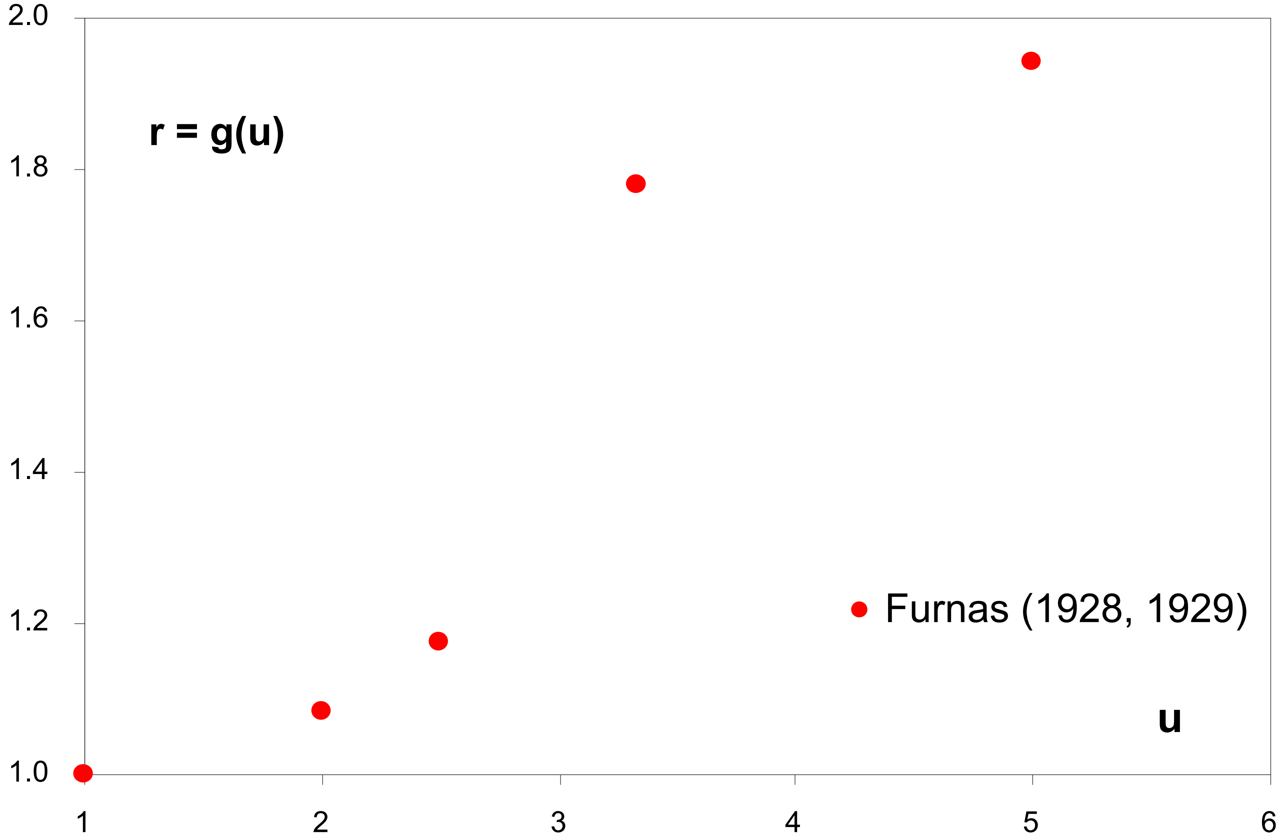


Figure 3.- Relation between voids and size composition in two-component systems of broken solids, when voids of mixed components = 0.50

Furnas (1928, 1929)

Volume ratio of optimum packing



← c_L/c_S = $1/\varphi_1 = 2$

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Bimodal discrete (u → 1)

$$\beta = -\frac{1}{\varphi_1(1-\varphi_1)}\left.\frac{dh}{du}\right|_{u=1,c_L=0.5} = -\left.\frac{dH}{du}\right|_{u=1,r=1}$$

φ_1 and β depend on:
- particle shape
- mode of packing (loose, dense)

only

Values of φ_1 and β

Material	Mode	Shape	φ_1	β
Steel	rcp	spherical	0.375	0.140
Simulation	rcp	spherical	0.360	0.204
Steel	rlp	spherical	0.500	0.125
Plastic	rcp	cubical	0.433	0.134
Quartz	rcp	fairly angular	0.497	0.374
Feldspar	rcp	plate-shaped	0.503	0.374
Dolomite	rcp	fairly rounded	0.505	0.347
Sillimanite	rcp	distinctly angular	0.531	0.395
Flint	rlp	angular	0.55	0.160

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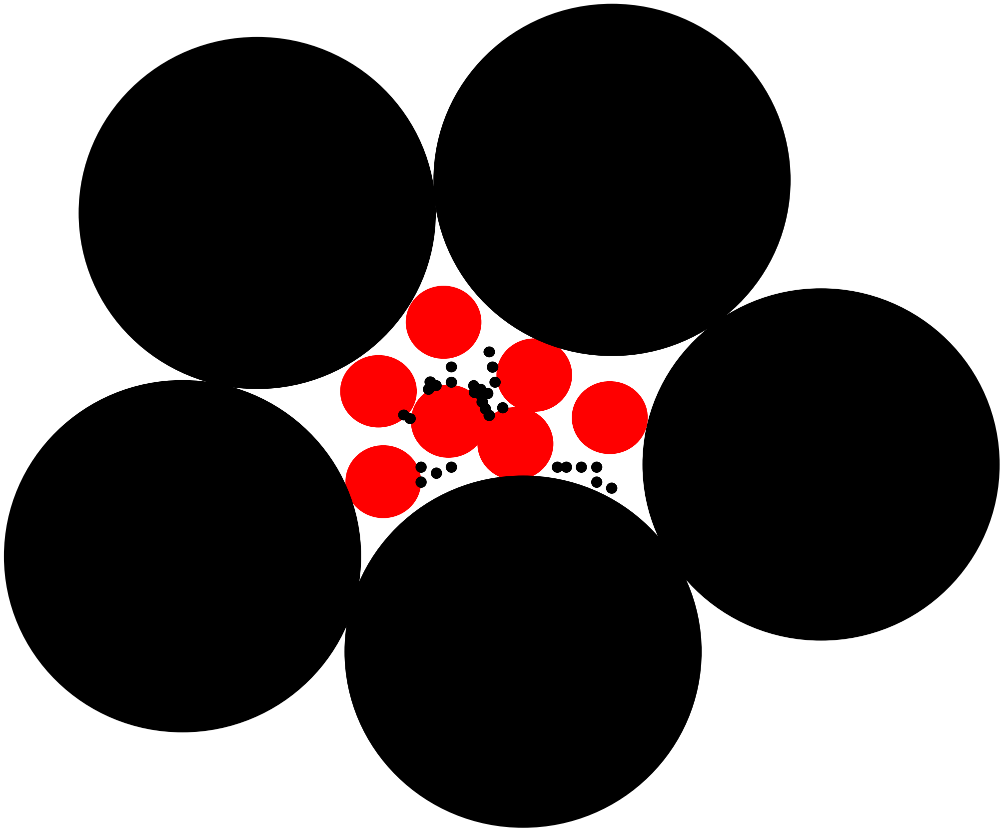
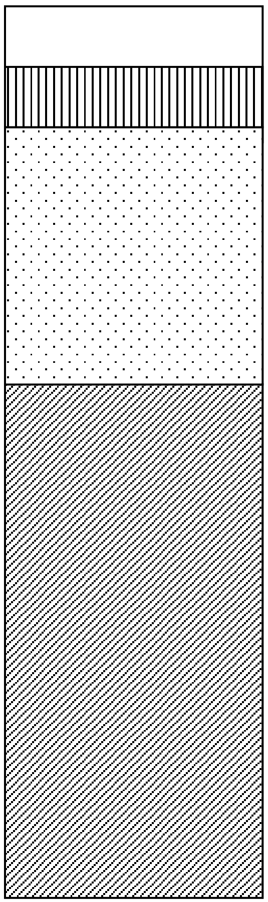
Polydisperse discrete (saturated)



Polydisperse discrete (saturated)



$\varphi_n = \varphi_1{}^n$

$f_n = 1 - (1 - f_1)^n$

f_1

$$c_i = \frac{f_i - f_{i-1}}{f_n} = \frac{\varphi_1^{i-1}(1-\varphi_1)}{1-\varphi_1^n}$$

$i = 1, 2, \ldots n$

Bimodal (n = 2):

$$c_1 = \frac{1-\varphi_1}{1-\varphi_1^2} = \frac{1}{1+\varphi_1}$$

$$c_2 = \frac{\varphi_1(1-\varphi_1)}{1-\varphi_1^2} = \frac{\varphi_1}{1+\varphi_1}$$

$r = c_i/c_{i+1} = 1/\varphi_1$

Polydisperse saturated discrete packing is geometric:

- diameter/size ratio of subsequent fractions is constant: u
- quantity/population ratio of subsequent fractions is constant: r

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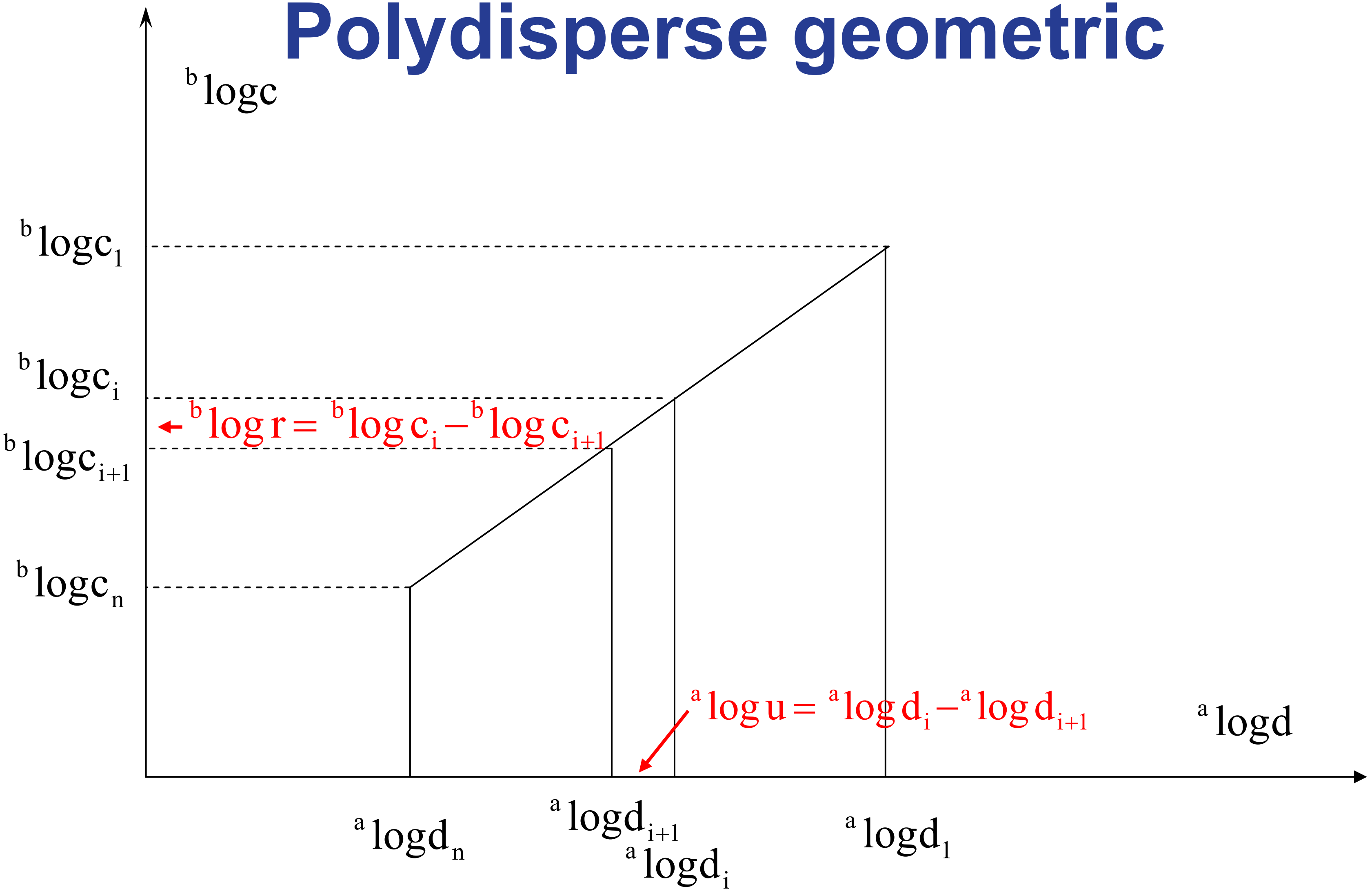
Polydisperse geometric



Polydisperse discrete geometric

$$d_i = d_1\left(u^{1-i}\right); c_i = c_1\left(r^{1-i}\right)$$

$$F(d_i) = \frac{\sum_i^n c_i}{\sum_1^n c_i} = \frac{c_i + c_{i+1} + ... + c_{n-1} + c_n}{c_1 + c_2 + ... + c_{n-1} + c_n}$$

$$= \frac{r^{n-i}c_n + r^{n-i-1}c_n + ... + rc_n + c_n}{r^{n-1}c_n + r^{n-2}c_n + ... + rc_n + c_n} = \frac{1 + r + r^2 + ... + r^{n-i}}{1 + r + r^2 + ... + r^{n-1}} = \frac{r^{n-i+1} - 1}{r^n - 1}$$

Polydisperse discrete geometric

$$y = \frac{d_1}{d_{n+1}} = u^n \Rightarrow n = {}^u\log y = {}^u\log\left[\frac{d_1}{d_{n+1}}\right]$$

$$n - i + 1 = {}^u\log\left[\frac{d_i}{d_{n+1}}\right]$$

$$F(d_i) = \frac{r^{n-i+1} - 1}{r^n - 1} = \frac{r^{{}^u\log(d_i/d_{n+1})} - 1}{r^{{}^u\log(d_1/d_{n+1})} - 1} = \frac{d_i^\alpha - d_{n+1}^\alpha}{d_1^\alpha - d_{n+1}^\alpha}$$

$\alpha = {}^u\log r$ Saturated rlp: $r = 2$ $(= 1/\varphi_1)$, $u \approx 10$

Polydisperse discrete geometric (void fraction)

$$\varphi = \varphi_1 \left(\frac{h(u,r)}{\varphi_1} \right)^{n-1} = \varphi_1 \left(\frac{\varphi_1^2}{\varphi_1} \right)^{n-1} \qquad \text{saturated}$$

$$= \varphi_1^n = \varphi_1 \cdot \varphi_1^{\,{}^{u}\log(d_1/d_n)} = \varphi_1 \left(\frac{d_1}{d_n} \right)^{{}^{u}\log \varphi_1}$$

$$\varphi = \varphi_1 \left(\frac{h(u,r)}{\varphi_1} \right)^{n-1} \qquad \text{unsaturated}$$

