INFLUENCE OF PARTICLE SHAPE AND CLUSTER FORMATION ON ELASTIC PROPERTIES OF PARTICLE REINFORCED COMPOSITES

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ABSTRACT

Numerical models were developed to evaluate the impact of different particle shape forms on elastic properties of particle reinforced composites. The studied particle shape forms are based on the particles obtained by the scanning electron microscopy (SEM) and were numerically recreated using the Spherical Harmonics function as well as the equations to describe super ellipsoids. Semi-analytic methods such as Mori-Tanaka and Lielens as well as numerical model were used to calculate the elastic properties of two-phase particle reinforced composites. The SEM analysis had shown that particles generally form clusters when embedded in the matrix material for manufacturing. A numerical FE model was developed to evaluate the effects on the elastic material properties of such cluster formations in the composite material.

1 INTRODUCTION

Particle reinforced polymer composites are applied in a variety of different industries to satisfy the individual requirements of the intended applications. The form and distribution of the particles throughout the matrix has an impact on the mechanical behaviour of the composite material. Thus, there is a high variation potential in the development process like changing the specific particles form, particle and matrix material, the particle volume fraction or particle distribution throughout the matrix in order to achieve the predefined material properties. A variety of composites can be obtained this way, which then need to be evaluated by mechanical testing. This experimental approach usually involves high efforts for producing the different composites and their specimens, testing their mechanical properties and evaluating the results.

Another possible way is predicting the mechanical behaviour through numerical studies. Thereby, the mentioned effort can be reduced and the development process can be shortened. Even though every composite is created to meet specific requirements and therefore is not easily replaceable with other particle reinforced composites, they do share the mechanics at the microscopic level. Thus, a theory has been developed that describes the mechanics at the microscopic level to predict the material behaviour at a macroscopic scale. For this, studies of particle reinforced composites at a micro scale are carried out to increase the insight into the mechanical behaviour.

An approximation of the particles by use of ellipsoids allows the analytical evaluation of the elastic properties of the composite, opening up two branches of composite evaluation methods, making it possible to compare results. On the one hand, using the Eshelby solution for ellipsoidal inclusions [1], semi-analytic homogenization methods such as proposed by Mori-Tanaka [2] and by Lielens [3] can be used as homogenization methods, to evaluate the elastic properties of the composite. On the other hand, numerical methods such as the FEM analysis can be used to study the effects of various particles onto the composite [4, 5] properties.

In this research we utilized the numerical evaluation using FE method. For the numerical calculations Representative Volume Elements (RVEs) were created as discussed by Gitman et al. [6]. The algorithm to create RVEs consisting of multiple periodic distributed particles is based on the Random Sequential

Adsorption (RSA) algorithm proposed by Rintoul et al. [7]. Periodic boundary conditions were applied onto the RVE's surface. The conducted research assumed ideal bonding between the matrix and the particles, as well as no overlapping of the particles. The calculations were carried out considering a linear elastic material behaviour of the composite.

2 NUMERICAL MODELING OF THE MICROSTRUCTURE

2.1 Numerical Modeling of the Composite with Periodic Distributed Particles

A SEM analysis was carried out to study particle reinforced composites. A variety of different particle shapes were studied, some of the observed particle shapes are displayed in Fig. 1 below.

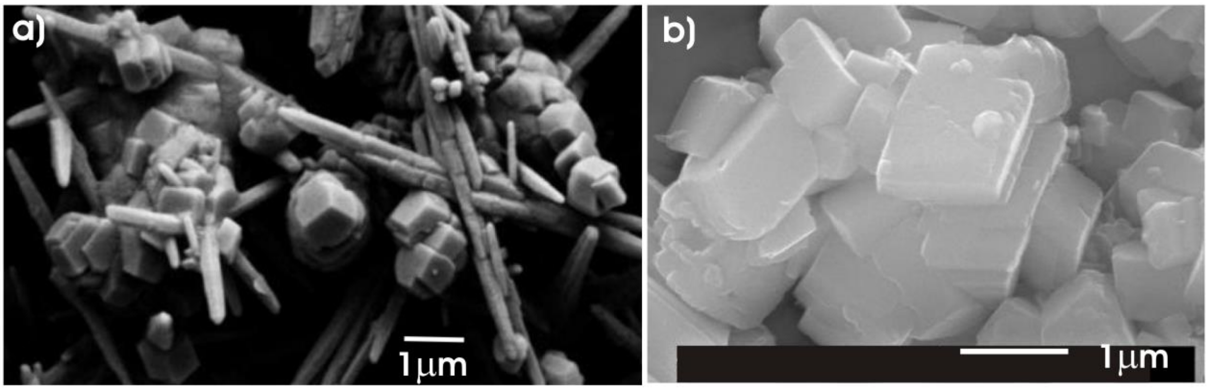

Figure 1: Examples of the observed particle shapes: a) Mixture of needles and cubes, b) Tile shaped particle form.

