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# GERM-GRAIN MODEL OF SHORT-FIBRE COMPOSITES

Karol Pelikán, Ivan Saxl[1], Petr Ponížil

Faculty of Technology, Technical University of Brno, TGM Square 275,
CZ-762 72 Zlín, Czech Republic
[1]Mathematical Institute, Academy of Sciences of the Czech Republic, Žitná 25,
CZ-115 67 Praha 1, Czech Republic

## ABSTRACT

The computer simulated 3D simple sequentional inhibition model of short-fibre strengthened composite materials is presented. Short fibers are approximated as cylinders with hemispherical caps, their spatial arrangement is described by the distribution function of spherical contact distance. The simulated SSI model is compared from this point of view with some well known theoretical models (Boolean and lattice models of balls and cylinders). The possibility of modelling randomly distributed particles by a lattice model with different intensity as well as the influence of the particle shape is discussed.

Key words: composite material, computer simulation, distance, germ-grain model, stochastic geometry, random closed sets.

## INTRODUCTION

Technically important group of composite materials are short-fibre composites, in which particles of fiber-like shape are more or less randomly distributed in the bulk of material. Examples of such a type of materials are polymer filled by glass, graphite or metallic particles, ceramics materials with whiskers or metals strengthened by elongated particles. Strength, toughness and other mechanical and/or physical properties of such materials depend on the size, shape and spatial arrangement of particles, in particular on the size and shape of particle-free regions in the matrix. A suitable characteristic of these regions is the spherical contact distribution function (SCDF) $F(l)$. Its form is well known for several theoretical models (Stoyan et al., 1987; Saxl, 1993). For the SSI model of fibre-like particles, it must be estimated on the basis of computer simulations. The comparison of obtained estimates with the theoretical results for selected germ-grain models is the main goal of the present paper.

## GERM-GRAIN MODELS

The starting point for all examined models is the germ-grain model of a random closed set $X=\bigcup_0^\infty (\Xi_n + x_n)$, where $x_n$ are germs and $\Xi_n$ are grains - particles. Three basic arrangements of germs will be investigated:

a) $x_n$ are points of a Poisson point process of intensity $\lambda$,
b) $x_n$ are points of a translation lattice $L(\mathbf{A})$,
c) $x_n$ are reference points of an SSI model obtained by a simulation.
The primary grains uniform in size and shape will be considered in all cases. The basic shape is $\Xi(s,R) = S \oplus B(R)$, where $B(R)$ is a ball (centred in the origin) of radius $R$ and $S$ is a line segment of length $s$. Thus $\Xi(s,R)$ is a cylinder of height $s$ and radius $R$ with hemispherical caps and may be considered either as a spherical dilation od a straight segment $S$ or as a linear dilation by S of $B(R)$. The important characteristics of $\Xi(s,R)$ are its volume $\upsilon(\Xi)$, surface area $\sigma(\Xi)$, mean width $\omega(\Xi)$, slimness (the total height to diameter ratio) $\eta(\Xi)$, the isoperimetric ratio $I_R(\Xi) = \sigma^3(\Xi)/(36\pi\upsilon^2(\Xi)$ (for an arbitrary $\Xi$ is $I_R(\Xi) \geq I_R(B) = 1$, which expreses the well known fact that the ball has the smallest surface area from all bodies of a given volume), and are summarized in Tab 1. The quantity $\zeta(\Xi)$ describes the volume increase of $\Xi$ with the length $s$.

Table 1. Grain parameters.

| $\upsilon(\Xi)$ | $\sigma(\Xi)$ | $\omega(\Xi)$ | $\eta(\Xi)$ | $\zeta(\Xi)$ | $I_R(\Xi)$ |
|---|---|---|---|---|---|
| $4\pi R^3\zeta/3$ | $4\pi R^2\eta$ | $(\eta+1)R$ | $(s+2R)/(2R)$ | $(3\eta+1)/2$ | $\eta^3/\zeta^2$ |