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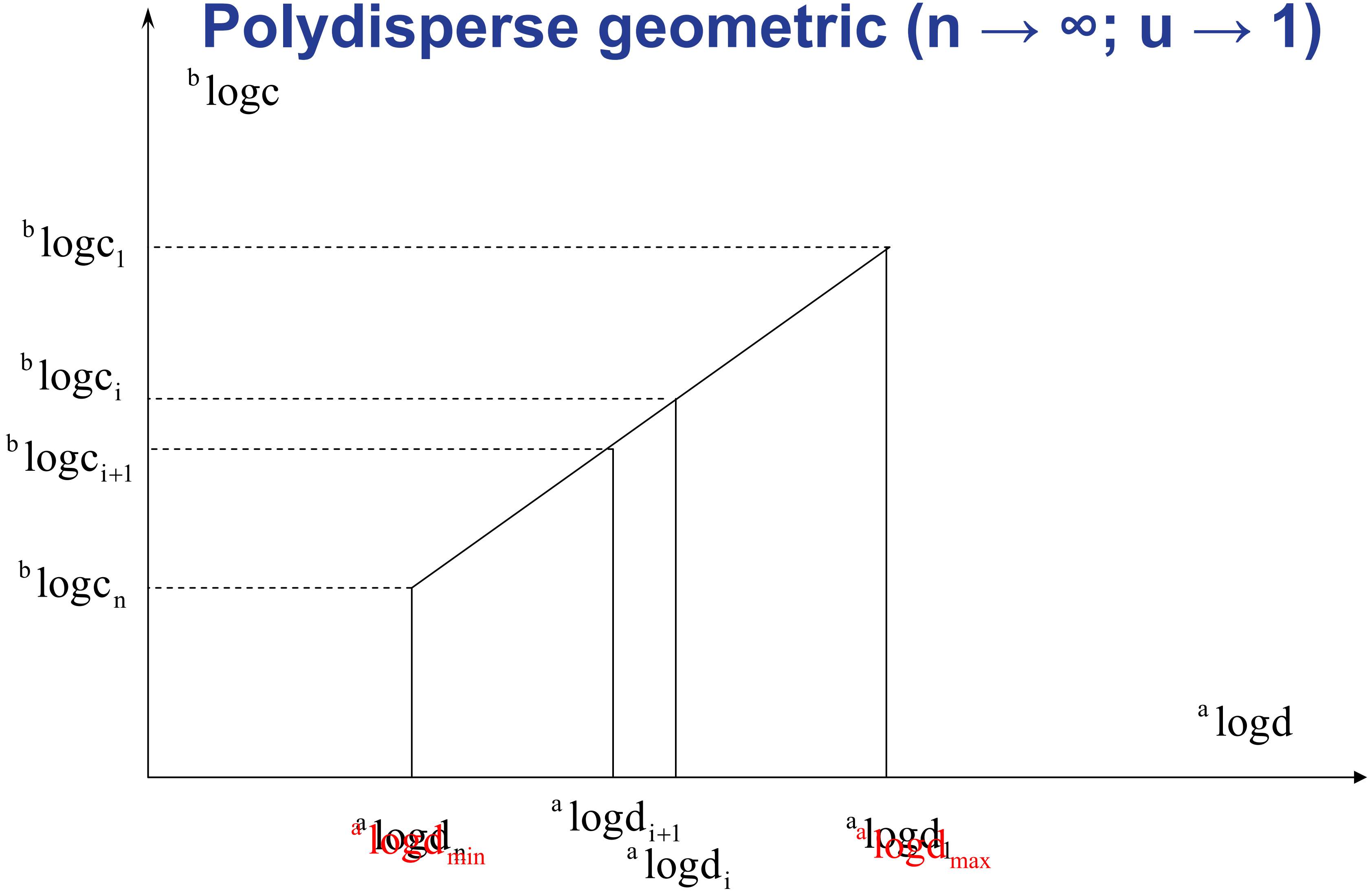
Polydisperse geometric (n → ∞; u → 1)



Polydisperse geometric ($n \to \infty$; $u \to 1$)

$$y = \frac{d_{max}}{d_{min}} = u^n \Rightarrow u = y^{\frac{1}{n}} \approx 1 + \frac{1}{n} \ln y + O(\frac{1}{n^2})$$

$$\alpha = {}^{u}\log r$$

$$r = y^{\frac{\alpha}{n}} \approx 1 + \frac{\alpha}{n} \ln y + O(\frac{1}{n^2})$$

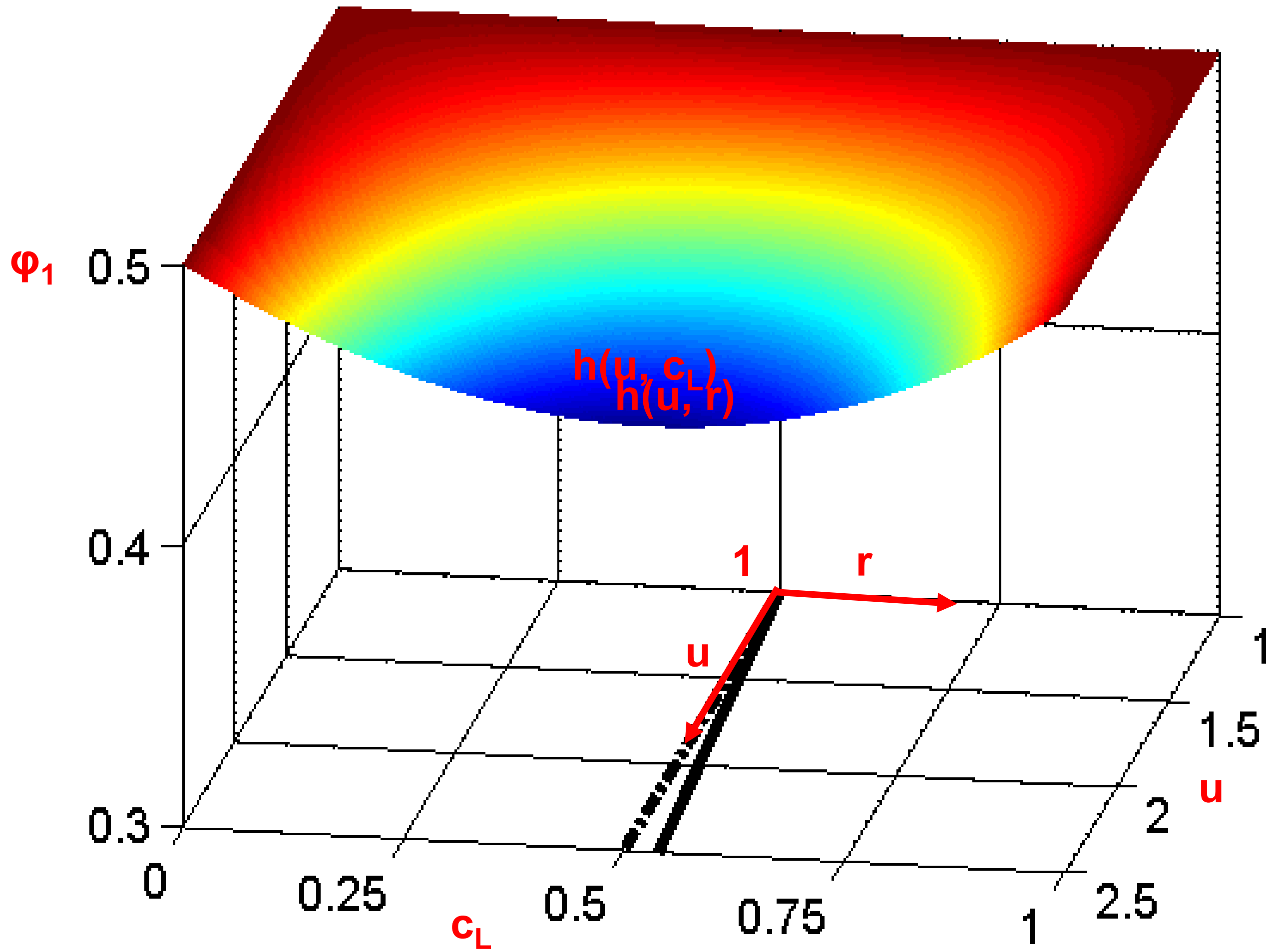
Polydisperse geometric (u → 1)

$$\lim_{u \to 1} \alpha = \lim_{u \to 1} {}^{u}\log r = \left.\frac{dr}{du}\right|_{u=1}$$

$$F(d) = \frac{d^{\alpha} - d_{min}^{\alpha}}{d_{max}^{\alpha} - d_{min}^{\alpha}} \qquad \alpha \neq 0$$

$$F(d) = \frac{\ln d - \ln d_{min}}{\ln d_{max} - \ln d_{min}} \qquad \alpha = 0$$

Polydisperse geometric (u → 1)



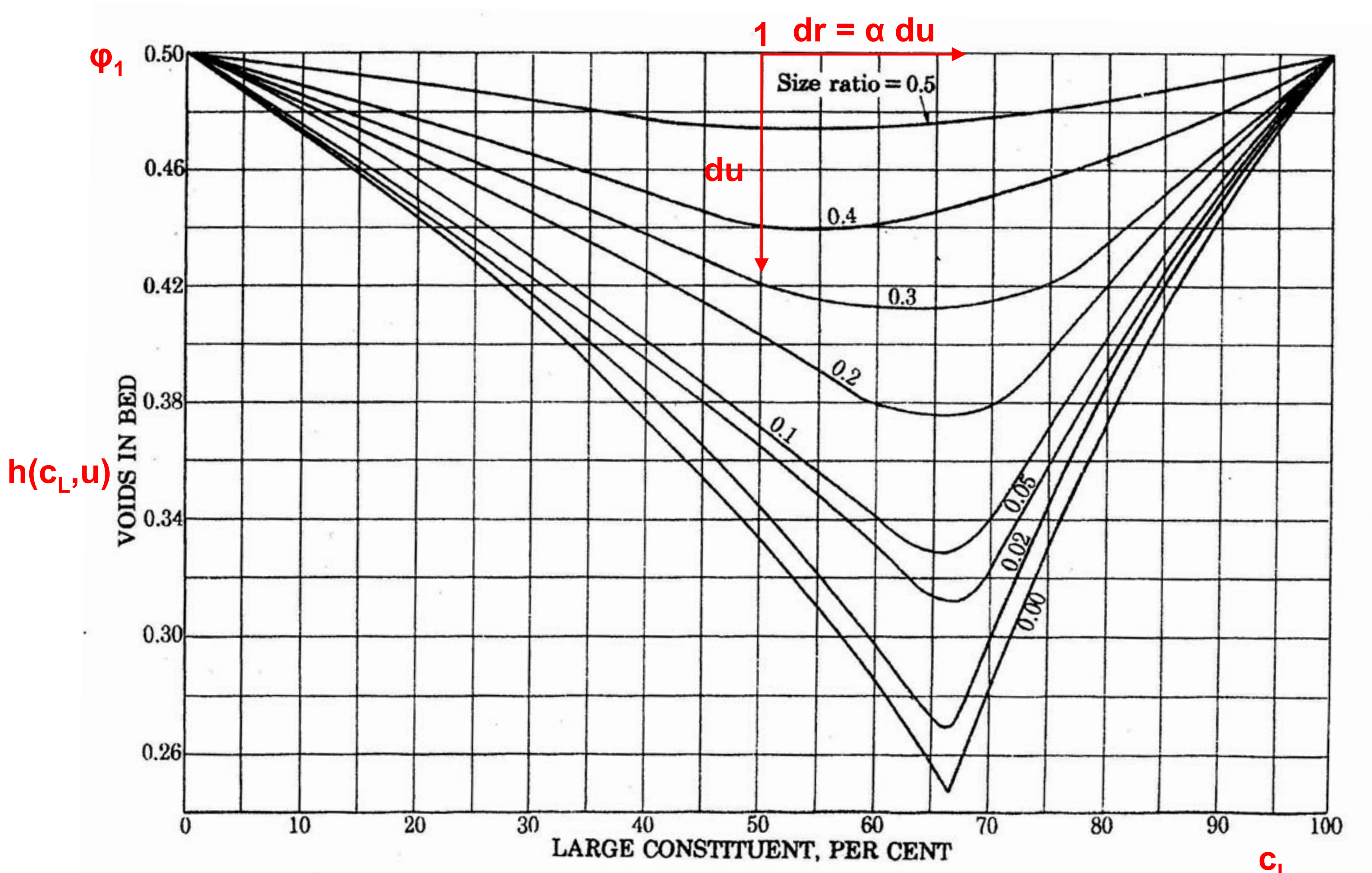
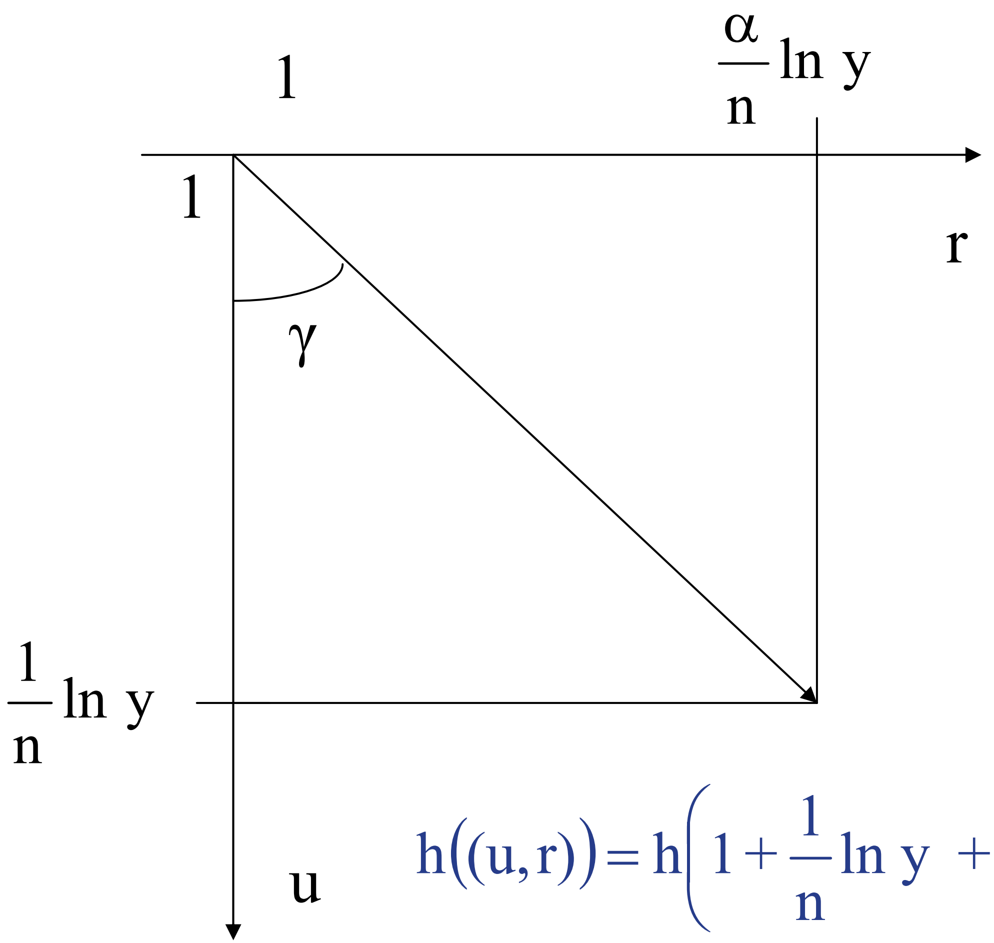


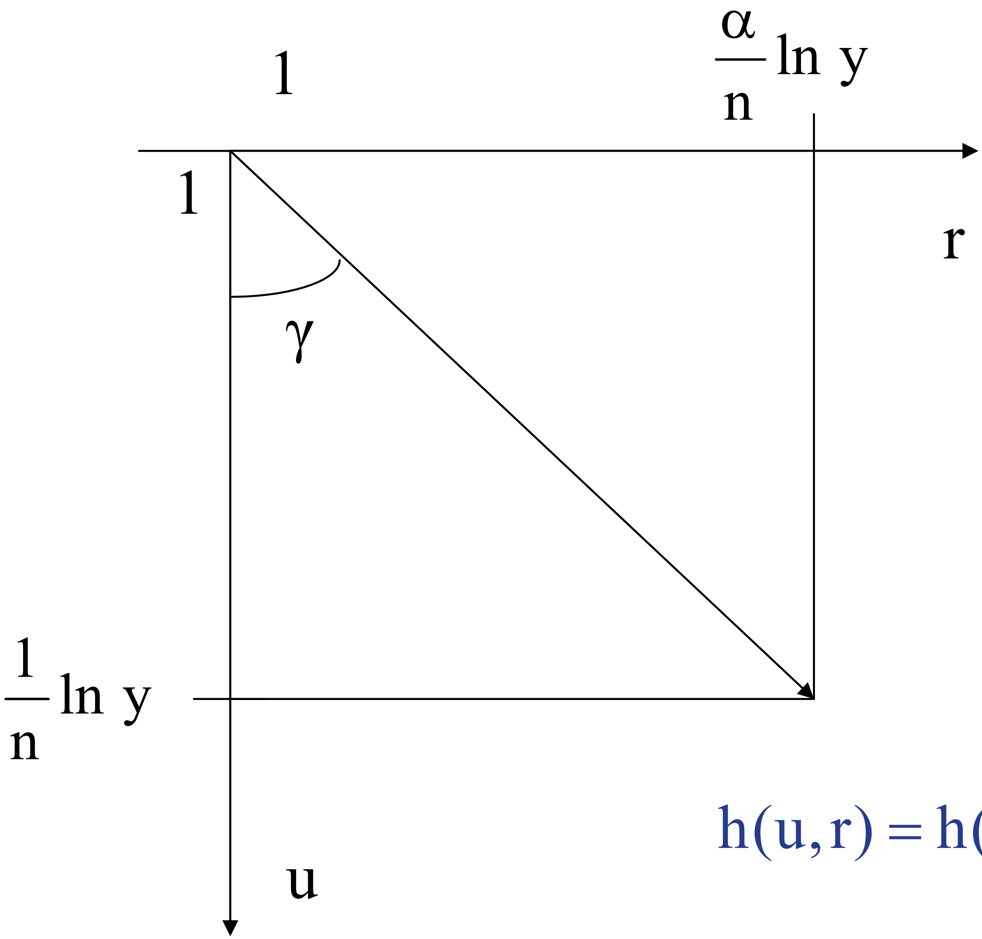
Figure 3.- Relation between voids and size composition in two-component systems of broken solids, when voids of mixed components = 0.50