The particle shapes namely sphere, ellipsoid, cube and cube with smooth edges were identified as the most common particle shapes among the studied materials and used for following FEM analysis. The particle shapes were recreated using the Python software package [8]. The equation for super ellipsoids as described by Jaklič et al. [9] were used to create the cube and the cube with smooth edges (see Fig. 2 a and b).

$$\left(\frac{|x|}{a}\right)^n + \left(\frac{|y|}{b}\right)^m + \left(\frac{|z|}{c}\right)^k = 1, m, n, k \in \mathbb{R}_+ . \tag{1}$$

Particle shown in Fig. 2 b was created with the values for the parameters as $n = m = k = 20$ and $a = b = c = 3$. Furthermore, the particles of spherical and ellipsoidal shape were created as well (see Figure 2 c and d).

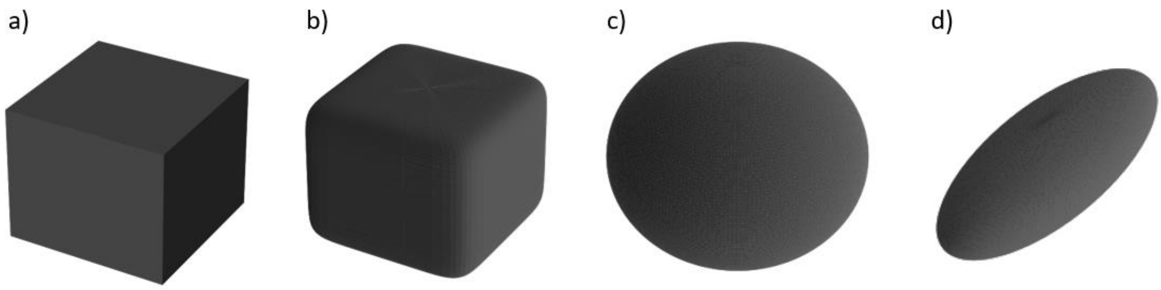

Figure 2: Particles studied in this research: a) cubic, b) cubic with smooth edges, c) spherical, d) ellipsoidal.

The RVE was created by either placing one particle (results for these studies are displayed in Fig. 3) or by placing multiple (results for these studies are displayed in Fig. 4 to Fig. 12) inside the matrix material. Six loading cases were applied, three of them being uniaxial loading and three being shear deformation, and the stress volume averages were calculated. Lastly, the Young's moduli were evaluated as proposed by Drach et al. [10]. The specific numeric calculations were done in the ABAQUS software [11].

The Young's modulus of the composite has been normalized by the Young's modulus of the matrix material along with calculating ψ, the surface to volume particle ratio, as proposed by Wadell [12] with slight modifications. The modified equation (Eq. (2)) is written below. Here S_P and V_P are the surface and volume of the particle respectively.

$$\Psi = \frac{S_P}{\sqrt[3]{\pi(6V_P)^2}} \; . \tag{2}$$

The results are displayed in Fig. 3 below.