Implanting grains in germs produced by the above listed processes, the Boolean models BM($k\Xi$) (Stoyan et al., 1987), lattice models $L(\mathbf{A},\Xi)$ (translation lattices of bodies, see Santaló, 1976) and SSI model $X(\Xi)$ (Diggle, 1983; Penttinnen and Stoyan, 1989; Mecke et al., 1990) are obtained - Tab.2. The orientation of primary grains is isotropic random in Boolean and SSI cases and fixed (parallel to an edge of the basic lattice cell) in the lattice models. The basic characteristics of a model $Z(\Xi_z)$ with a uniform grain $\Xi_z$ are intensity $\lambda_z$, volume fraction $p_z = V_V(Z)$ and surface to volume ratio $\Sigma_z = S_V(Z)$; the volume fraction of the complement (matrix) $Z^c$ is $q_z = 1 - p_z$, whereas $S_V(Z^c) = \Sigma_z$. The SSI model $X(\Xi)$ obtained by the simulation is considered as a "master" process and all quantities related to it will be used without indices, i.e. $p, q, R, \eta, I_R$ etc. Various models $Z(\Sigma_z)$ are characterized by their relation to $X$, i.e. by the choice of quantities matching that ones of $X$. Consequently, primary grain $k_z\Xi$, $k_z > 1$, must be used in Boolean model of intenzity $\lambda_z = \lambda$ if either $p_z = p$ or $\Sigma_z = \Sigma$ should hold. For the comparison, also Boolean and lattice models of balls $B(\nu_z R)$ have been considered. The quantities $k_z$, $\kappa_z$, $\nu_z$ follow from the relations $-\ln q_z = \lambda_z\upsilon_z$, $\Sigma_z = q_z\lambda_z\sigma_z$ valid for the Boolean models, and $p_z = \lambda_z\upsilon_z$, $\Sigma_z = \lambda_z\sigma_z$ holding for lattice and SSI models. The shape and size of the lattice used in lattice models is subject to two conditions only; namely the volume of the basic lattice cell $\upsilon_P$ is inversely proportional to the intensity $\lambda$ of the germ process and its shape must be such that the whole grain can be embedded into it. The most simple choice of the lattice cell for fibre-like particles $\Xi$ is a rectangular prism $P(a,a,a+s)$ with a square base of edge $a$, which is a solution of the equation $a^3 + a^2 s - \lambda^{-1} = 0$; its height is $c = a + s$, the model U) and it becomes a cube when $s = 0$ (the lattice models of balls - D and W).
The geometrical properties of the matrix $Z^c$ will be characterized by the spherical contact distribution function (SCDF) $F(l)$, which can be interpreted as the conditional probability $\Pr\{B(z,l) \cap Z \neq \emptyset | z \in Z^c$ that a ball $B(z,l)$ of radius $l$ centred in a point $z \in Z^c$ chosen uniformly at random hits the boundary of $Z^c$. Or equivalently, $F(l)$ is the distribution function of Euclidean distances of points $z \in Z^c$ from $Z$. The knowledge of the SCDF enables us to calculate its moments and related quantities describing the distribution of spherical distances and hence also the geometry of $Z^c$. For example, the first moment of $F(l)$ is the expected distance of a typical point of $Z^c$ from its boundary, it is from the closest grain $\Xi$. The

SCDF for the SSI model $X$ must be estimated on the simulation, in the remaining cases is known from the theory.

Table 2. Models and their parameters.