Polydisperse geometric (n → ∞; u → 1)



$$h((u,r)) = h\left(1+\frac{1}{n}\ln y + O\left(\frac{1}{n^2}\right), 1+\frac{\alpha}{n}\ln y + O\left(\frac{1}{n^2}\right)\right)$$

Polydisperse geometric ($n \to \infty$; $u \to 1$)



$$\cos\gamma = \frac{1}{1+\alpha^2}$$

$- \beta(1-\varphi_1)\,\varphi_1$

$$h(u,r) = h(1,1) + \frac{\cos\gamma \ln y}{n} \cdot \left.\frac{dh}{du}\right|_{u=1,r=1}$$

φ_1

Polydisperse geometric continuous

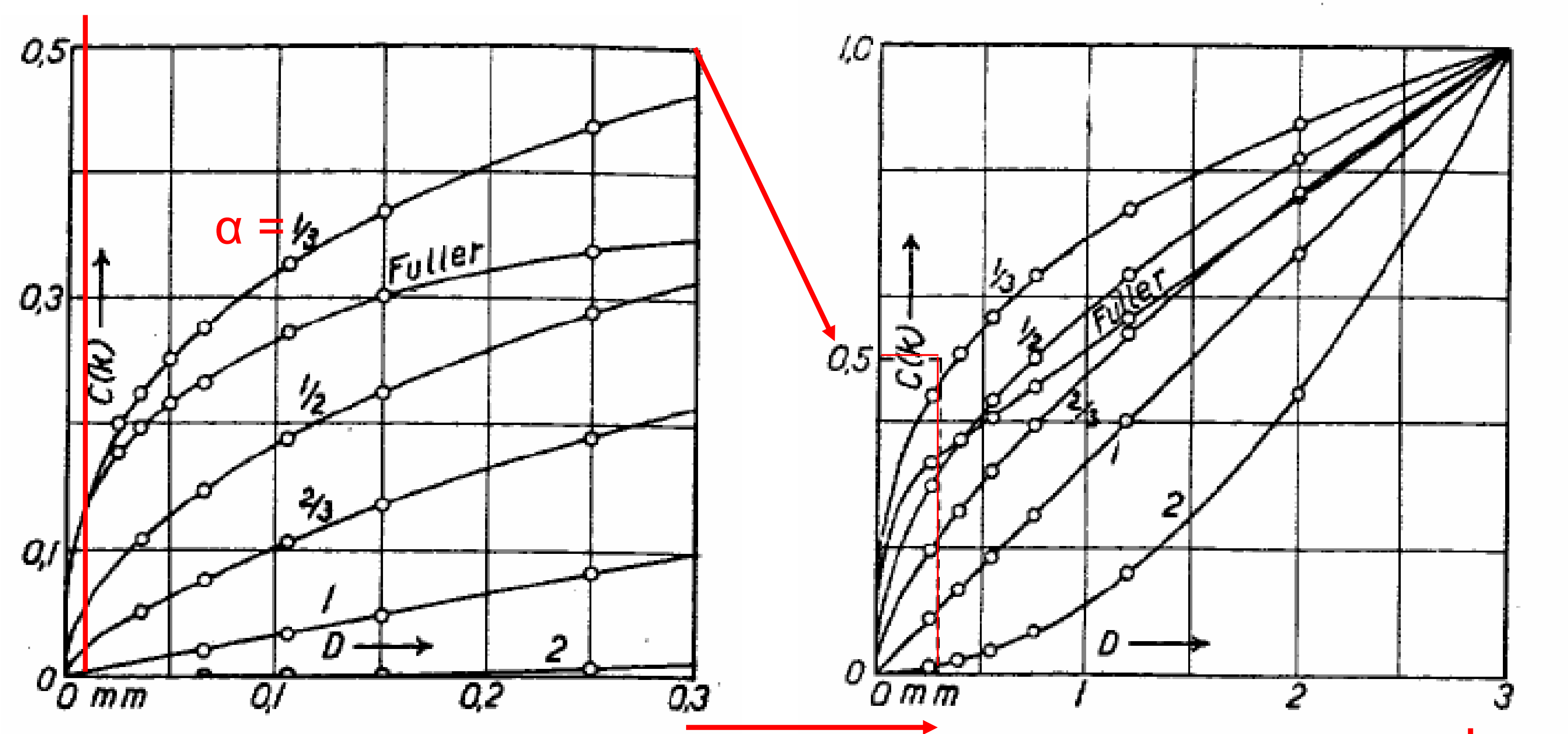
$$\varphi = \varphi_1 \left(\frac{h(u,r)}{\varphi_1} \right)^{n-1} \qquad \varphi_1^2 \le h \le \varphi_1$$

$$\varphi = \varphi_1 \lim_{n \to \infty} \left(1 - \frac{\beta(1-\varphi_1)}{n(1+\alpha^2)} \ln y + O\left(\frac{1}{n^2}\right) \right)^{n-1}$$

$$= \varphi_1 y^{\frac{-(1-\varphi_1)\beta}{(1+\alpha^2)}} = \varphi_1 \left(\frac{d_{max}}{d_{min}} \right)^{\frac{-(1-\varphi_1)\beta}{(1+\alpha^2)}} \approx \varphi_1 \left(\frac{d_{max}}{d_{min}} \right)^{-\frac{1}{5}}$$

Caquot (1937)

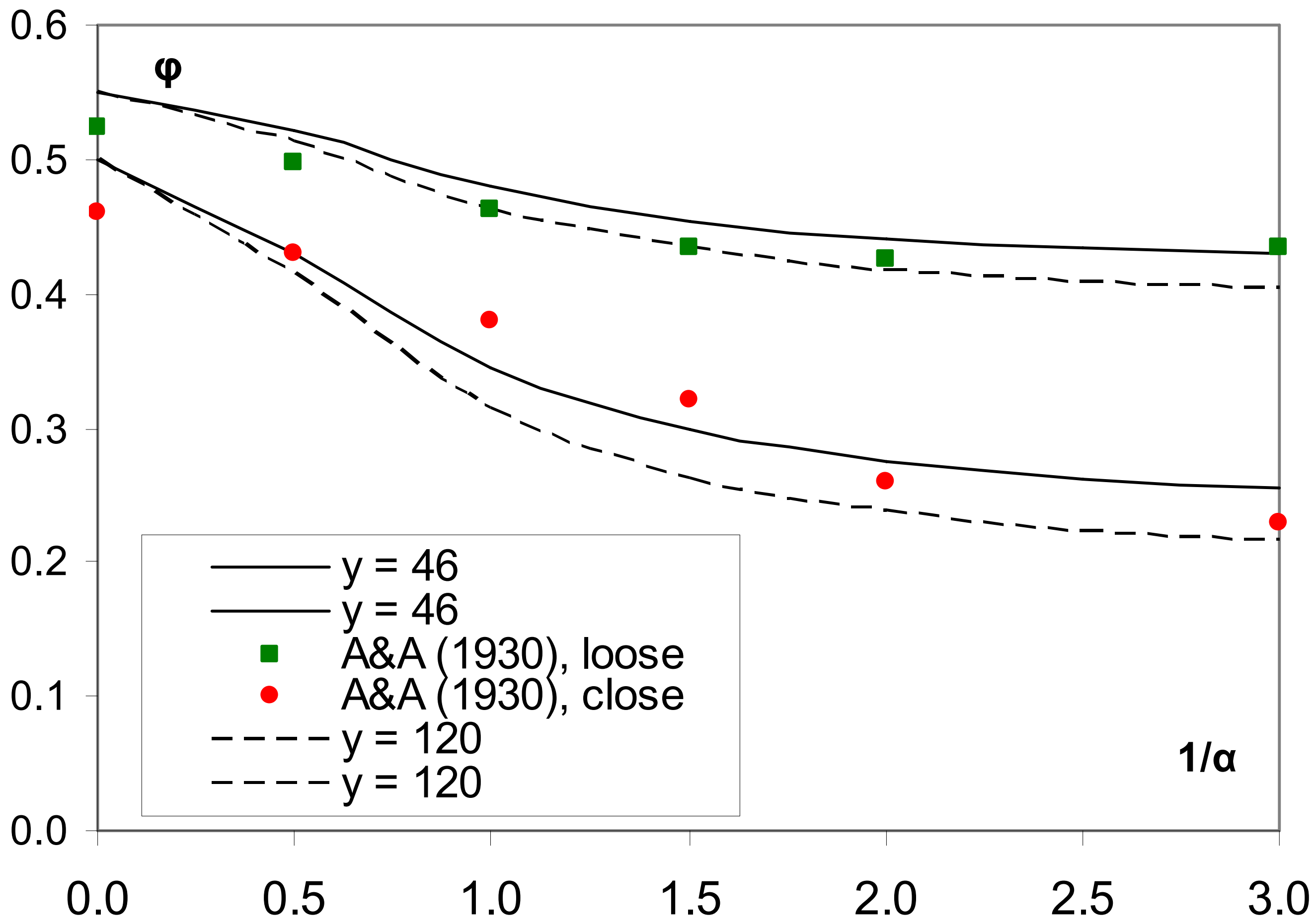
Andreasen and Andersen (1930)



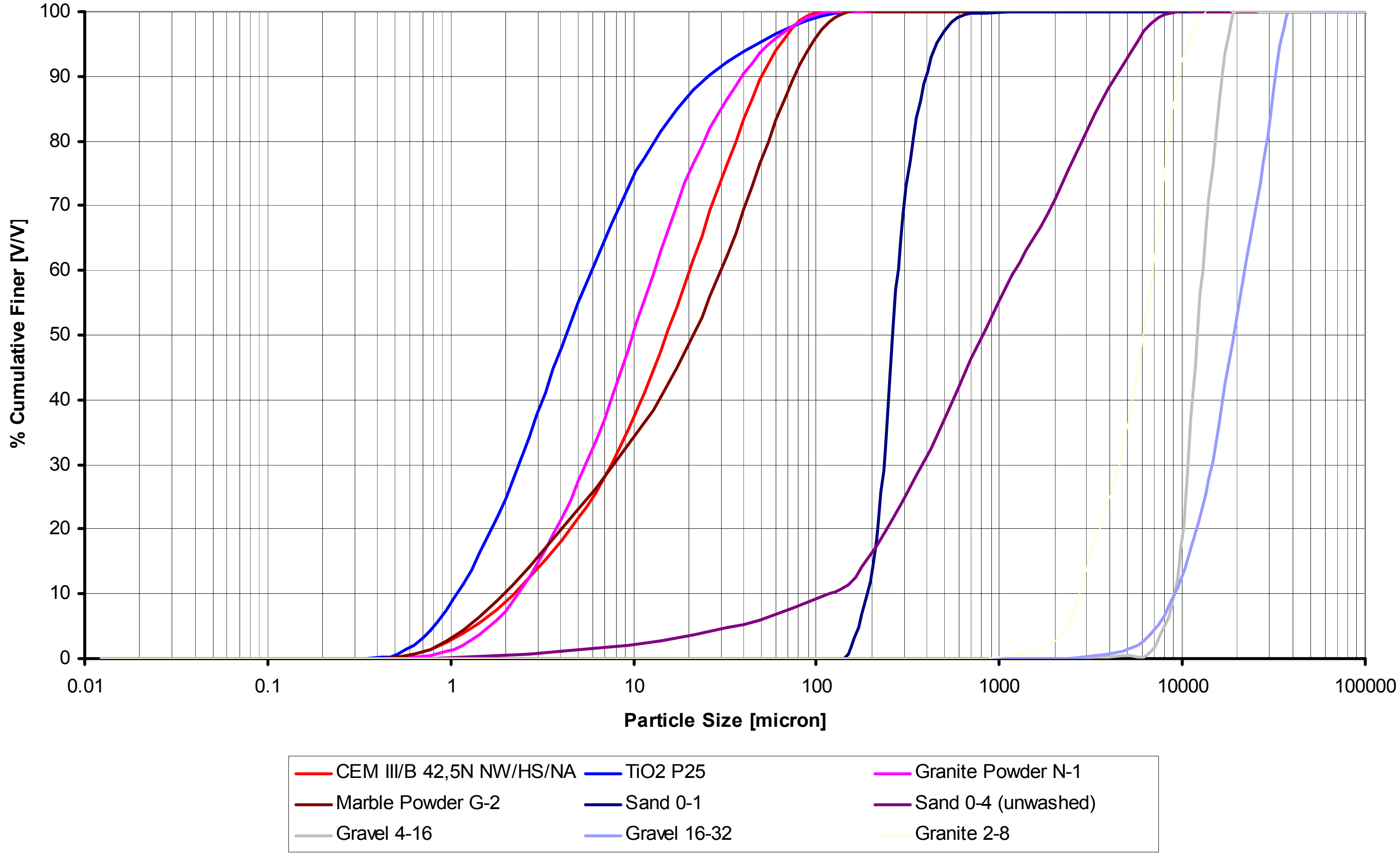
$$F(d) = \left(\frac{d}{d_{max}} \right)^{\alpha}$$

$$F(d) = \frac{d^{\alpha} - d_{min}^{\alpha}}{d_{max}^{\alpha} - d_{min}^{\alpha}}$$

Andreasen and Andersen (1930)