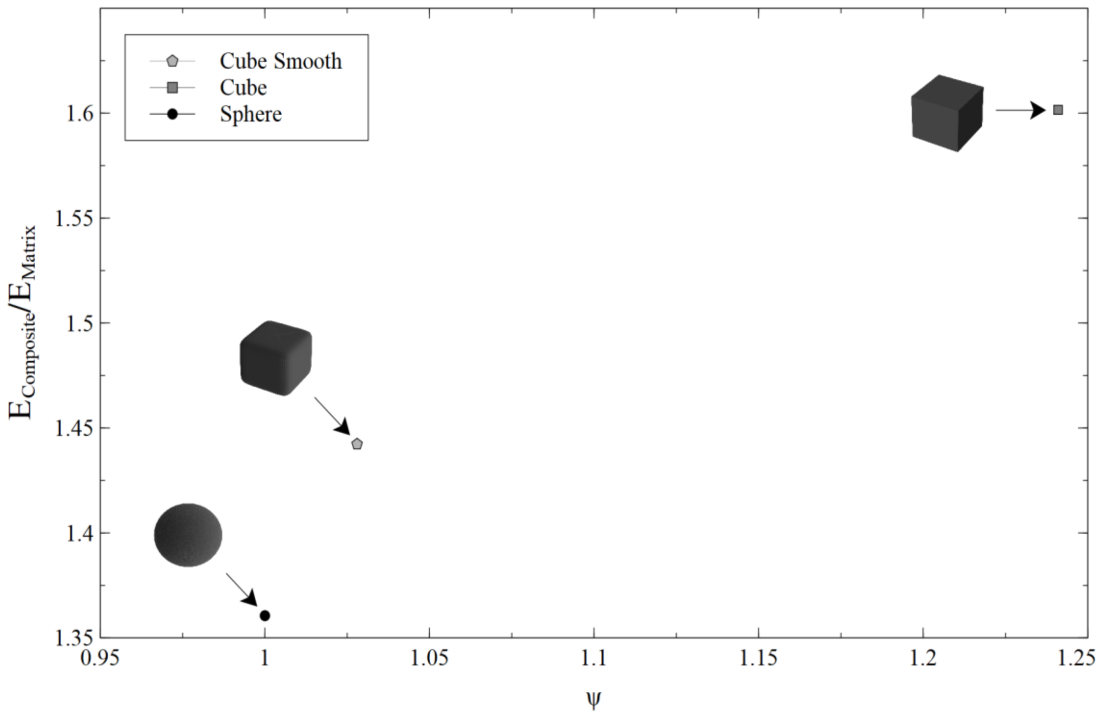

Figure 3: Normalized Young's modulus for specific particle form over surface to volume ratio.

The shape of the particles have a measurable influence onto the normalized Young's modulus of the particle reinforced composite, as is displayed in Fig. 3. Therefore the particle shape has to be taken into consideration, when approximating the microstructure of the composite.

2.2 Numerical Modeling for Multiple Particles

The shape of the reinforcing particle has an influence onto the effective Young's modulus of the composite, as was shown in the previous section. Up to this point only single particles embedded in the matrix material forming the RVE were considered. This method of creating an RVE can be used if the volume fracture of the particles in the composite is small. Most of the time this is not the case; usually particles are located close together, so that the interactions should be taken into account. Furthermore, simulations must include the formation of agglomerates, which are considered in the following by forming particle clusters throughout the matrix.

The particles utilized for the previous calculations were used to create RVEs containing multiple particles. The particles were distributed randomly throughout the RVE, no periodicity of the particles was applied here. The employed algorithm places particles inside the cube until the pre-set volume fraction is achieved, as proposed by Seguardo et al. [18]. Studies were conducted to estimate the appropriate amount of particles sufficient for obtaining the RVE. For a random homogenous distribution of a cube like particle the obtained RVE is depicted in Fig. 4.

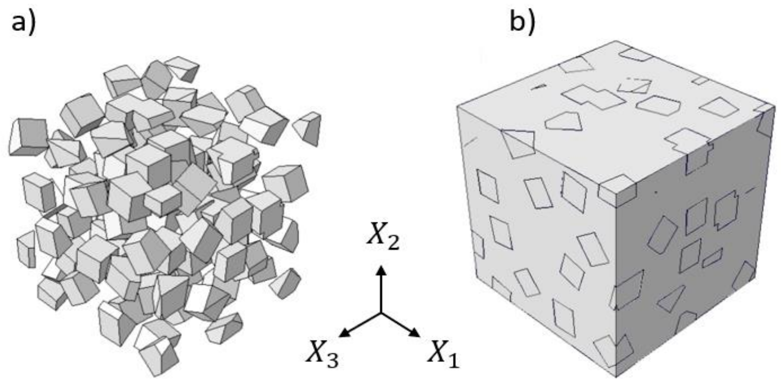

Figure 4: RVE for random homogenous distribution of a) cube particles, b) the same RVE with particles embedded in the matrix.

Calculations were carried out for different particle forms and particle volume fractions considering the case of the random homogenous distribution. A closer look was taken onto the influence of the orientation of the particles on resulting elastic properties. The particles generated in the previous section were placed randomly throughout the matrix and oriented along axis, if needed (as done for 'Cube Oriented ($\pm 10°$)'). The following particles were studied: 'Cube', 'Cube Smooth Edges' and 'Sphere', see Fig. 5.