| Model | Characteristics | $k_z$ | $\kappa_z$ | $\nu_z$ | Note |
|---|---|---|---|---|---|
| $X: SSI(\Xi)$ | $p, \Sigma, \lambda$ | 1 | 1 | 1 | |
| $S: BM(k_S\Xi)$ | $p_s = p, \lambda_s = \lambda, \Sigma_s$ | $(\vartheta/q)^{1/3}$ | 1 | – | $\Sigma_s = qk_s^2\Sigma \le \Sigma$ *as* $0 \le qk_s^2 \le 1$ |
| $T: BM(B(\nu_t R))$ | $p_t = p, \lambda_t = \lambda, \Sigma_t$ | – | 1 | $(\vartheta\zeta/q)^{1/3}$ | $\Sigma_t = qk_s^2\Sigma I_R^{-1/3} \le \Sigma_s \le \Sigma$ *as* $I_R \ge 1$ |
| $U: L(\Xi)$ | $p_u = p, \lambda_u = \lambda, \Sigma_u = \Sigma$ | 1 | 1 | – | $a^3 + a^2 s = \lambda^{-1}, c = s + a$ |
| $W: L(B(\nu_w R))$ | $p_w = p, \lambda_w = \lambda, \Sigma_w$ | – | 1 | $\zeta^{1/3}$ | $\Sigma_w = \Sigma I_R^{-1/3} \le \Sigma,\ a = \lambda^{-1/3}$ |
| $A: BM(k_a\Xi)$ | $p_a = p, \Sigma_a = \Sigma, \lambda_a = \kappa_a\lambda$ | $\vartheta$ | $1/(q\vartheta^2)$ | – | $\lambda_a \ge \lambda$ *as* $1 \le \kappa_a \le \infty$ *for* $0 \le q \le 1$ |
| $C: BM(B(\nu_c R)$ | $p_c = p, \Sigma_c = \Sigma, \lambda_c = \kappa_c\lambda$ | – | $I_R/(q\vartheta^2)$ | $\vartheta\zeta/\eta$ | $\lambda_c \ge \lambda_a \ge \lambda$ *as* $I_R \ge 1$ |
| $D: L(B(\nu_d R))$ | $p_d = p, \Sigma_d = \Sigma, \lambda_d = \kappa_d\lambda$ | – | $I_R$ | $\zeta/\eta$ | $\lambda_d \ge \lambda$ *as* $I_R \ge 1$, *a as in W* |
| $E: BM(k_e\Xi)$ | $\lambda_e = \lambda, \Sigma_e = \Sigma, p_e$ | $q^{-1/2}$ | 1 | – | $p_e = 1 - \exp(-k_e^3 p) \ge p$ *as* $k_e \ge 1$ |
| $F: BM(B(\nu_f R))$ | $\lambda_f = \lambda, \Sigma_f = \Sigma, p_f$ | – | 1 | $(\eta/q)^{1/2}$ | $p_f = 1 - \exp\left(-k_e^3 I_R^{1/2} p\right) \ge p$ |

$\vartheta = -\ln q/(q^{-1} - 1)$

The function $F(l)$ for considered Boolean models is $F(l) = 1 - \exp(-\lambda Q(l)$ , where the polynomial

$$Q(l) = \upsilon(\Xi_z \oplus B(l)) - \upsilon(\Xi_z) = 4\pi l^3/3 + 2\pi\omega_z l^2 + \sigma_z l$$

(Stoyan et al., 1987), the moments of this distribution must be calculated numerically. In lattice models, $F(l)$ depends on that part of the spherical dilation $\Xi_z \oplus B(l)$ that is included in the zone of influence $\vartheta_z$ of the particle; here $\vartheta_z$ is the union of all points of $Z^c$, that are loser to a given particle than to any other particle. In a translation lattice of bodies, the zones of influence are translation equivalent and $F(l) = \upsilon(\Xi_z \oplus B(l) \cap \vartheta_z)/\upsilon(\vartheta_z)$ - Saxl (1993). For the lattice model U, this distribution function is given in Saxl(1994):

$$F(l; \Xi_u, \lambda_u) = \{a_u^2\lambda_u[aF^{(3)}(l+R; a_u) + sF^{(2)}(l+R; a_u)] - p_u\}/(1 - p_u) \qquad (1)$$

where $F^{(2)}(t; a)$, $F^{(3)}(t; a)$ are the SCDF's in a square and cubic point lattices of parameter $a$, respectively. The formulae for SCDF $F^{(2)}(t; 2)$, $F^{(3)}(t; 2)$ in lattices of parameter $a$=2 are given in Saxl (1993) and $F^{(d)}(t; a) = F^{(d)}(2t/a; 2)$. The moments of $F(l; \Xi_u, \lambda_u)$ in a $d$-dimensional space are given in Saxl (1994). For $d$=3 we obtain