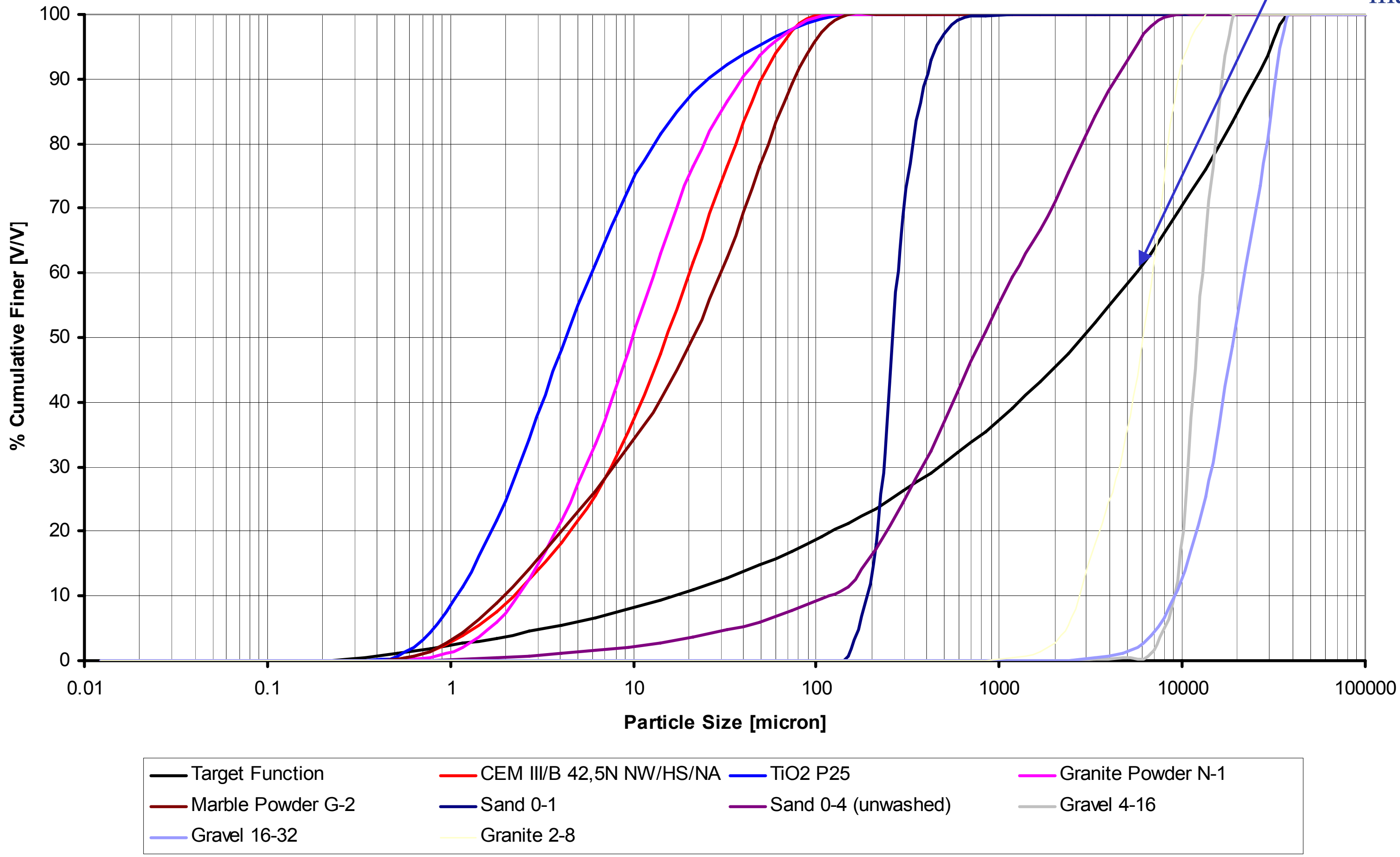


Mix design tool



Mix design tool

$$F(d) = \frac{d^{\alpha} - d_{min}^{\alpha}}{d_{max}^{\alpha} - d_{min}^{\alpha}}$$



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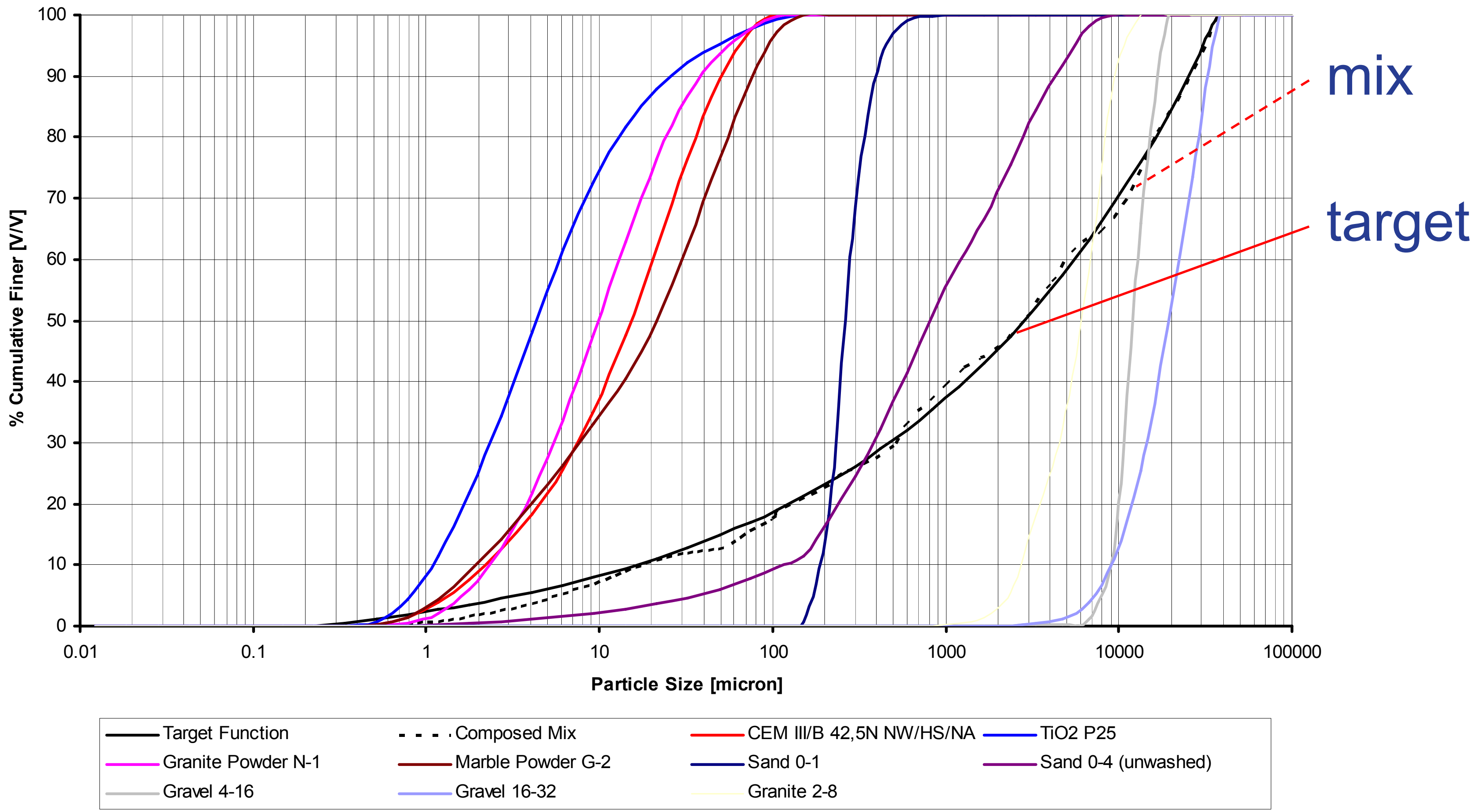

Slump flow with/without J-Ring

$$\text{Blocking factor (B)} = 2 \cdot \left(h_{in} - h_{ex}\right) - \left(h_{c} - h_{in}\right)$$

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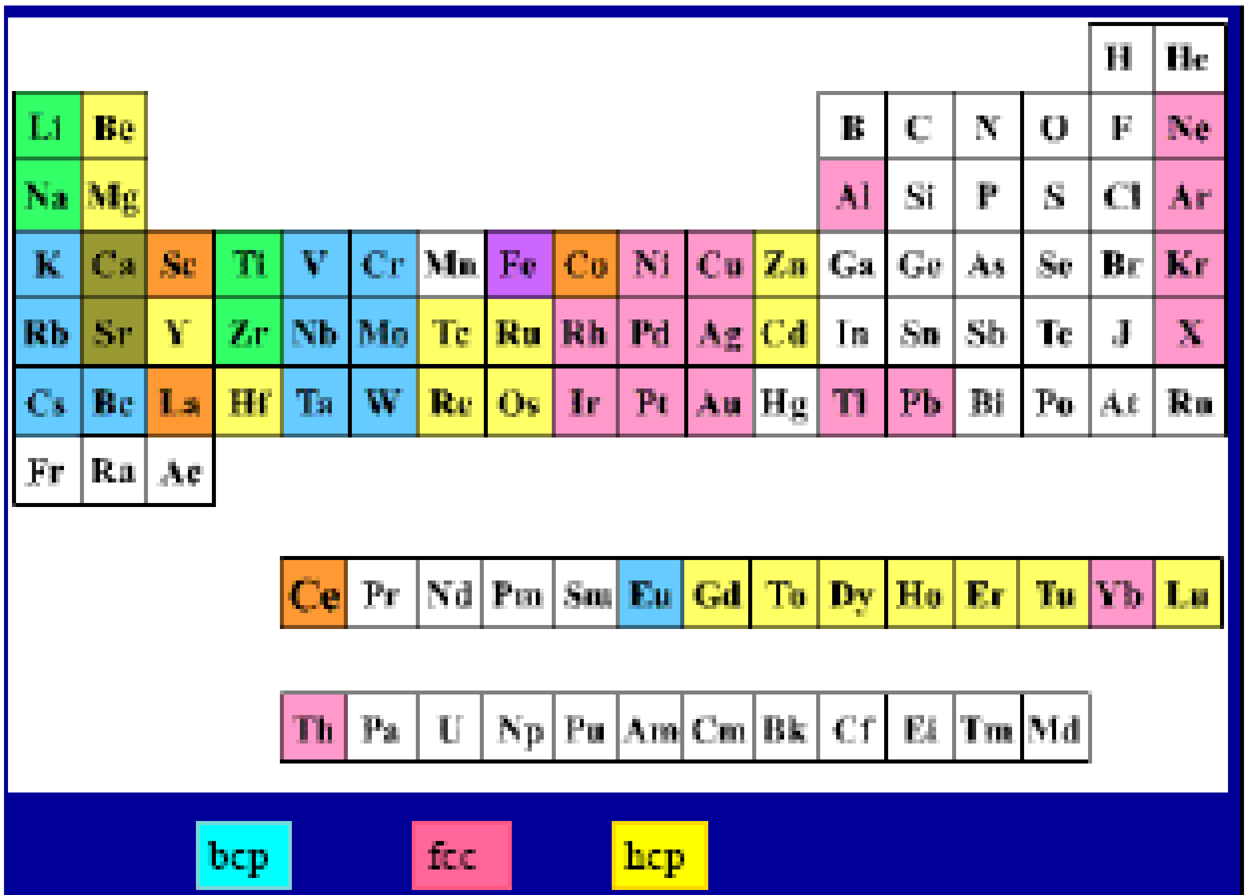
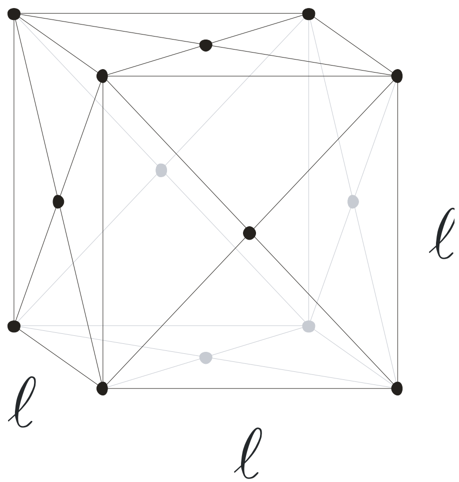
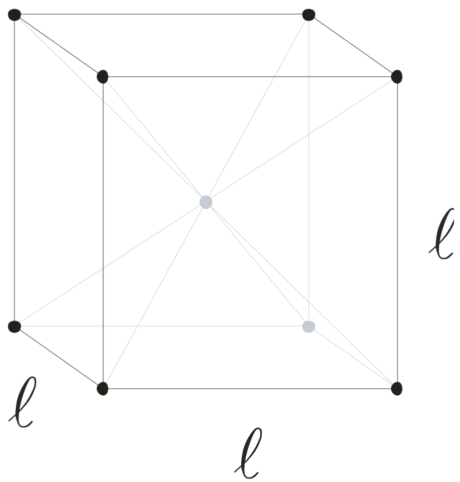
Crystalline structure elements



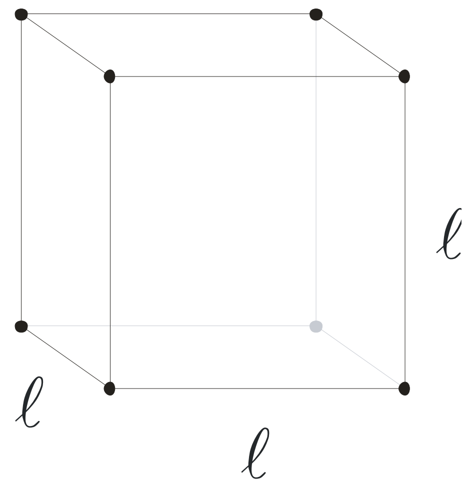
Bravais lattices (u = 1) cubic system



fcc
A1, α

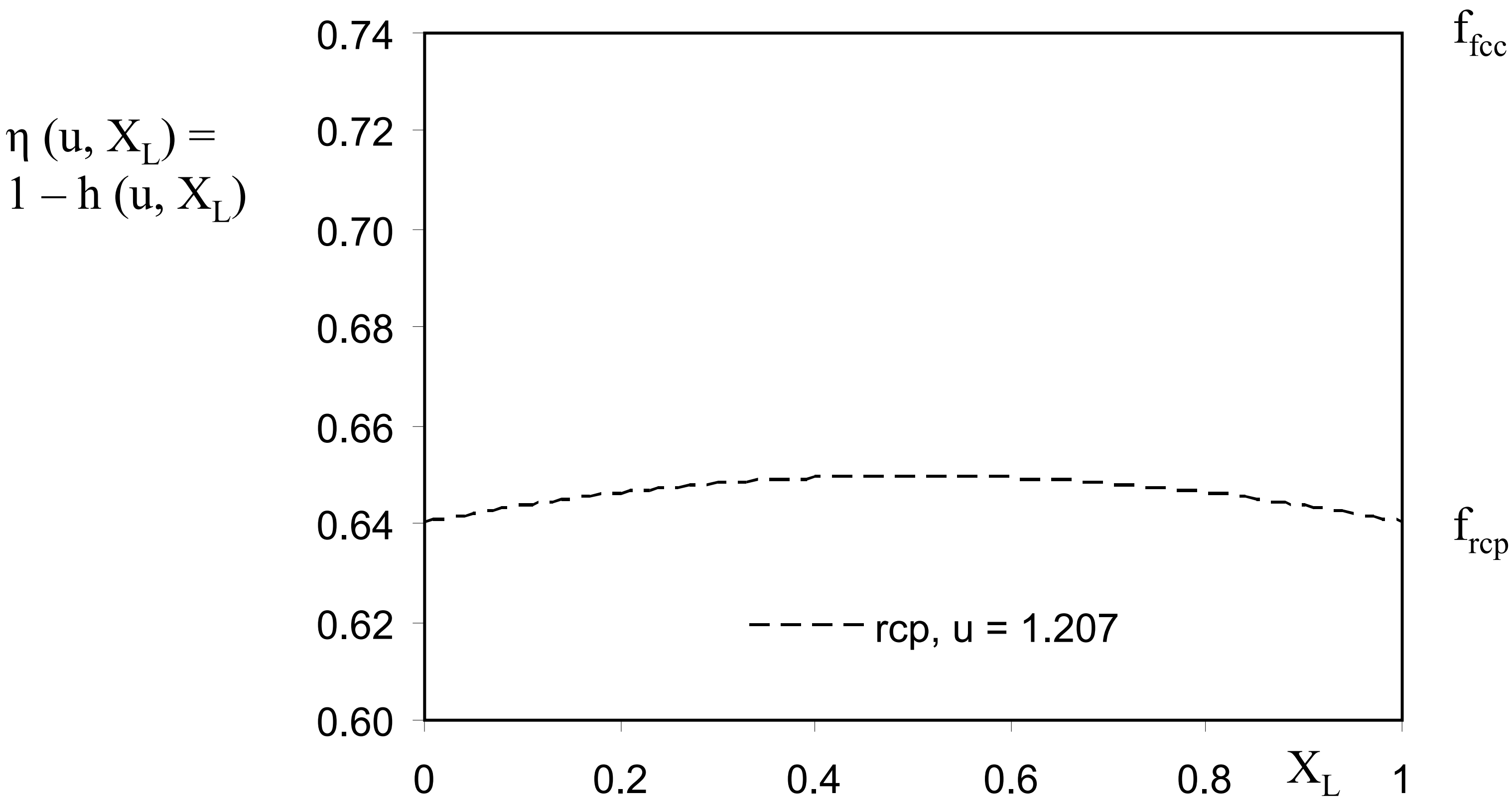


bcc
A2, β



sc

Bimodal random discrete spheres



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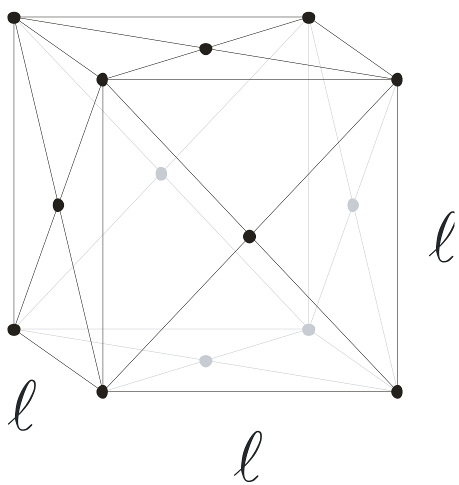
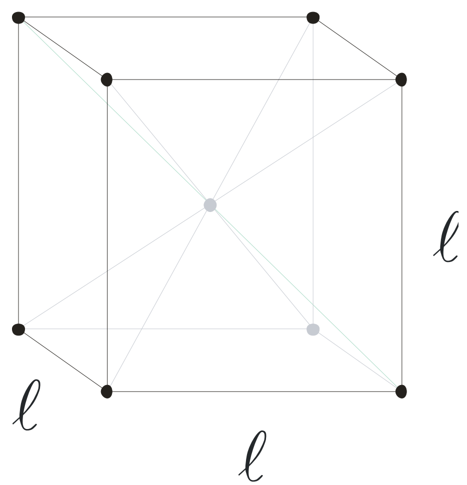
u = 1: monosized crystalline (cubic)