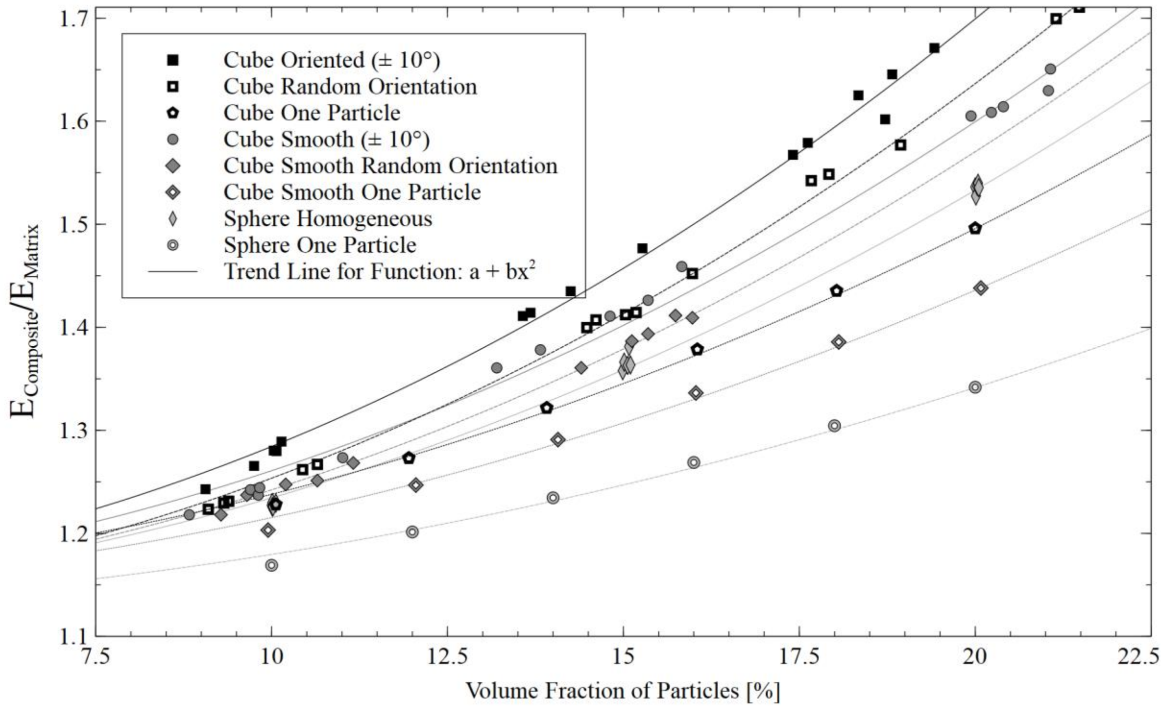

Figure 5: Normalized effective Young's modulus of the composite for different particle shapes and distributions for X1 direction. Trend line was obtained by minimizing chi-squared.

The elastic properties of the composite for each particle shape were evaluated using the ABAQUS software. The values of the normalized Young's modulus of the composite considering different particle shapes can be seen in Fig. 5, with $E_{Composite}$ being the Young's modulus of the composite and E_{Matrix} being the Young's modulus of the matrix material. The multiple inclusion set ups were also compared with their single inclusion counterpart. It can be seen, that the multiple particles set up achieves higher Young's moduli than the periodic distributed single particles in general.

The approximation of the real particle shape considering an RVE containing multiple particles has an influence onto the obtained Young's modulus of the composite. Furthermore, the slight deviation between particles of cube like shape with smooth and sharp edges can be observed.

Finally, a study was carried out on the effects of agglomerates onto the Young's modulus of the composite material. For this the algorithm generating the microstructure was edited to place the particles in a way so that they form a specific agglomerate type. Here two agglomerate types (cluster types) were studied. On the one hand a chain cluster of the particles and on the other hand cloud like agglomerate. For the chain cluster each particle is placed next to the previously placed one. The specific location for the subsequent particle is randomly selected. The general chain cluster is depicted in Fig. 6 a.

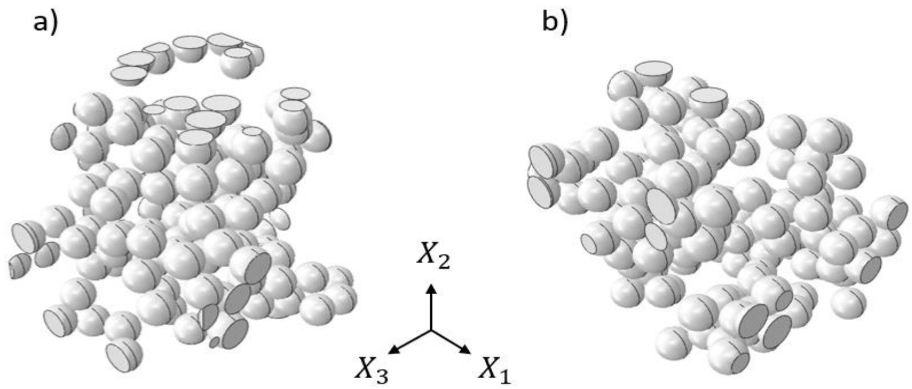

Figure 6: RVE with a) chain cluster, b) cloud cluster for spherical particles.

