Structure and dynamics of densely packed ellipsoidal particles

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Packing problems, such as how densely objects can fill a volume are among the most basic and challenging problems in the physics of liquids and glasses. It is for example well known, that the phase diagram of hard spheres colloids depends on the volume fraction only. The highest packing fraction of ϕ=0.74 can be achieved only in the crystalline fcc structure [1]. Random close packing leads to lower volume fractions (ϕ=0.64) [2]. with amorphous structures which are of particular relevance for the glass transition of simple liquids [3]. Introducing an additional degree of freedom in the system (ellipsoidal particles) allows packing amorphous structures much more densely than simple spheres as shown by simulations and experiments [4]. Such ellipsoidal systems are expected to build up different amorphous structures depending on their aspect ratio.

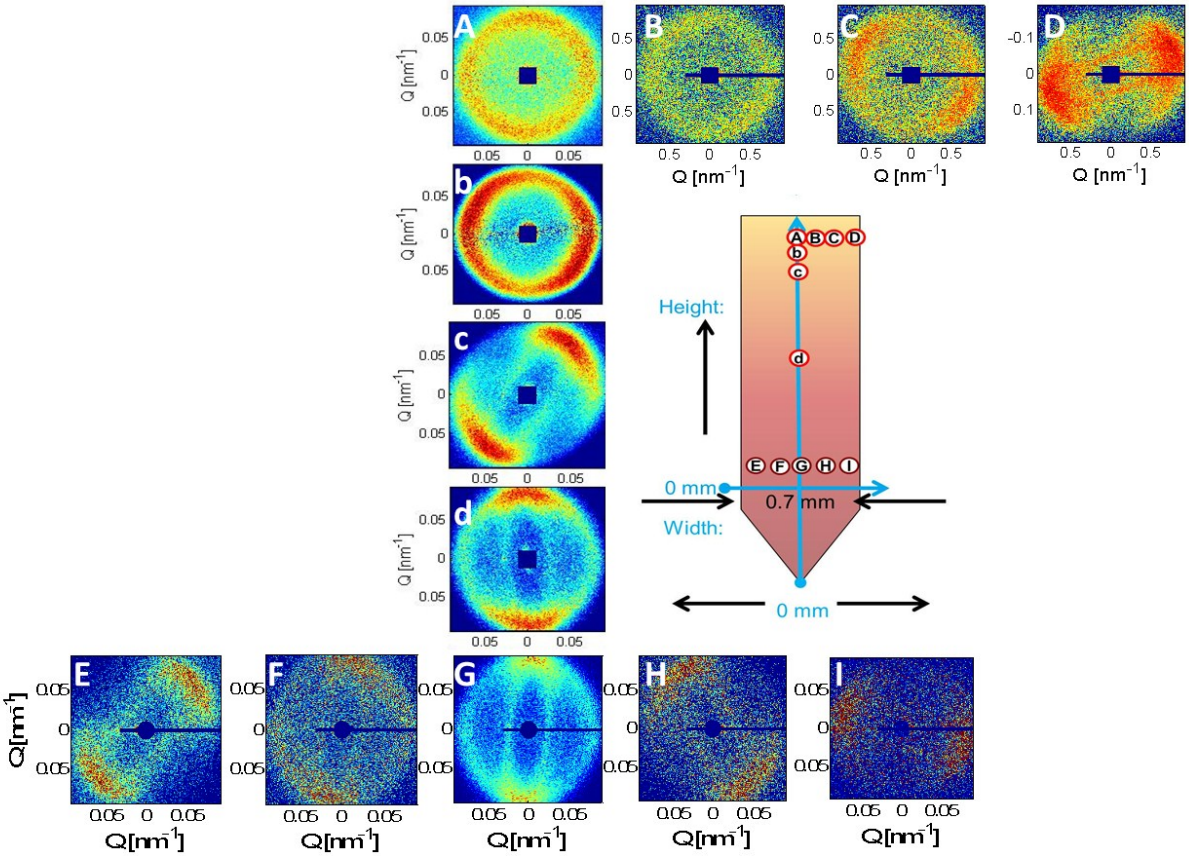

FIGURE 1: Sketch of the capillary used in the experiment (thickness 0.7 mm) and 2D pattern of the hematite particles measured in the dilute regime (ϕ=0.144) at spots between **A** → **D** and at high concentration (ϕ=0.187) from **G** → **I**. The concentration gradient was measured from **A** → **G**, via (ϕ=0.145) **b**, (ϕ=0.1575) **c** and (ϕ=0.165) **d**.

During the experiment we investigated the influence of confinement to a wall- due to the sample container a 0.7 mm quartz capillary - to the orientation of the elongated hematite particles by measuring spatially resolved 2D-SAXS patterns. For this purpose hematite particles with an aspect ratio of about ~3.5 have been centrifuged in order to achieve a volume gradient

To investigate the influence of the confinement due to the capillary wall the sample was measured at different distances to the capillary wall in the dilute regime at a concentration about ϕ=0.144 (Fig. 1 **A** → **D**) and concentrated regime with ϕ=0.187 (Fig. 1 **E** → **I**). In the dilute phase the anisotropic particles are almost completely randomly oriented in the middle of the capillary (Fig. 1 **A**). If the x-ray beam hits the sample closer to the wall of the capillary (Fig. 1 **A** → **D**), the isotropic pattern changes and two peaks appear. The particles align parallel to the wall, here we define the angle of their preferred orientation as φ=0.

In the concentrated phase the particles are stronger horizontally pre-aligned (Fig. 1 **G**) than in the dilute regime (Fig. 1 **A**) in the middle of the capillary. Here still some isotropic background from randomly oriented particles or domains can be seen in the pattern, especially at higher Q-values (Fig. 1 **G**). Closer to the wall the peaks gets sharper and the particles align parallel to the wall again like in the dilute phase (Fig. 1 **G→E** and **G→I**).

In order to determine the effect of volume fractions, diffraction patterns were taken at different spots from low **A** at ϕ=0.144 to high concentration ϕ=0.187 **G** in the middle of the capillary (Fig 1 **A→G**). The volume fraction was determined via the x-ray transmission of the sample under the assumption of a 0.7 mm capillary which is filled with iron oxide particles in water. The absorption was calculated according to Henke et al [5]. At **A** the particles are randomly oriented and the scattering pattern has an isotropic shape **A** (Fig. 1). Further down at ϕ=0.145 **b** the particles change their preferred direction to (φ=1.38) and the particles gets more ordered. At even higher concentration at ϕ=0.158 (Fig. 1 **C**) the particles change their preferred orientation to φ=2.63 and there are almost perfectly ordered. At concentrations higher than ϕ=0.158 the particles align horizontally **d** and **G** (Fig. 1).

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