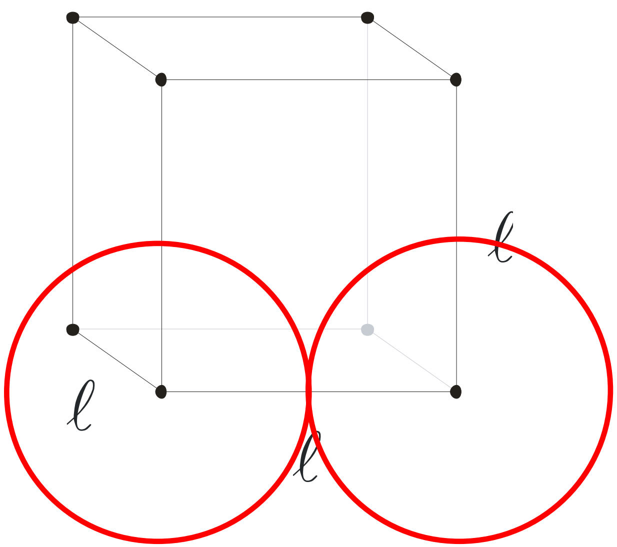
fcc



bcc



sc

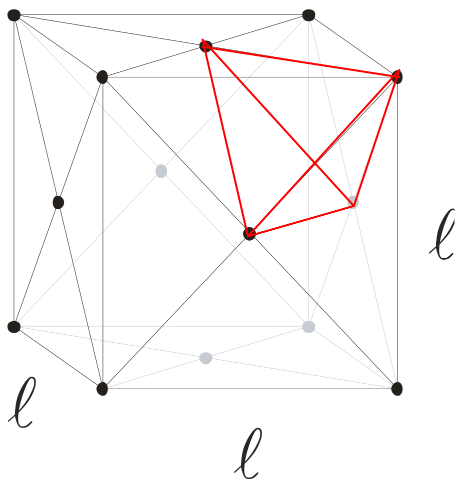


$$f_{fcc} = \frac{4\frac{\pi}{6}d^3}{\ell^3} = \frac{4\frac{\pi}{6}d^3}{(d\sqrt{2})^3} = \frac{\pi\sqrt{2}}{6} \approx 0.74$$

$$f_{bcc} = \frac{2\frac{\pi}{6}d^3}{\ell^3} = \frac{2\frac{\pi}{6}d^3}{(2d/\sqrt{3})^3} = \frac{\pi\sqrt{3}}{8} \approx 0.68$$

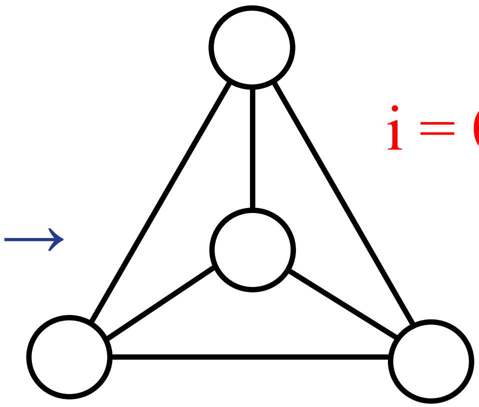
$$f_{sc} = \frac{\frac{\pi}{6}d^3}{\ell^3} = \frac{\frac{\pi}{6}d^3}{d^3} = \frac{\pi}{6} \approx 0.52$$

Building block fcc



Tetrahedron (n = 4)

Graph →



i = 0 and 4 (n)

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \lambda(\ell_L^3 - \ell_S^3)\right)\right] - \lambda(X_L^n + (1-X_L)^n)(\ell_L^3 - \ell_S^3)$$

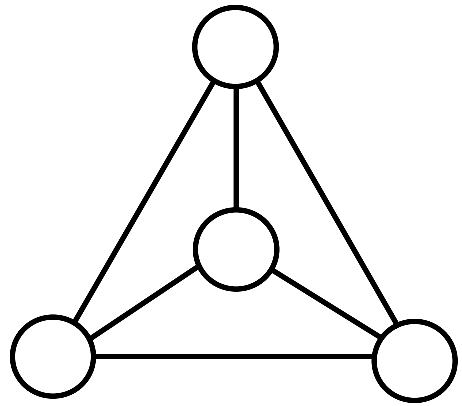
$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

Bimodal building block fcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3\right) + \psi_i(\ell_L^3 - \ell_S^3)\right]$$

$$i = 0;\ \psi_i = 0$$

$$V_{cell} = \binom{4}{0} X_L^4 \ell_L^3 = X_L^4 \ell_L^3$$



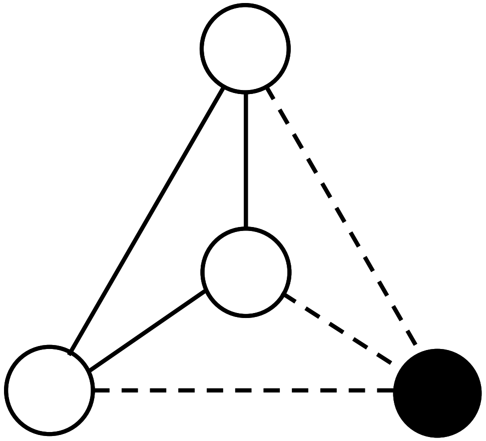
Bimodal building block fcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$i = 1;\ \psi_i = 3C/6 = C/2$

$$V_{cell} = \binom{4}{1} X_L^3(1-X_L)\left(\tfrac{3}{4}\ell_L^3 + \tfrac{1}{4}\ell_S^3 + \tfrac{C}{2}(\ell_L^3 - \ell_S^3)\right) =$$

$$4X_L^3(1-X_L)\left(\tfrac{3}{4}\ell_L^3 + \tfrac{1}{4}\ell_S^3 + \tfrac{C}{2}(\ell_L^3 - \ell_S^3)\right)$$



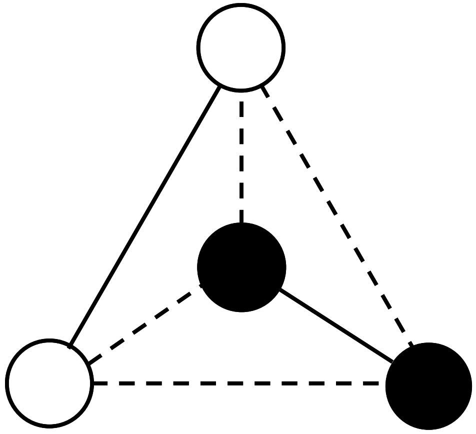
Bimodal building block fcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$i = 2;\ \psi_i = 4C/6 = 2C/3$

$$V_{cell} = \binom{4}{2} X_L^2(1-X_L)^2\left(\tfrac{2}{4}\ell_L^3 + \tfrac{2}{4}\ell_S^3 + \tfrac{2C}{3}(\ell_L^3 - \ell_S^3)\right) =$$

$$6X_L^3(1-X_L)\left(\tfrac{1}{2}\ell_L^3 + \tfrac{1}{2}\ell_S^3 + \tfrac{2C}{3}(\ell_L^3 - \ell_S^3)\right)$$



Bimodal building block fcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$$\sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3\right)\right] = X_L\ell_L^3 + (1-X_L)\ell_S^3$$

Retgers

$$\sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\psi_i(\ell_L^3 - \ell_S^3)\right] = 2C\,X_L(1-X_L)(\ell_L^3 - \ell_S^3)$$

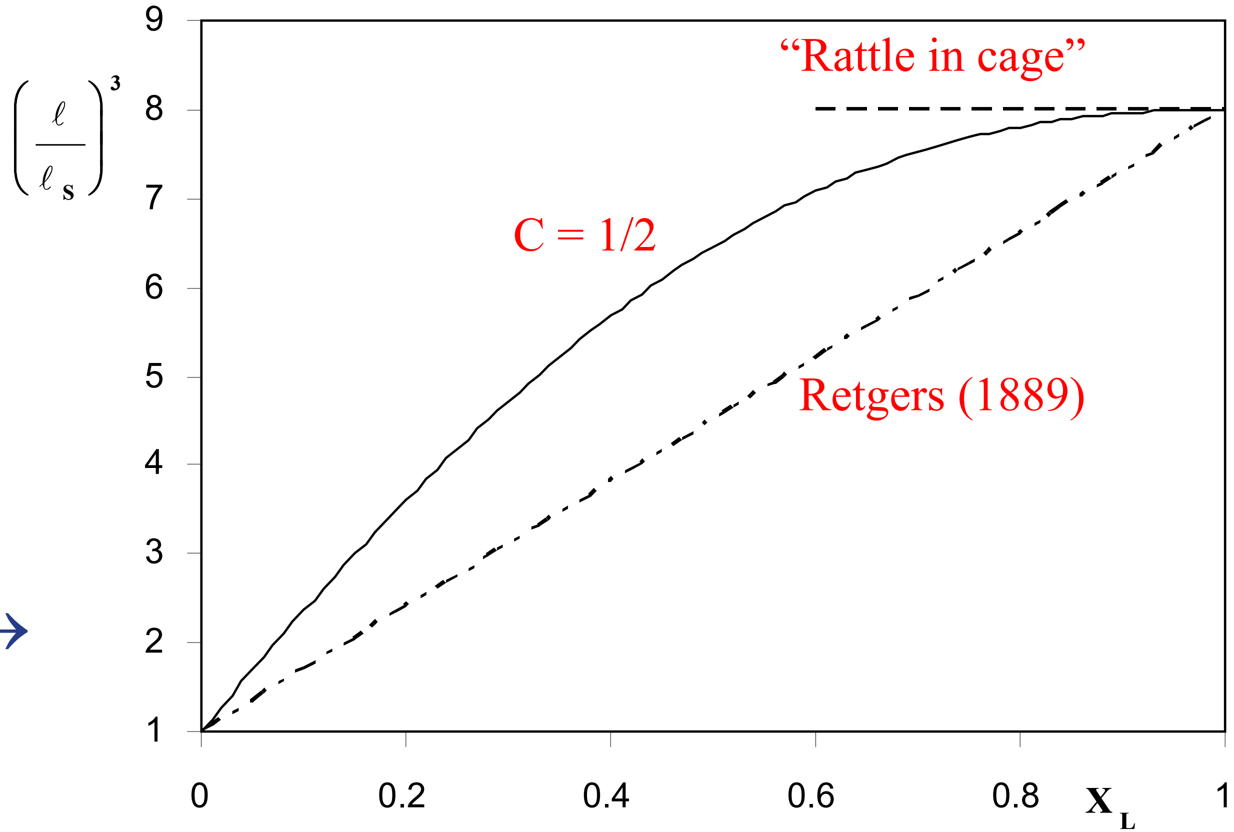
$$V_{cell} = X_L\ell_L^3 + (1-X_L)\ell_S^3 + 2C\,X_L(1-X_L)(\ell_L^3 - \ell_S^3)$$

Bimodal cell volume

$$\left.\frac{dV_{cell}}{dX_L}\right|_{X_L=1} = 0$$

$$\rightarrow C = 1/2$$

$$\ell_L / \ell_S = u = 2 \rightarrow$$



Bimodal fcc cell volume (C = ½)

$$V_{\mathrm{cell}} = \ell^3 = \boxed{X_L \ell_L^3 + (1 - X_L)\ell_S^3} \boxed{+ X_L(1 - X_L)(\ell_L^3 - \ell_S^3)}$$

c_L	ℓ_L (nm)	ℓ_S (nm)	u	X_L	measured (nm)	model (nm)	$\ell_{\mathrm{Re\,tgers}}$ (nm)
0.500	414	375	1.104	0.426	403	402	393
0.901	472	375	1.259	0.048	385	386	381

Colloidal crystallization data: Luck, Klier & Wesslau (1963)

Packing fraction bimodal fcc

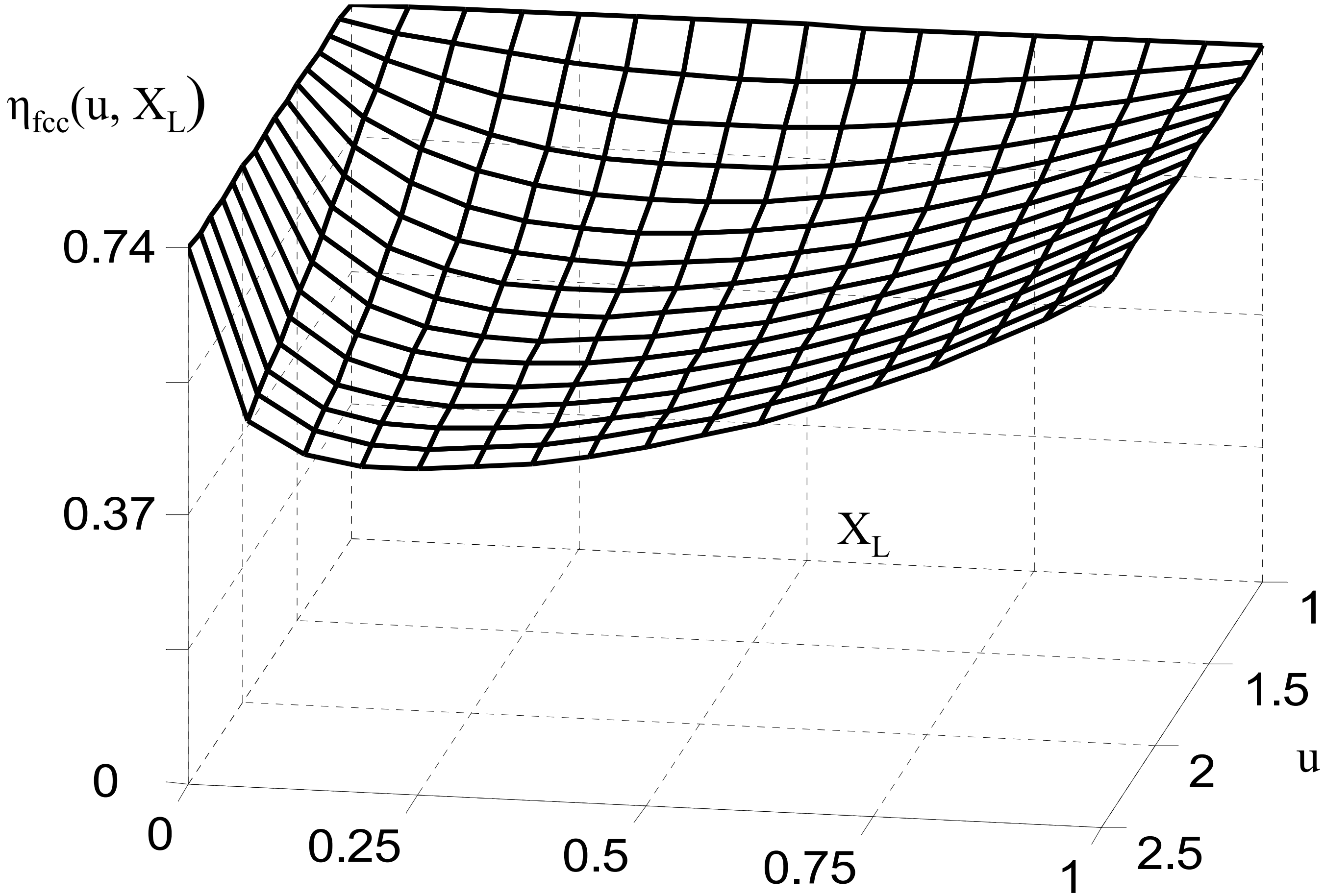
$$V_{cell} = \ell^3 = X_L \ell_L^3 + (1 - X_L)\ell_S^3 + X_L(1 - X_L)(\ell_L^3 - \ell_S^3)$$

$$d^3 = X_L d_L^3 + (1 - X_L) d_S^3$$

$$\frac{d_L}{d_S} = u;\ \ell_S = d_S\sqrt{2};\ \ell_L = d_L\sqrt{2} \Rightarrow \frac{\ell_L}{\ell_S} = u$$