$$\mu_k'(\Xi_u, \mathbb{A}_u) = q_u^{-1}\left\{\sum_{j=0}^{k-1}\binom{k}{j}(-1)^j\left[\mu_{k-j}'(s)R^j - R^k\right] + \frac{\lambda(-R)^{k+1}}{\binom{k+2}{k}}\left[\frac{4\pi R^2}{k+3} + \pi sR\right]\right\}, \qquad (2)$$

where $\mu'_{k-j}(s) = \left[ a^3 \mu'^{(3)}_{k-j}(O,a) + a^2 s \mu'^{(2)}_{k-j}(O,a)/\upsilon_p \right]$ are the moments of SCDF of $S$ in $P(a,a,a+s)$; $\mu'^{(d)}_{k-j}(O,a)$ are the moments of SCDF in a point cubic lattice of dimension $d$ and edge length $a$ (e.g. $\mu'^{(3)}_1(O,a) = 0.4803a$, $\mu'^{(2)}_1(O,a) = 0.3826a$ are the first and $\mu'^{(3)}_2(O,a) = 0.25a^2$, $\mu'^{(2)}_2(O,a) = 0.16\bar{6}a^2$ are the second moments, respectively). Setting $s = 0$, inserting $a_z^3 = 1/\lambda$ and $\nu_z R$ for $R$, we can write a simple formula for the moments of SCDF in lattices of balls $D$, $W$.

## RESULTS

Simulation of the SSI model was accomplished using the "simple rejection" algorithm:

step 1: the particle $\Xi_1$ with the axis along an isotropic random direction is implanted in a uniform random point of chosen bounded volume $V$

step $n$: the $n$-th particle $\Xi_n$ is implanted by the same manner as in step 1 and then tested for intersection with alredy accepted particles: if $\Xi_n \cap \bigcup_{i=1}^{n-1} \Xi_i = \emptyset$ , then $\Xi_n$ is accepted, otherwise the whole step $n$ is repeated. The procedure was stopped, when the intensity of particles centres reached the chosen value.

The particles were generated in a volume of cubical shape, the guard layer width was 7% of the cube edge length; hence the active zone comprised 64% of generated particles. Such a protecting layer does not fully excludes edge effects introduced by the absence in the simulation of those particles that have reference points outside of $V$ and still hit $V$. Consequently, the protecting layer is overfilled , the active volume underfilled and the spherical distancesbased on measurements performed mainly within the active volume are overestimated; the effect increases with growing volume fraction $p$ and growing slimness $\eta(\Xi)$. The estimate (by random point method) of the actually attained $p$ within the active volume did not revealed any substantial difference in $p$ between the protecting layer and active volume bellow $p$=0.1 even at $\eta(\Xi)$=10.

The formation of clusters containing several particles with a similar orientation has been observed, in particular at high $\eta(\Xi)$ and $p$. Defining a cluster by the condition, that any particle belonging to it must have the Euclidean distance to at least one other particle of the same sluster smaller than chosen value, $d$ say, they can be simply recognized. Fig. 1a presents example of three such clusters at $p$=0.19 defined by $d$=0.11$R$. Nevertheless, the global isotropy of particle axes has been approximately conserved.

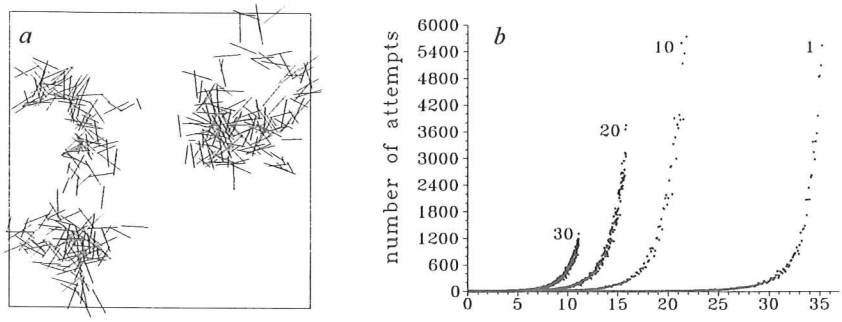


Fig.1.a: Mean number of attempts preceding the acceptance of a new particle into the simulated SSI model for various shapes of particles ($\eta(\Xi) = 1, 10, 20, 30$).

b: Plane projection of three selected clusters with $d$=0.11$R$ at $p$=0.19, $\eta(\Xi)$=10.