For the cloud cluster all particles are placed next to the initial particle. The specific location of the initial particle and every subsequent one is randomly chosen. This configuration is depicted in Fig. 6 b.

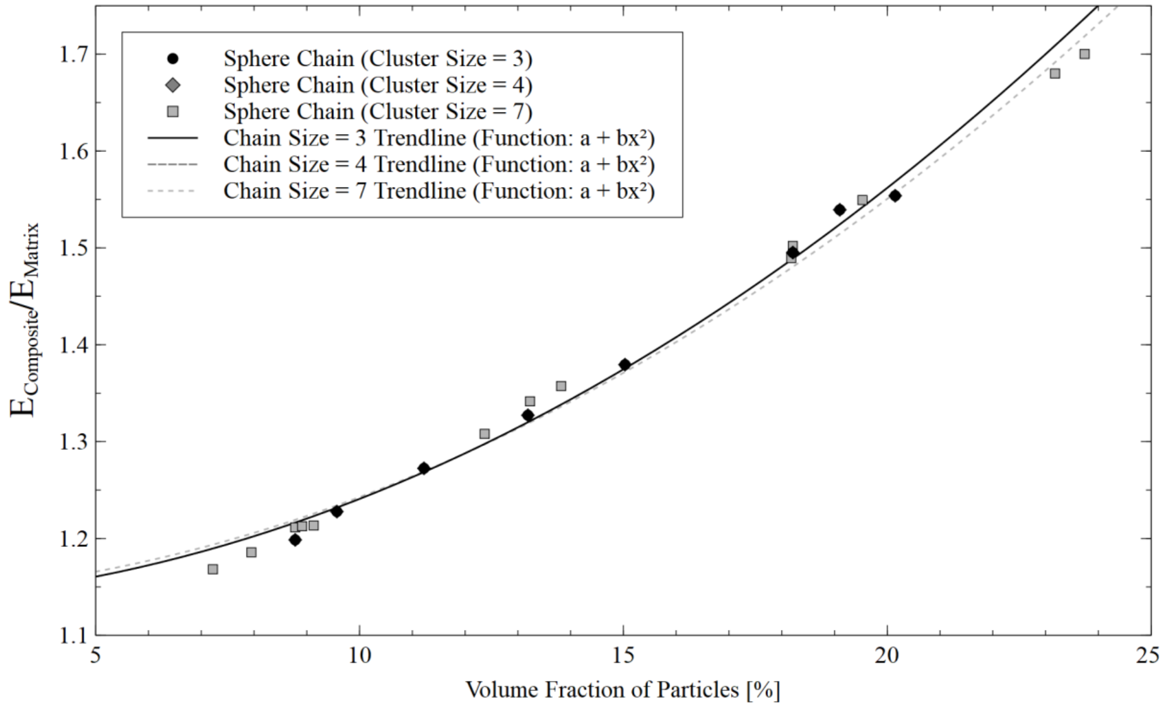

Figure 7: Normalized effective Young's modulus of the composite for chain consisting of 3, 4 and 7 particles for X1 direction. Trend line was obtained by minimizing chi-squared.

Of further interest is the size of the particle cluster and their effects on the overall elastic material properties. For this a study was carried out, which compares the effective Young's moduli of the composites for different chain lengths (Fig. 7) and cloud cluster sizes (Fig. 8).

The lengths of the chains do not seem to have an effect on the overall elastic material properties. In the case of cloud cluster, a slight deviation can be observed.