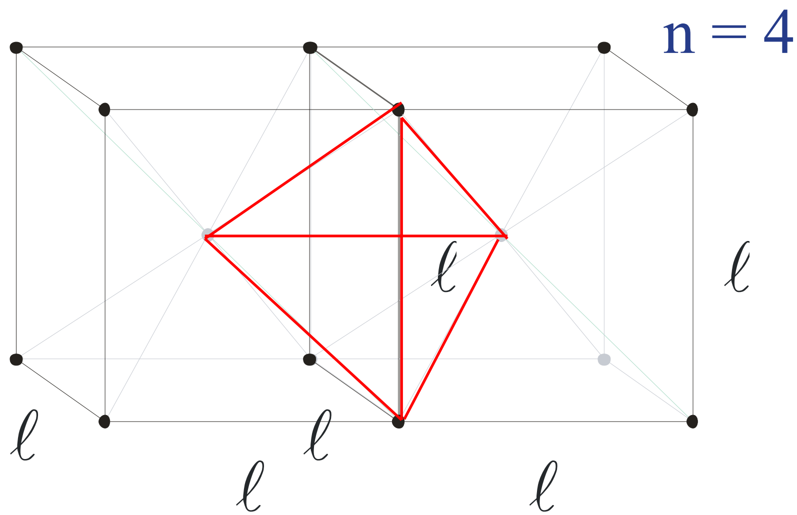
$$\eta_{fcc} = \frac{4\frac{\pi}{6}d^3}{\ell^3} = f_{fcc}\left(\frac{X_L(u^3 - 1) + 1}{X_L(u^3 - 1) + 1 + X_L(1 - X_L)(u^3 - 1)}\right)$$

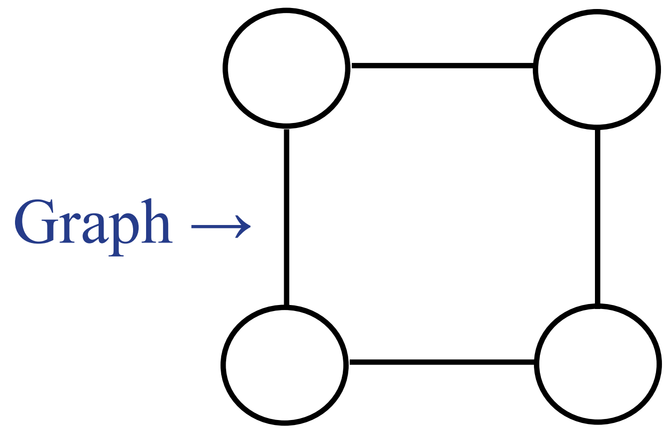
Packing fraction bimodal fcc



Building block bcc

i = 0 and 4 (n)





$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \lambda(\ell_L^3 - \ell_S^3)\right)\right] - \lambda\left(X_L^n + (1-X_L)^n\right)(\ell_L^3 - \ell_S^3)$$

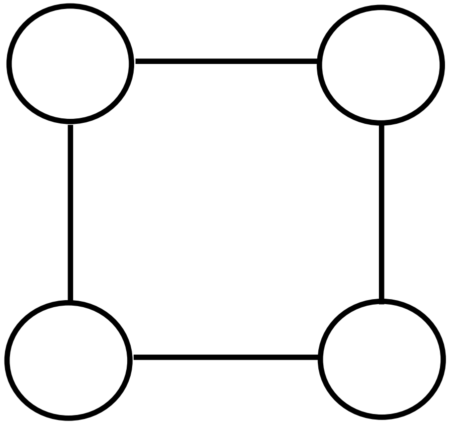
$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

Bimodal building block bcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3\right) + \psi_i(\ell_L^3 - \ell_S^3))\right]$$

$$i = 0;\ \psi_i = 0$$

$$V_{cell} = \binom{4}{0} X_L^4 \ell_L^3 = X_L^4 \ell_L^3$$



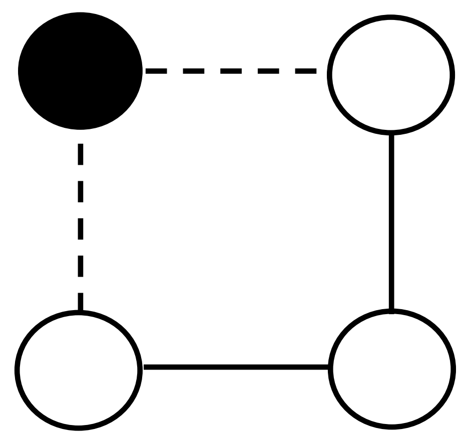
Bimodal building block bcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$i = 1;\ \psi_i = 2C/4 = C/2$

$$V_{cell} = \binom{4}{1} X_L^3(1-X_L)\left(\tfrac{3}{4}\ell_L^3 + \tfrac{1}{4}\ell_S^3 + \tfrac{C}{2}(\ell_L^3 - \ell_S^3)\right) =$$

$$4X_L^3(1-X_L)\left(\tfrac{3}{4}\ell_L^3 + \tfrac{1}{4}\ell_S^3 + \tfrac{C}{2}(\ell_L^3 - \ell_S^3)\right)$$



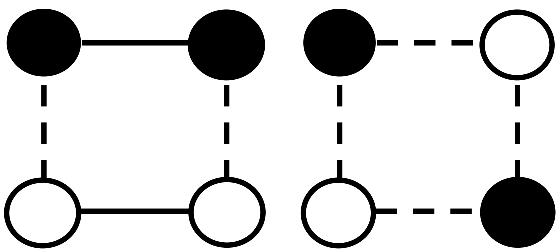
Bimodal building block bcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$i = 2; \psi_i = C\ (2/3 \text{ x } 2/4 + 1/3 \text{ x } 4/4) = 2C/3$

$$V_{cell} = \binom{4}{2} X_L^2(1-X_L)^2\left(\frac{2}{4}\ell_L^3 + \frac{2}{4}\ell_S^3 + \frac{2C}{3}(\ell_L^3 - \ell_S^3)\right) =$$

$$6X_L^3(1-X_L)\left(\frac{1}{2}\ell_L^3 + \frac{1}{2}\ell_S^3 + \frac{2C}{3}(\ell_L^3 - \ell_S^3)\right)$$



p = 2/3   p = 1/3

Bimodal building block bcc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$$\sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3\right)\right] = X_L\ell_L^3 + (1-X_L)\ell_S^3$$

$$\sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\psi_i(\ell_L^3 - \ell_S^3)\right] = 2C\,X_L(1-X_L)(\ell_L^3 - \ell_S^3)$$

$$V_{cell} = X_L\ell_L^3 + (1-X_L)\ell_S^3 + 2C\,X_L(1-X_L)(\ell_L^3 - \ell_S^3)$$

Packing fraction bimodal bcc

$$\left.\frac{dV_{cell}}{dX_L}\right|_{X_L=1} = 0 \Rightarrow C = 1/2$$

$$V_{cell} = \ell^3 = X_L \ell_L^3 + (1 - X_L)\ell_S^3 + X_L(1 - X_L)(\ell_L^3 - \ell_S^3)$$

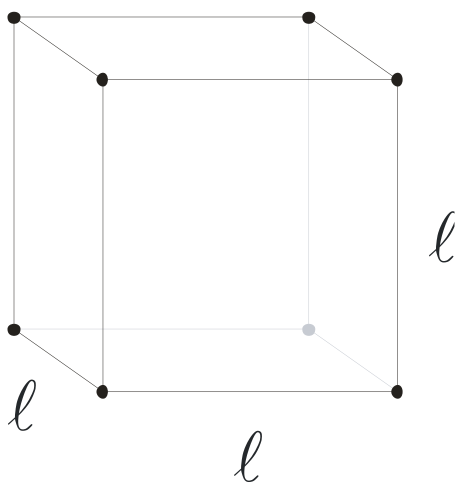
$$d^3 = X_L d_L^3 + (1 - X_L) d_S^3 \qquad \frac{d_L}{d_S} = u;\ \ell_S = 2d_S/\sqrt{3};\ \ell_L = 2d_L/\sqrt{3} \Rightarrow \frac{\ell_L}{\ell_S} = u$$

$$\eta_{bcc} = \frac{2\frac{\pi}{6}d^3}{\ell^3} = f_{bcc}\left(\frac{X_L(u^3 - 1) + 1}{X_L(u^3 - 1) + 1 + X_L(1 - X_L)(u^3 - 1)}\right)$$

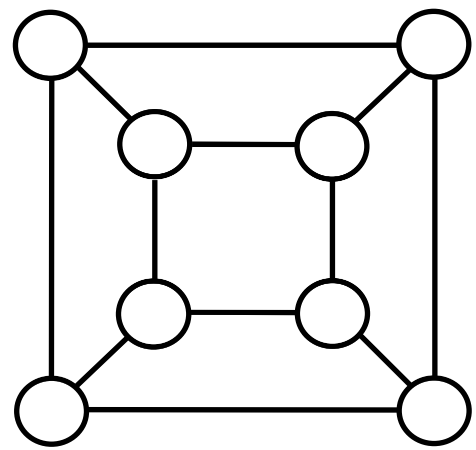
Building block sc

i = 0 and 8 (n)

n = 8



Graph →



$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \lambda(\ell_L^3 - \ell_S^3)\right)\right] - \lambda(X_L^n + (1-X_L)^n)(\ell_L^3 - \ell_S^3)$$

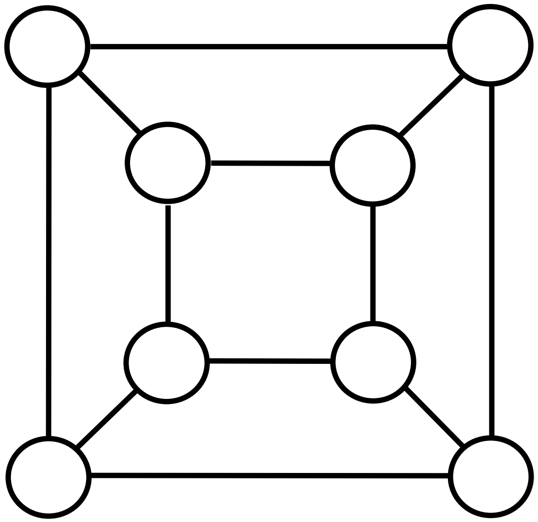
$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

Bimodal building block sc

$$V_{cell} = \sum_{i=0}^{n} \left[\binom{n}{i} X_L^{n-i} (1 - X_L)^i \left(\frac{n-i}{n} \ell_L^3 + \frac{i}{n} \ell_S^3 \right) + \psi_i (\ell_L^3 - \ell_S^3) \right]$$

$$i = 0; \psi_i = 0$$

$$V_{cell} = \binom{8}{0} X_L^8 \ell_L^3 = X_L^8 \ell_L^3$$



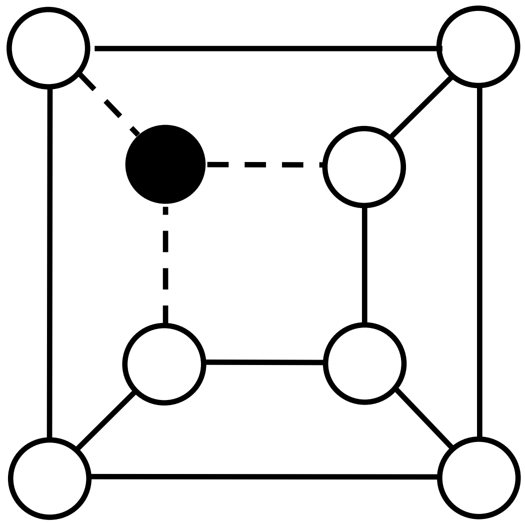
Bimodal building block sc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\tfrac{n-i}{n}\ell_L^3 + \tfrac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$$i = 1;\ \psi_i = C/4$$

$$V_{cell} = \binom{8}{1} X_L^7(1-X_L)\left(\tfrac{7}{8}\ell_L^3 + \tfrac{1}{8}\ell_S^3 + \tfrac{C}{4}(\ell_L^3 - \ell_S^3)\right) =$$

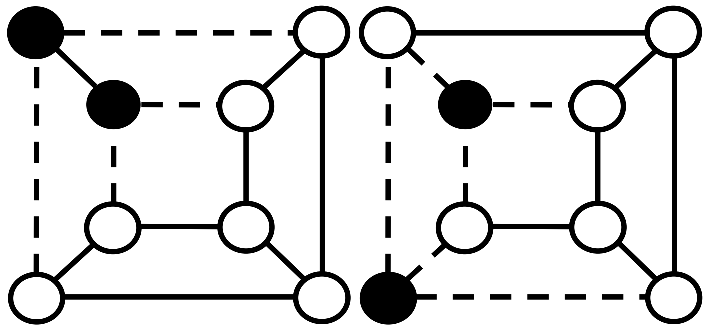
$$8X_L^3(1-X_L)\left(\tfrac{7}{8}\ell_L^3 + \tfrac{1}{7}\ell_S^3 + \tfrac{C}{4}(\ell_L^3 - \ell_S^3)\right)$$



Bimodal building block sc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$i = 2;\ \psi_i = C\ (3/7 \times 4/12 + 4/7 \times 6/12) = 3C/7$



p = 3/7 p = 4/7

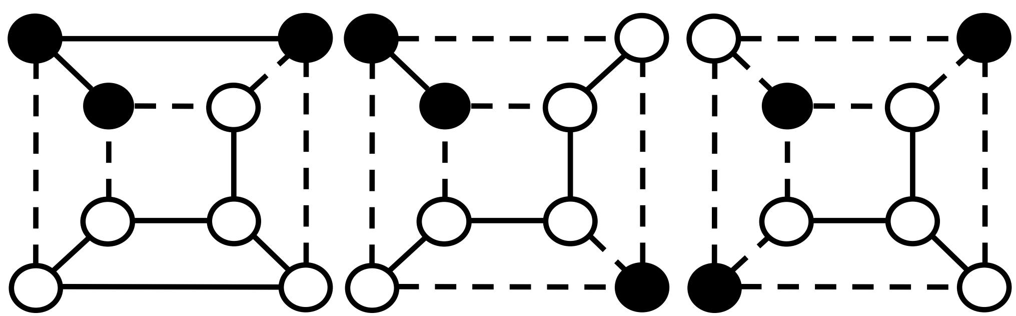
$$V_{cell} = \binom{8}{2} X_L^6(1-X_L)^2\left(\frac{6}{8}\ell_L^3 + \frac{2}{8}\ell_S^3 + \frac{3C}{7}(\ell_L^3 - \ell_S^3)\right) =$$

$$28 X_L^3(1-X_L)\left(\frac{3}{4}\ell_L^3 + \frac{1}{4}\ell_S^3 + \frac{3C}{7}(\ell_L^3 - \ell_S^3)\right)$$

Bimodal building block sc

$$V_{cell} = \sum_{i=0}^{n} \left[\binom{n}{i} X_L^{n-i} (1 - X_L)^i \left(\tfrac{n-i}{n} \ell_L^3 + \tfrac{i}{n} \ell_S^3 + \psi_i (\ell_L^3 - \ell_S^3) \right) \right]$$