The number of unsuccesful attempts preceding the implantation of the $n$-th particle depends not only on the attained packing density $\tau \approx (n-1)\upsilon(\Xi)/V$ but also on the shape of $\Xi$ characterized by $\eta(\Xi)$ - see Fig.1. The value of the maximum attainable packing density $\tau_{max}$ for $\eta(\Xi) = 1$ (balls) is in good agreement with the estimate $\tau_{max} = 0.381$ for $V \to \infty$ and a slighly more sophisticated SSI algorithm of "complete packing" (Tanemura,1992). SSI model with $\eta(\Xi) = 10$ as a typical value for a short-fibre composite was used as the "master model" in the present study, the corresponding value of $\tau_{max} \approx 0.24$. If no checking for intersections were carried out and any particle were accepted at step $n$, then the Boolean model with isotropic primary grain $\Xi$ would be generated - the planar sections of the both Boolean and SSI 3D models are compared in Fig.2 (to obtain the same volume fraction at the same grain size, the intensity of Boolean model is adequately higher).

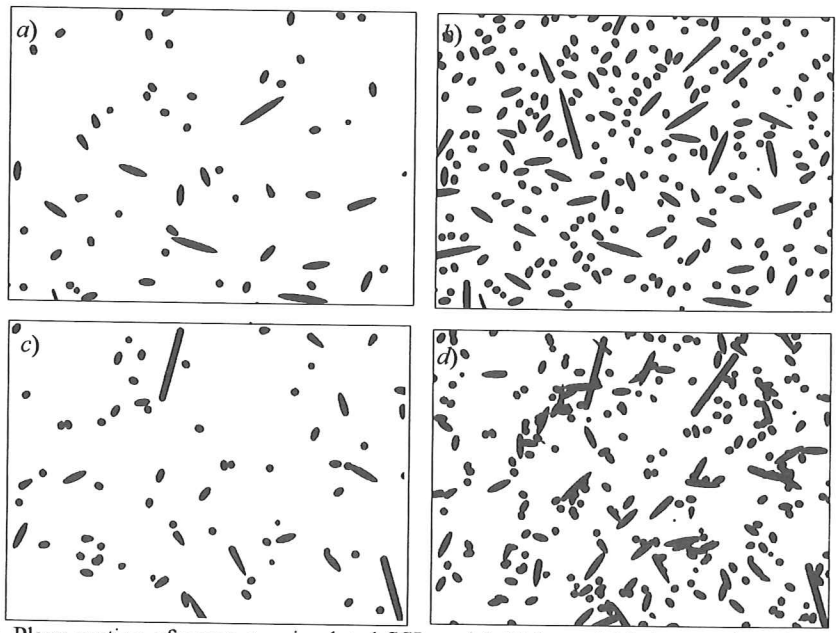


Fig.2. Plane section of computer simulated SSI model X (a: $p$=0.05; b: $p$=0.2) and Boolean model with the same volume content and grain size(c: $p$=0.05; d: $p$=0.2).

Five different realizations of the SSI model with $p \equiv p_x$ =0.01, 0.05, 0.10, 0.15 and 0.20 were investigated in detail. For each of them, $5.10^3$ distances from uniform random matrix points to the closest particles were computed and used to estimate the shape of the p.d.f. $f_x(l)$ 's and the values of moments $\mu'_{k,x}(s)$, $k = 1, 2, 3, 4$. The number of particles comprised in the active zone was 640 at $p$=0.01 (the total number of generated particles $10^3$) and $12.8\text{x}10^4$ at $p$=0.2; consequently, the specimen was oversampled at $p$=0.01. The maximum observed spherical contact distance exceeds the guard layer width only at $p$=0.01, in the all other cases was considerably smaller. For the remaining models, the functions $f_z(l)$ and the moments $\mu'_{k,z}$ were computed from the formulae given above.