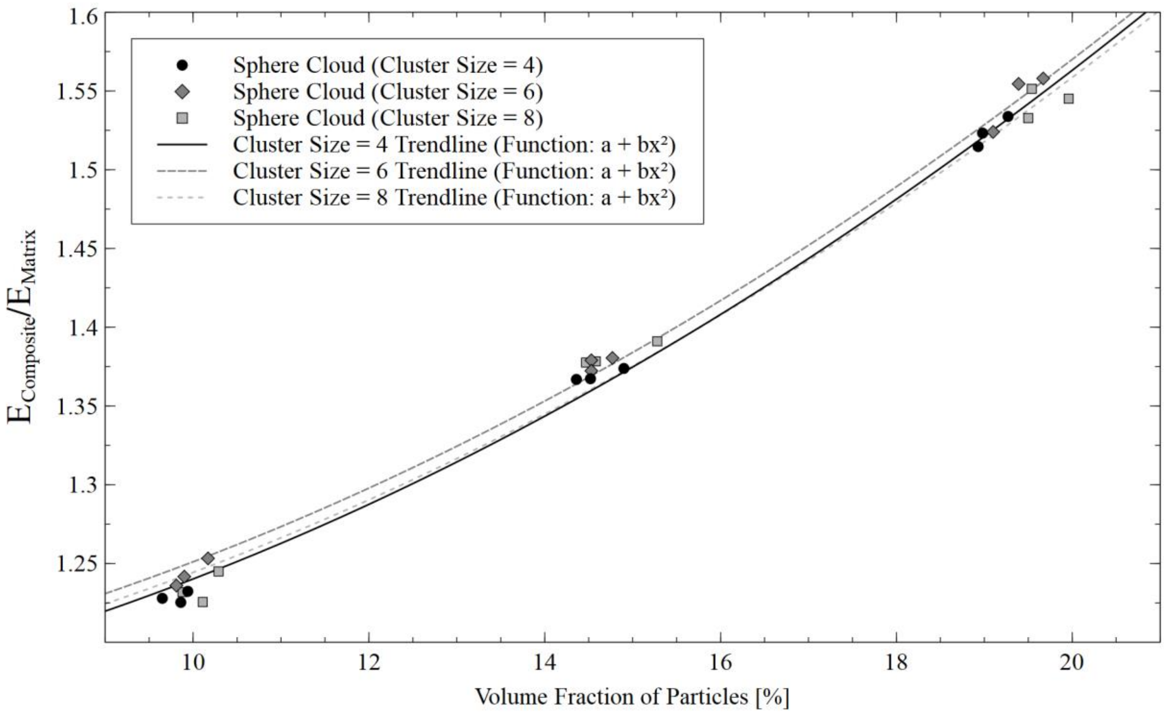

Figure 8: Normalized effective Young's modulus of the composite for cloud clusters consisting of 4, 6 and 8 particles for X1 direction. Trend line was obtained by minimizing chi-squared.

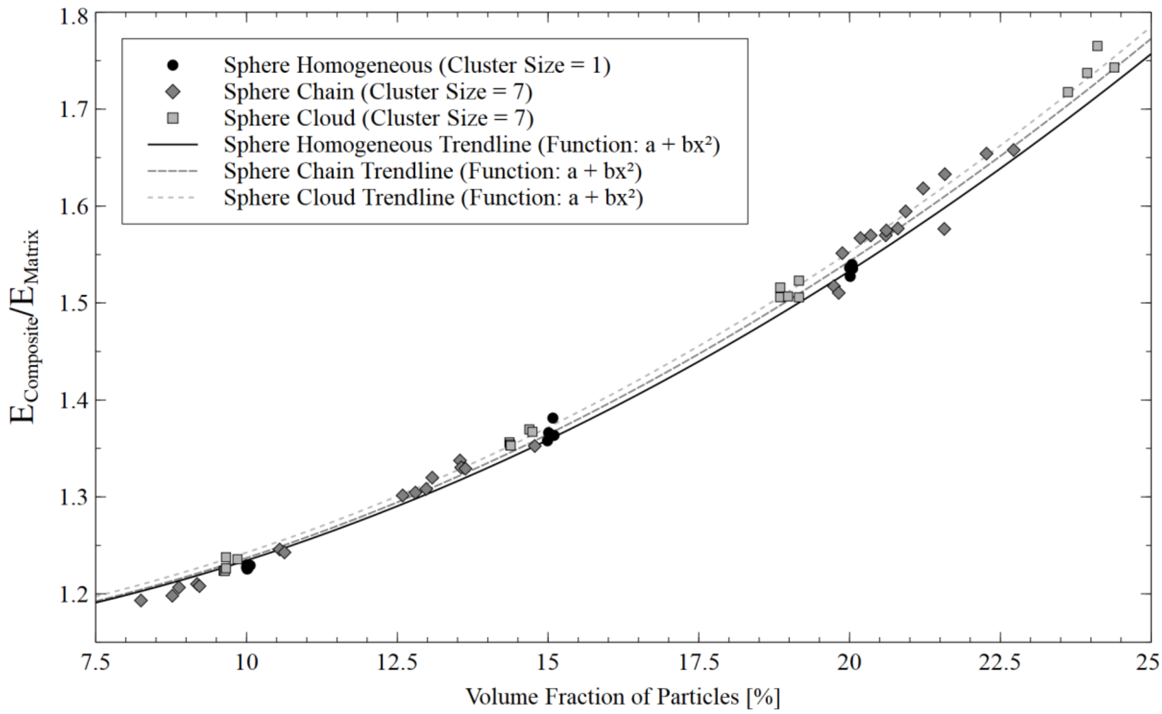

Figure 9: Normalized effective Young's modulus of the composite for different distributions of the spherical particles in X1 direction. Trend line was obtained by minimizing chi-squared.