$i = 3$; $\psi_i = C\ (3/7 \times 5/12 + 3/7 \times 7/12 + 1/7 \times 9/12) = 15C/28$



p = 3/7 p = 3/7 p = 1/7

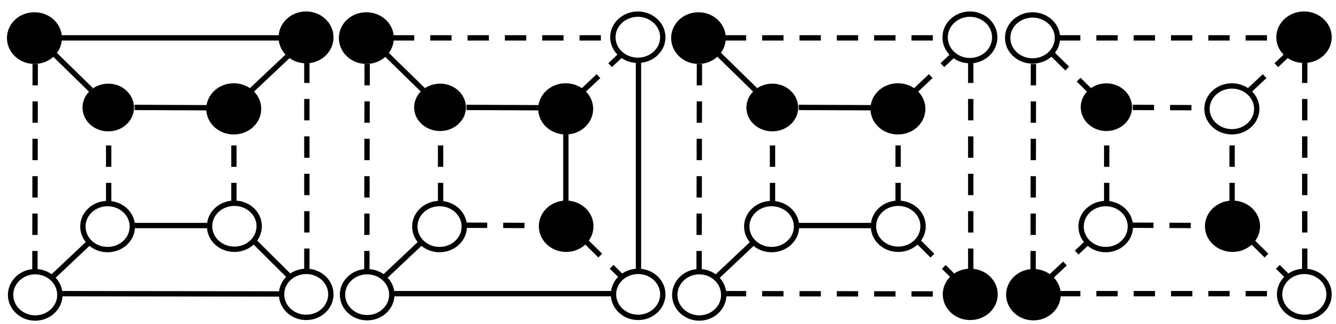
$$V_{cell} = \binom{8}{3} X_L^5 (1 - X_L)^3 \left(\tfrac{5}{8} \ell_L^3 + \tfrac{3}{8} \ell_S^3 + \tfrac{15C}{28} (\ell_L^3 - \ell_S^3) \right) =$$

$$56 X_L^3 (1 - X_L) \left(\tfrac{5}{8} \ell_L^3 + \tfrac{3}{8} \ell_S^3 + \tfrac{15C}{28} (\ell_L^3 - \ell_S^3) \right)$$

Bimodal building block sc

$$V_{cell} = \sum_{i=0}^{n} \left[\binom{n}{i} X_L^{n-i} (1 - X_L)^i \left(\tfrac{n-i}{n} \ell_L^3 + \tfrac{i}{n} \ell_S^3 + \psi_i (\ell_L^3 - \ell_S^3) \right) \right]$$

$i = 4;\ \psi_i = C\ (4/35 \times 4/12 + 2/5 \times 6/12 + 16/35 \times 8/12 + 1/35) = 4C/7$



p = 4/35 p = 2/5 p = 16/35 p = 1/35

$$V_{cell} = \binom{8}{4} X_L^4 (1 - X_L)^4 \left(\tfrac{4}{8} \ell_L^3 + \tfrac{4}{8} \ell_S^3 + \tfrac{4C}{7} (\ell_L^3 - \ell_S^3) \right) =$$

$$70\, X_L^3 (1 - X_L) \left(\tfrac{1}{2} \ell_L^3 + \tfrac{1}{2} \ell_S^3 + \tfrac{4C}{7} (\ell_L^3 - \ell_S^3) \right)$$

Bimodal building block sc

$$V_{cell} = \sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3 + \psi_i(\ell_L^3 - \ell_S^3)\right)\right]$$

$$\sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\left(\frac{n-i}{n}\ell_L^3 + \frac{i}{n}\ell_S^3\right)\right] = X_L\ell_L^3 + (1-X_L)\ell_S^3$$

$$\sum_{i=0}^{n}\left[\binom{n}{i} X_L^{n-i}(1-X_L)^i\psi_i(\ell_L^3 - \ell_S^3)\right] = 2C\,X_L(1-X_L)(\ell_L^3 - \ell_S^3)$$

$$V_{cell} = X_L\ell_L^3 + (1-X_L)\ell_S^3 + 2C\,X_L(1-X_L)(\ell_L^3 - \ell_S^3)$$

Packing fraction bimodal sc

$$\left.\frac{dV_{cell}}{dX_L}\right|_{X_L=1} = 0 \Rightarrow C = 1/2$$

$$V_{cell} = \ell^3 = X_L \ell_L^3 + (1 - X_L)\ell_S^3 + X_L(1 - X_L)(\ell_L^3 - \ell_S^3)$$

$$d^3 = X_L d_L^3 + (1 - X_L) d_S^3$$

$$\frac{d_L}{d_S} = u;\ \ell_S = d_S;\ \ell_L = d_L \Rightarrow \frac{\ell_L}{\ell_S} = u$$

$$\eta_{sc} = \frac{\frac{\pi}{6} d^3}{\ell^3} = f_{sc}\left(\frac{X_L(u^3 - 1) + 1}{X_L(u^3 - 1) + 1 + X_L(1 - X_L)(u^3 - 1)}\right)$$

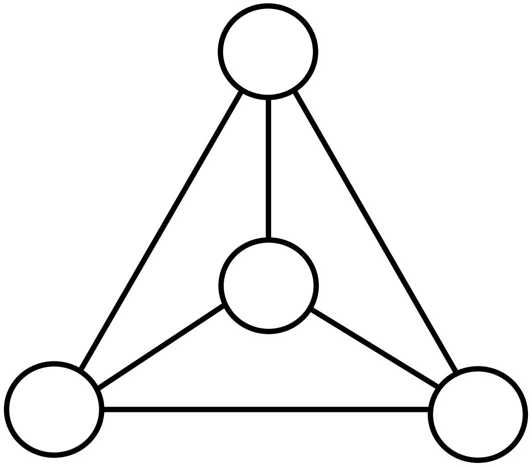
General equation for bimodal graphs?

$$V_{cell} = X_L \ell_L^3 + (1 - X_L)\ell_S^3 + 2C\, X_L (1 - X_L)(\ell_L^3 - \ell_S^3)$$

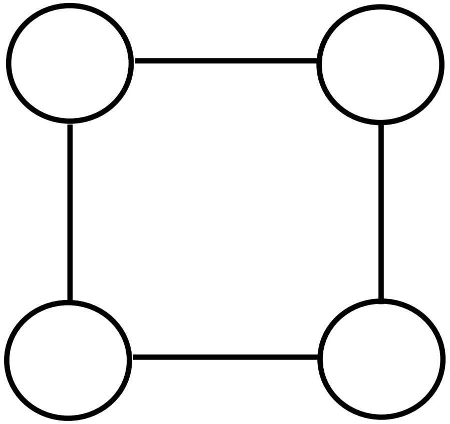
$$\left.\frac{dV_{cell}}{dX_L}\right|_{X_L = 1} = 0 \Rightarrow C = 1/2$$

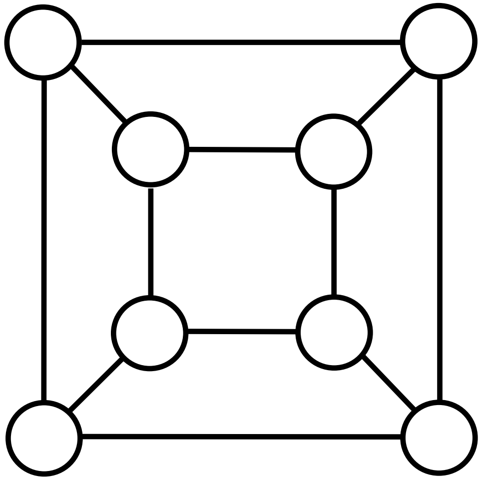
$$V_{cell} = \ell^3 = X_L \ell_L^3 + (1 - X_L)\ell_S^3 + X_L (1 - X_L)(\ell_L^3 - \ell_S^3)$$

True for n = 4 and n = 8 graphs



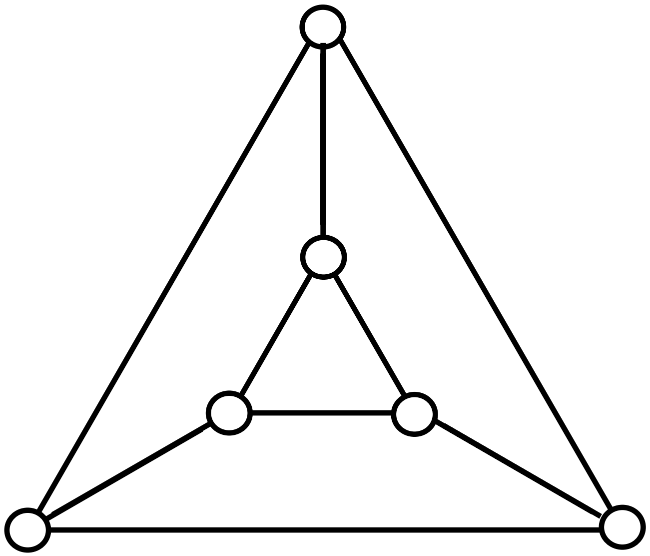
Tetrahedron

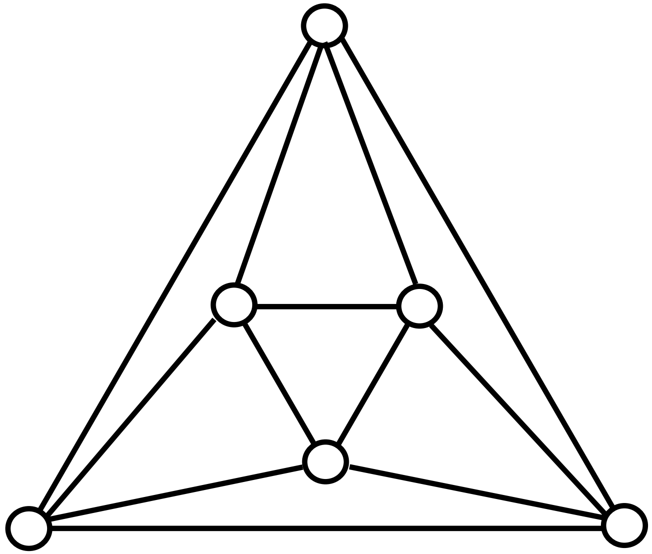




Hexahedron

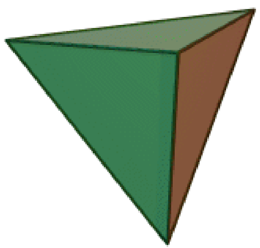
Also true for n = 6 graphs





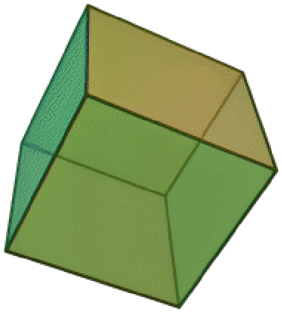
Octahedron

Five platonic solids



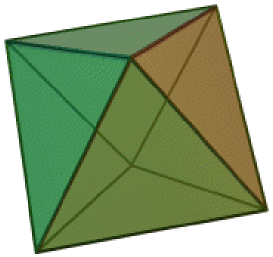
Tetrahedron

4 faces



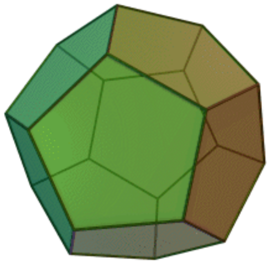
Hexahedron

6 faces



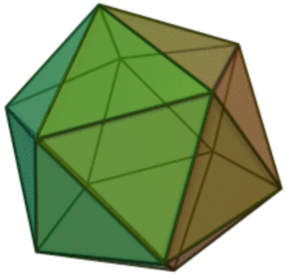
Octahedron

8 faces



Dodecahedron

12 faces

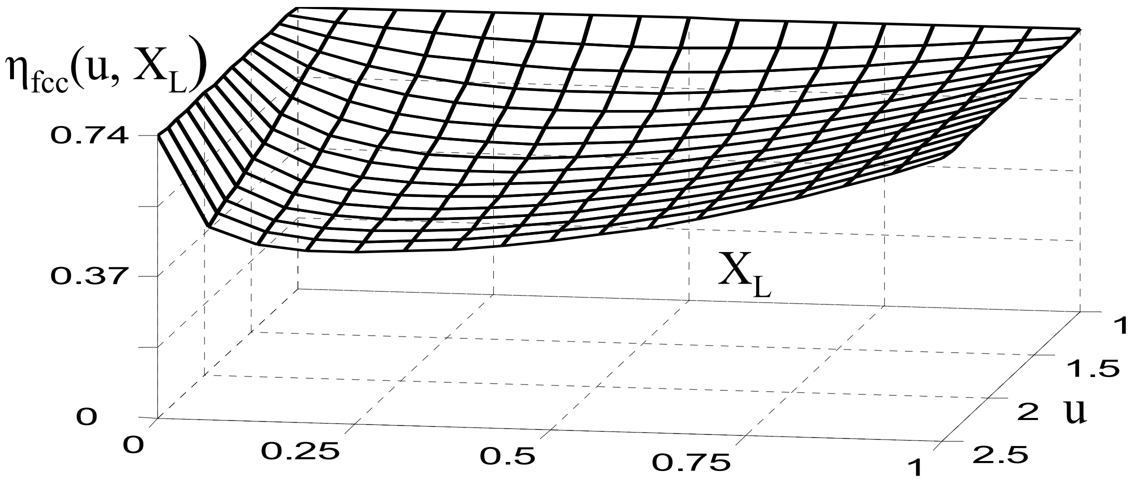


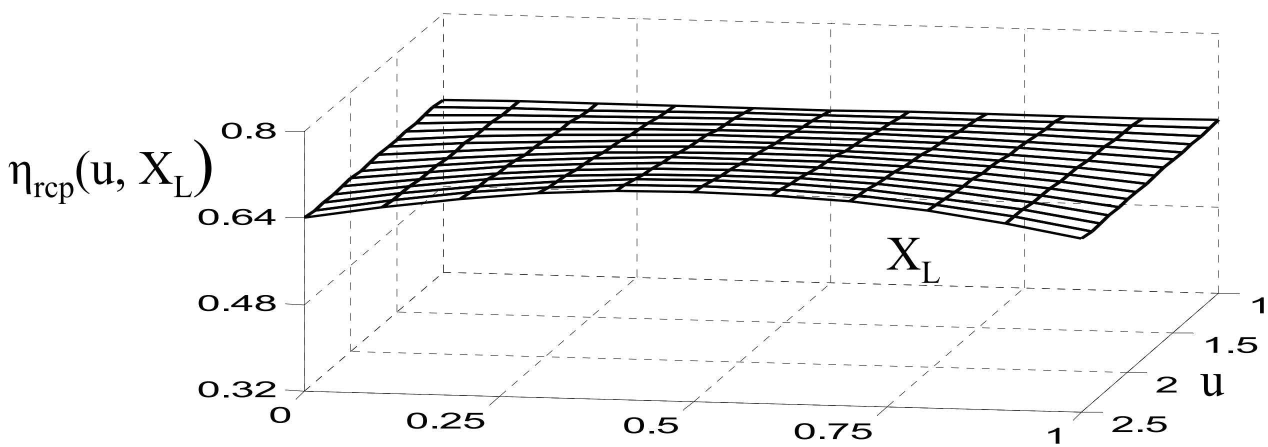
Icosahedron

20 faces

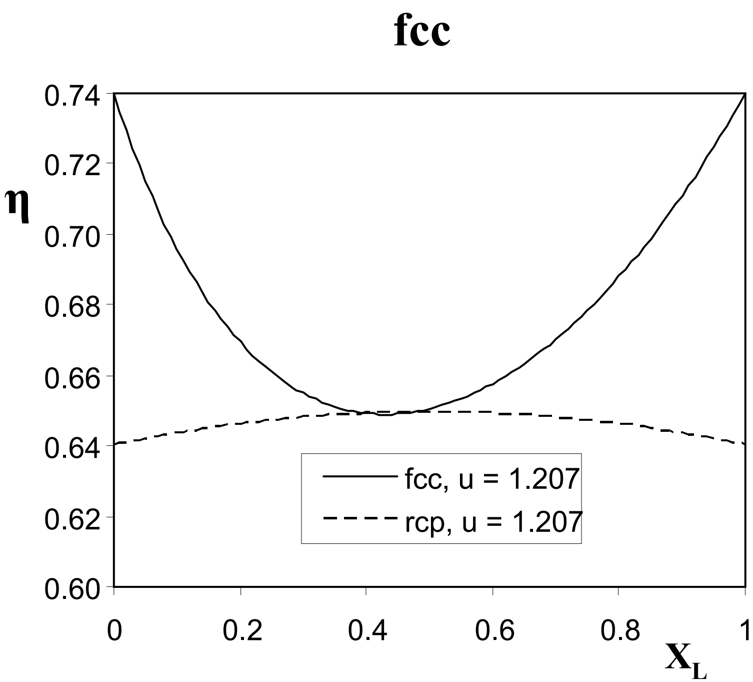
1. Polydisperse geometric packing
    1. Bimodal discrete random
    2. Polydisperse discrete random
    3. Continuous random
2. Amorphisation
    1. Bimodal discrete random
    2. Bimodal discrete crystalline
    3. Cross-over