The p.d.f.'s of the models U,W,S,T,X with the same intensity $\lambda$ for any given $p$ are compared in Fig.3, the normalized dimensionless quantities $f_z/\lambda^{1/3}$ and $l.\lambda^{1/3}$ are plotted in

order to make the shape comparison easier (consequently, the absolute value of the length unit in Fig.3d is ≈ 2.7 times shorter then in Fig.3a). A similar comparison of models with the same surface density $\Sigma = \Sigma_x$ is carried out in Fig.4.

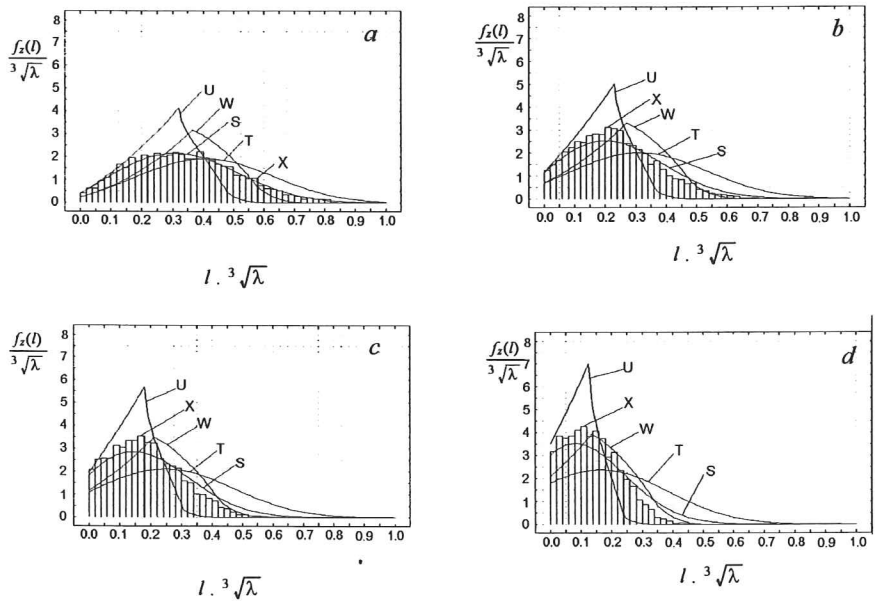


Fig.3. Probability density function of SCD for selected models (a: $p$=0.01; b: $p$ =0.05; c: $p$ =0.1; d: $p$ =0.2).

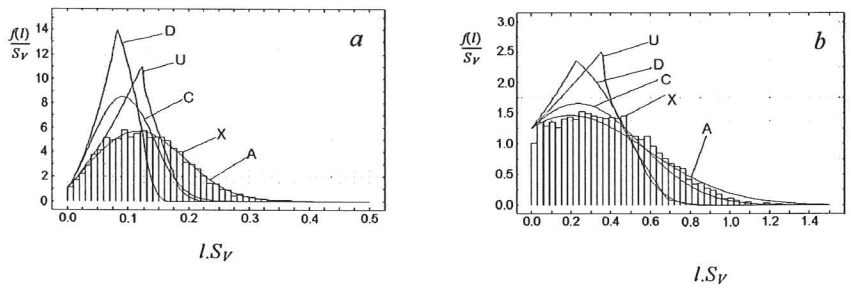


Fig.4. Probability density function of SCD for selected models (a: $p$=0.01; b: $p$ =0.2).

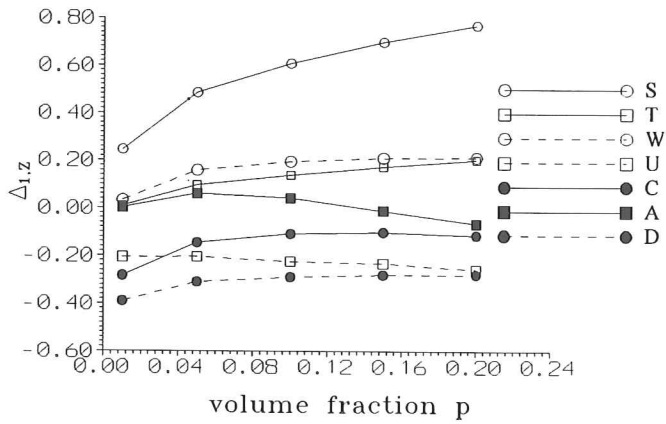


Fig.5. Relative differences $\Delta_{k,z} = \left(\mu'_{k,z} - \mu'_{k,x}\right)/\mu'_{k,x}$ for selected models.