Finally, the different particle distributions, homogeneous, chain and cloud, were compared with each other in Fig. 9. It shows normalized Young's modulus for homogeneously distributed particles, chain and the cloud clusters particle distribution.

It can be seen here that the results obtained with the cluster configurations deviate compared with the homogeneously distributed particles that do not form clusters. The difference in Young's modulus even grows with an increase in volume fraction of the particles.

A further interesting result of the evaluation is the difference between the clusters themselves. Different cluster formations do lead to deviations in the Young's modulus considering the different particle positioning methods, where the deviation grows with increase in the particle volume fraction considered (see Fig. 9).

In the subsequent steps, the influence of the ellipsoidal particles onto the Young's modulus of the composite was studied. The algorithm used for the placement of the sphere particles beforehand was changed to calculate the centre points of the ellipsoids. Both cluster types of the previous study were adopted for the following study, considering ellipsoids. The occurring microstructure is displayed in Fig. 9.

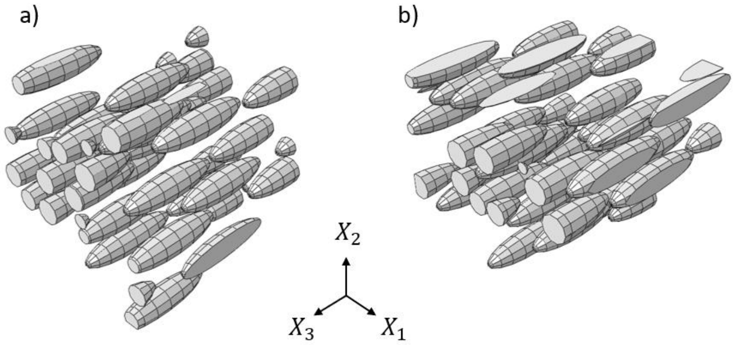

Figure 10: Multiple particle set up for ellipsoidal particles in a) chain cluster and b) cloud cluster.

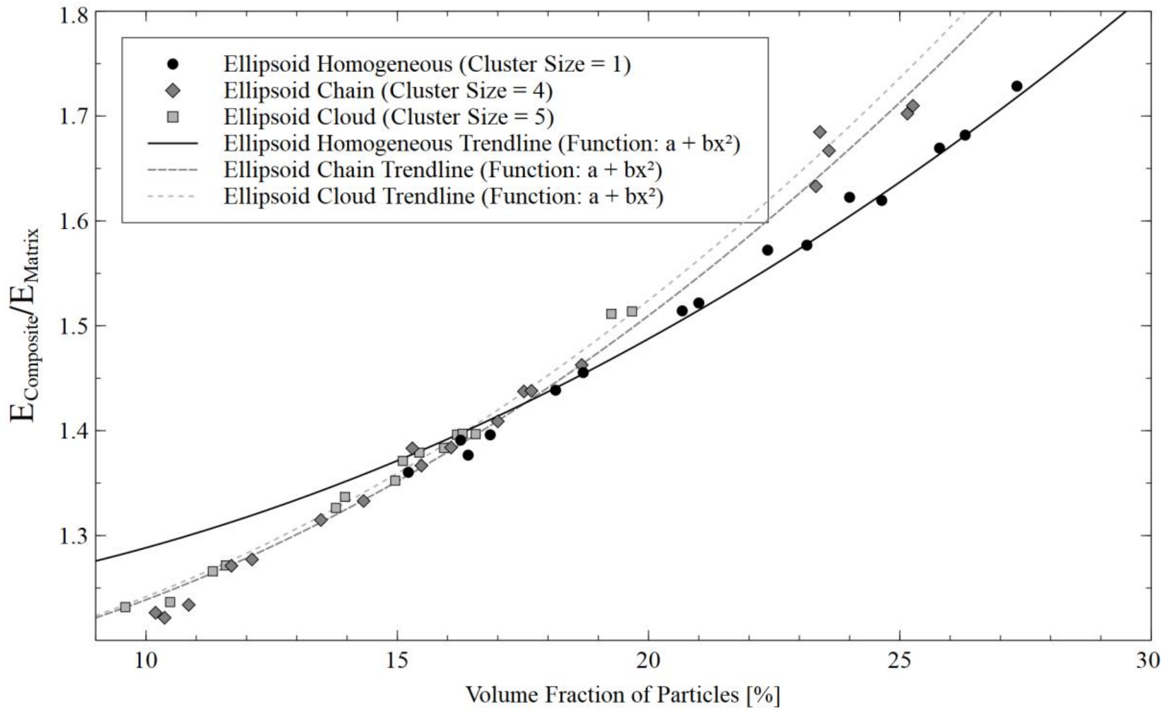

Figure 11: Normalized effective Young's modulus of the composite for different distributions of the needle-shaped particles in X1 direction. Trend line was obtained by minimizing chi-squared.