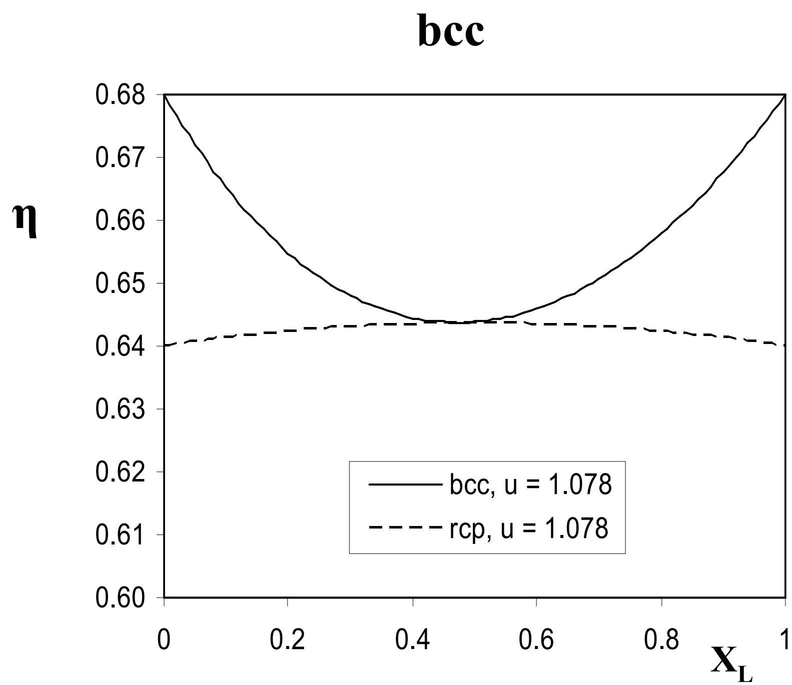
Crossing of packing fraction bimodal fcc/rcp





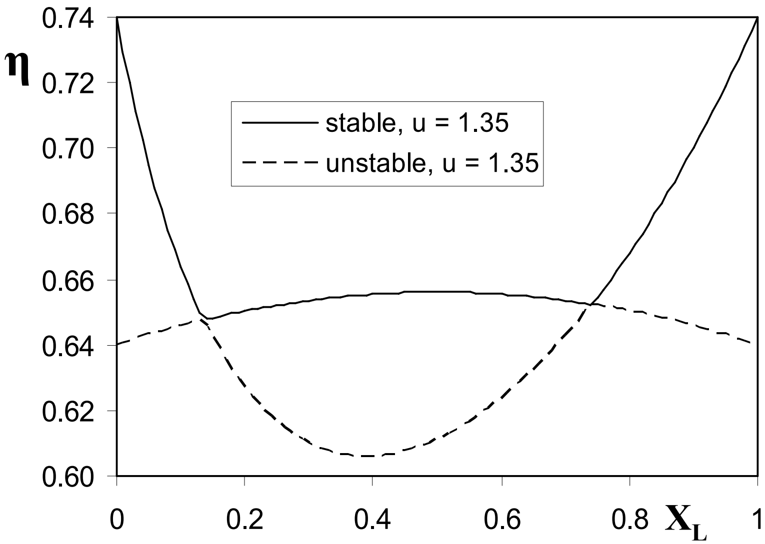
Crystalline and amorphous packing fraction



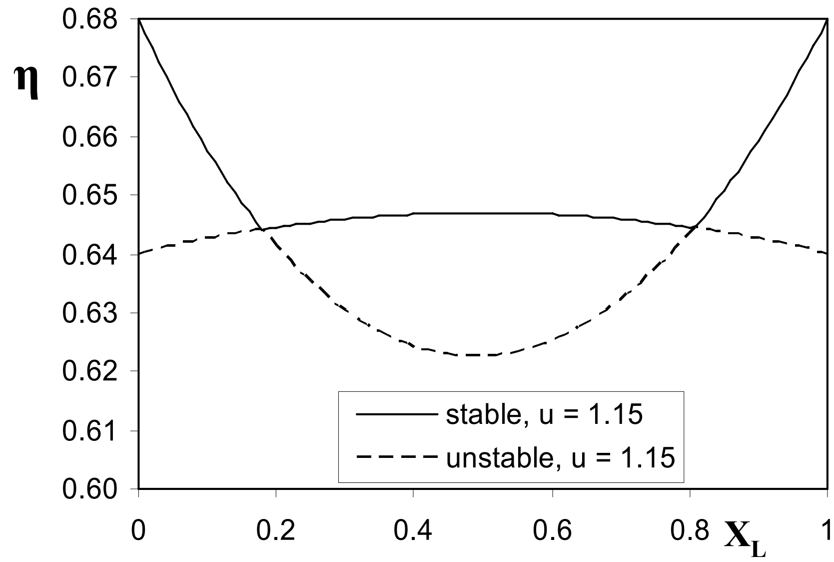


Crystalline and amorphous packing fraction

fcc



bcc



Amorphous-crystalline (fcc) crossover

$$\eta_{fcc} = f_{fcc}\left(\frac{X_L(u^3-1)+1}{X_L(u^3-1)+1+X_L(1-X_L)(u^3-1)}\right) =$$

$$f_{fcc}(1-X_L(1-X_L)(u^3-1))+O((u^3-1)^2)$$

$$\eta_{rcp} = f_{rcp} + \tfrac{4}{3}\beta f_{rcp}(1-f_{rcp})X_L(1-X_L)(u^3-1)$$

$$\eta_{rcp} = \eta_{fcc}$$

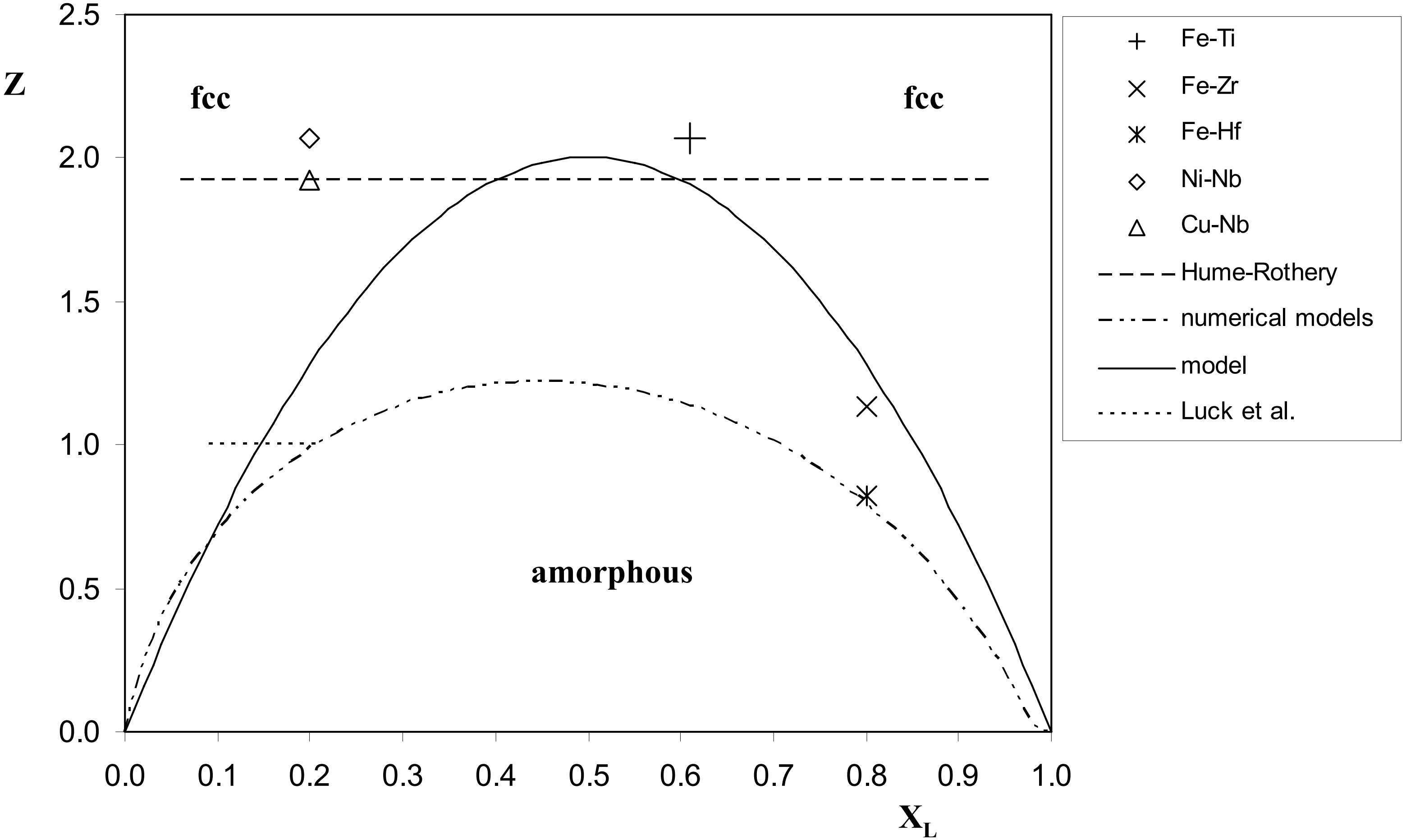
Amorphous-crystalline crossover

$$f_{fcc}(1 - X_L(1 - X_L)(u^3 - 1)) =$$

$$f_{rcp} + \tfrac{4}{3}\beta f_{rcp}(1 - f_{rcp})X_L(1 - X_L)(u^3 - 1)$$

$$\frac{1}{u^3 - 1} = z = (1 - X_L)X_L\left(\frac{\tfrac{4}{3}\beta\ f_{rcp}(1 - f_{rcp}) + f_{fcc}}{f_{fcc} - f_{rcp}}\right)$$

Map of closest packing fcc-rcp



Amorphous-crystalline (bcc) crossover

$$\eta_{bcc} = f_{bcc}\left(\frac{X_L(u^3-1)+1}{X_L(u^3-1)+1+X_L(1-X_L)(u^3-1)}\right) =$$

$$f_{bcc}(1-X_L(1-X_L)(u^3-1)) + O((u^3-1)^2)$$

$$\eta_{rcp} = f_{rcp} + \tfrac{4}{3}\beta f_{rcp}(1-f_{rcp})X_L(1-X_L)(u^3-1)$$

$$\eta_{rcp} = \eta_{bcc}$$

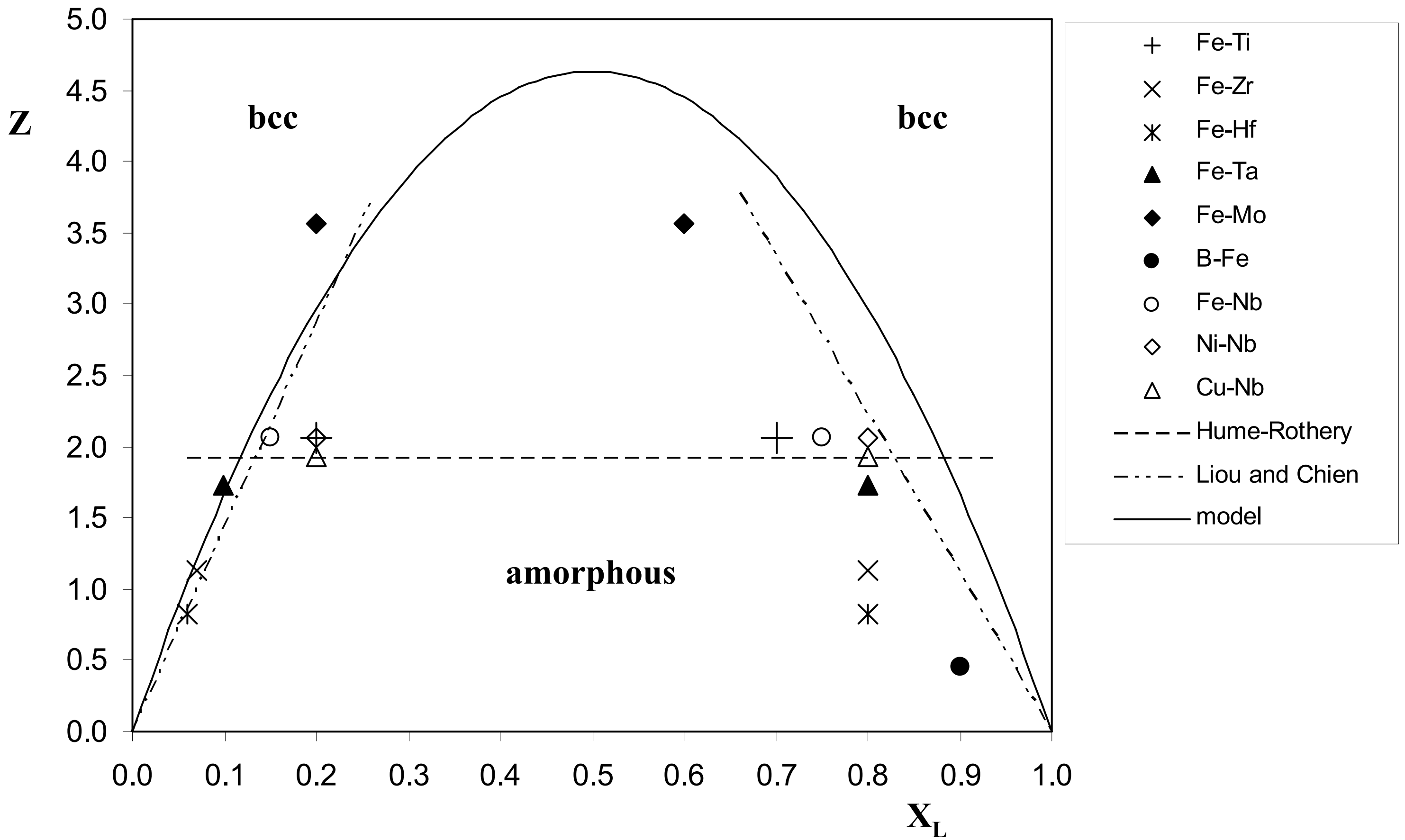
Amorphous-crystalline crossover

$$f_{bcc}(1-X_L(1-X_L)(u^3-1)) =$$

$$f_{rcp}+\tfrac{4}{3}\beta f_{rcp}(1-f_{rcp})X_L(1-X_L)(u^3-1)$$

$$\frac{1}{u^3-1} = z = (1-X_L)X_L\left(\frac{\tfrac{4}{3}\beta\, f_{rcp}(1-f_{rcp})+f_{bcc}}{f_{bcc}-f_{rcp}}\right)$$

Map of closest packing bcc-rcp



Conclusions

The onset of the monosized to bimodal packing of particles can be used to:

- study packing fraction of polydisperse geometric packings
- study amorphisation of crystalline materials

"Simple" hard particle/sphere packings can be applied to real and complicated systems.

Conclusion

- Acknowledgement: Dipl.-Ing. Götz Hüsken for Matlab assistance;
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- Post-Doc vacant position available;

Thank you for your kind attention !

Questions?