The results concerning the moments of SCD are illustrated in Fig. 5, where the relative difference $\Delta_{k,z} = \left(\mu'_{k,z} - \mu'_{k,x}\right)/\mu'_{k,x}$ is plotted *vs* the volume fraction $p$ for $k$=1. The corresponding results for higher moments are similar in the shape as $\Delta_{k,z}(p)$ dependences, but the values of $|\Delta_{k,z}|$ are greater. The typical difference between lattice and Boolean model is an excess of short and a lack of long distances in the former; the SSI model lies somewhere between. Consequently, the Boolean models A nad S are fairly good approximations, in particular at low values of $p$ and the lattice model U improves its matching with growing $p$.

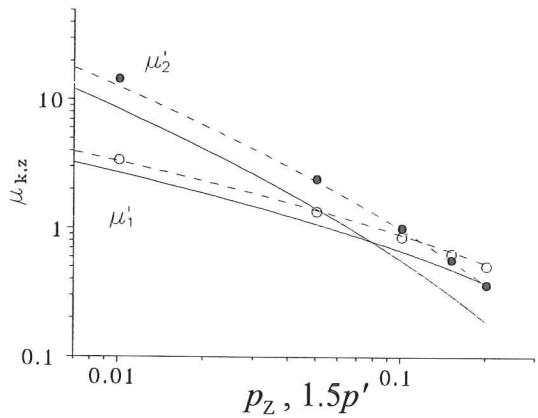


Fig.6. First and second moment of SCD (points: SSI; full line: U model; dashed line: U' model ≡ U model with $p' = 0.6\bar{6}p$.

From the point of view of moments, the model A must be preferred before S as $|\Delta_{k,a}| \leq 0.1$ in the whole examined range of $p$ whereas $\Delta_{k,s}$ in contrast to $\Delta_{k,a}$, steadily increases with $p$ and attains the values 0.2÷0.8 at $p$=0.2 for $k$=1,2. The behaviour of the lattice model U is quite

remarkable; even when the shape of the p.d.f. $f_u(l)$ differs substantially from $f_x(l)$, the relative difference $\Delta_{k,u}$ is nearly independent of $p$. Hence, $\mu'_{k,u}$ is approximately proportional to $\mu'_{k,x}$ (see Fig.5) and by a suitable reduction of $p_u$, namely $p_u = 0.6\bar{6}p$, an approximate coincidence of the moments $\mu'_{k,a}(0.6\bar{6}p)$ and $\mu'_{k,x}(p)$ can be obtained (see Fig. 6 $|\Delta_{k,s}(p)| \leq 0.1$ for $k$=1,2 and $0.03 \leq p \leq 0.2$). On the other hand, all the models with "equivalent balls" must be rejected due to considerable magnitude of $|\Delta_{k,z}|$ as well as due to its pronounced incorrigible dependence on $p$.

## CONCLUSIONS

The present simulation study proves the robustness of the Boolean model: if its parameters are suitably modified in order to account for overlapping and to match the important characteristics of a model with disjoint grains ($p$, $\lambda$ and $\Sigma$ in the present case), it can be used as a good approximation even at rather high volume fractions. Further, the behaviour of the lattice model U opens another possibility. At least in the case, that a physical process depending *e.g.* on heat and/or stress transfer between the matrix and particles along the shortest possible paths is investigated, there is a possibility to replace a random particle arrangement by a simple and easily tractable lattice model. The necessary reduction of the input parameters of the lattice model demostrates the well known rule, that a regular arrangement of particles is more "economical" than a random one in that sense, that effectively similar distribution of particle-free regions (or, of "interparticle distances" in well defined sense) is achieved by a lower volume fraction of particles.

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