Fig. 10 displays the two types of studied particle clusters, namely the chain cluster (see Fig. 10 a) and the cloud cluster (see Fig. 9 b). The particles are oriented according to the X3-axis. The method of up to 10° deviation from the major axis was not adopted here. The Young's moduli for the three different placement methods (homogeneous particle distribution, chain and cloud cluster distribution) were evaluated. The results for the X1 direction are depicted in Fig. 11, and those for the X3 direction are shown in Fig. 12.

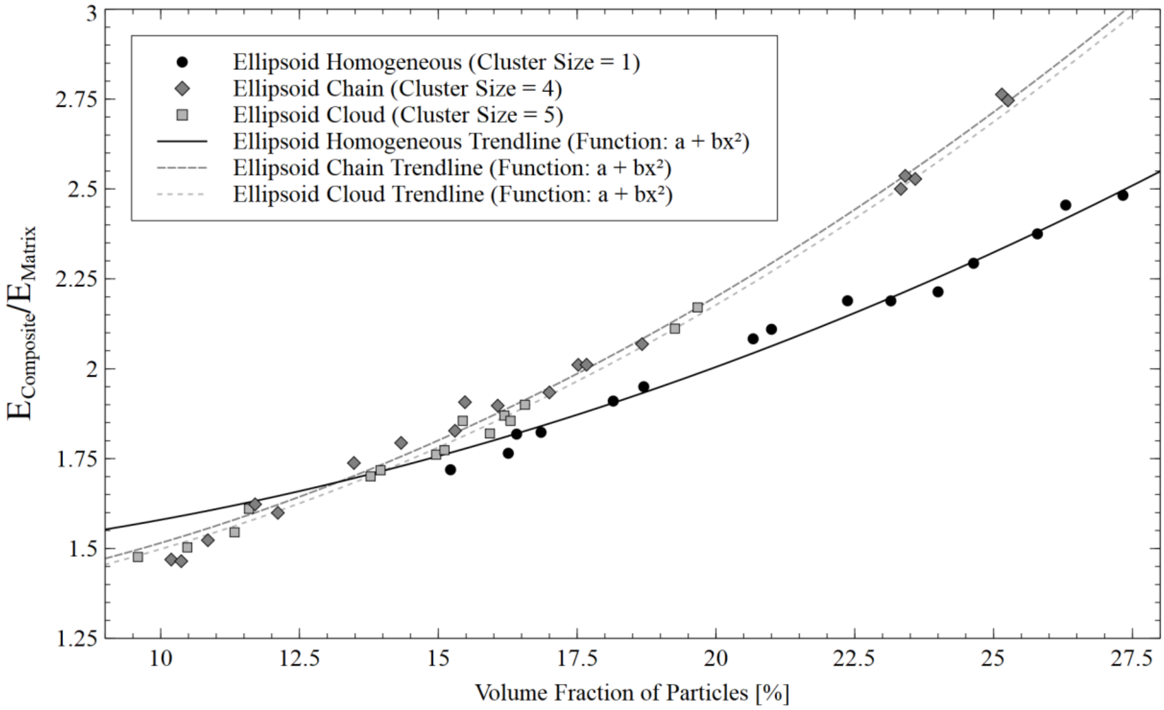

Figure 12: Normalized effective Young's modulus of the composite for different distributions of the needle-shaped particles in X3 direction. Trend line was obtained by minimizing chi-squared.

The differences between the cluster positioning methods and the homogenous particle distribution can be observed here as well. Clusters generally have a significant impact onto the obtained Young's modulus of the composite material. The presence of particle clusters throughout the matrix material must be taken into the consideration, when approximating the microstructure of a particle reinforced composite.

3 OUTLOOK

A numerical model for predicting the elastic properties of the composite was built and successfully validated in numerical calculations. In the next step, size and shape of the modelled particles as well as their orientation within the matrix will be adjusted to the above-mentioned new findings. Volume elements consisting of homogenous distributions of the particles with scattered clusters will be studied. In consequence, based on the adjusted design of the microstructure more realistic results are expected.

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