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Minkowski Tensors and Local Structure Metrics: Amorphous and Crystalline Sphere Packings


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Abstract. Robust and sensitive tools to characterise local structure are essential for investigations of granular or particulate matter. Often local structure metrics derived from the bond network are used for this purpose, in particular Steinhardt’s bond-orientational order parameters $q_l$. Here we discuss an alternative method, based on the robust characterisation of the shape of the particles’ Voronoi cells, by Minkowski tensors and derived anisotropy measures. We have successfully applied these metrics to quantify structural changes and the onset of crystallisation in random sphere packs. Here we specifically discuss the expectation values of these metrics for simple crystalline unimodal packings of spheres, consisting of single spheres on the points of a Bravais lattice. These data provide an important reference for the discussion of anisotropy values of disordered structures that are typically of relevance in granular systems. This analysis demonstrates that, at least for sufficiently high packing fractions above $\phi > 0.61$, crystalline sphere packs exist whose Voronoi cells are more anisotropic with respect to a volumetric moment tensor than the average value of Voronoi cell anisotropy in random sphere packs.

Keywords: granular matter; local structure; random close packing; sphere packs; order metrics
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The quantitative morphological description of local structure is a commonly required tool when studying amorphous particulate systems, such as granular matter or structural glasses, but also in cellular structures such as liquid soap froths or metal foams. Often, the task at hand will be the detection of local crystalline domains, e.g. in nucleation phenomena in sheared spherical bead packs [1]. A more challenging task is the description of local structure in systems that are far from an ordered state. For example, one may want to characterise the difference in local structure in systems that are amorphous throughout the sample but that spatially separate into domains of different typical local structural motifs, as has been observed recently in granular heaps [2]. Similarly, a disordered jammed or un jammed configuration may evolve, for example under some compaction protocol, with distinct changes to the local structure without ever reaching short- or long-range order. How does one characterise differences between different forms of disordered configurations?

The most commonly used method for quantifying local structure of spherical bead packs is by construction of a nearest-neighbour bond network on which quantitative structure metrics are computed, most notably the bond-orientational order parameters $q_l$ and $w_l$ introduced by Steinhardt et al [4], see also the discussion in [5].

An alternative approach for quantifying local structure is provided by analyses of the Voronoi diagram of the bead pack. The Voronoi diagram is the partition of space into the same number of convex cells as there are beads in the packing. The Voronoi cell of a sphere is the region of space closer to that given sphere than to any other sphere. In granular matter, Voronoi diagrams have been used to determine distributions of local packing fractions.
We have recently suggested that the shape of Voronoi cells, in particular the degree of anisotropy or elongation, provides insightful information about the local structure of sphere packings and sphere ensembles [11, 12, 13].

A comprehensive quantitative method for characterising the degree of anisotropy of a convex object $K$, here the Voronoi cell, is provided by so-called Minkowski tensors [14, 15], based on the solid foundation of integral geometry [16]. The Minkowski tensors of rank two comprise the moment tensor $W_0^{2.0} = \int_k r \otimes r dV$, similar to the tensor of inertia, the moment tensor of the bounding surface $W_1^{2.0} = \frac{1}{3} \int_{\partial K} r \otimes r dA$ and the interface tensor $W_1^{0.2} = \frac{1}{3} \int_{\partial K} n \otimes n dA$; here $r$ and $n$ are position and surface normal vectors, and $\partial K$ is the bounding surface of the object $K$. For 3D polyhedra, the set of Minkowski tensors is completed by moment tensors $W_1^{2.0} = \frac{1}{3} \int_{\partial K} H(r) r \otimes r dA$ and $W_2^{2.0} = \frac{1}{3} \int_{\partial K} G(r) r \otimes r dA$ whose support are the edges and vertices of the polyhedral surface and by a curvature-weighted interface tensor $W_2^{0.2} = \frac{1}{3} \int_{\partial K} H(r) n \otimes n dA$, see eq. (5-10) in ref. [14]; $H(r)$ and $G(r)$ are discrete versions of the mean and Gauss curvature which are non-zero only at edges and vertices of the polyhedron $K$, respectively. For the tensors $W_2^{0.2}$, we choose the sphere centres as the origin.

Each of these six tensors characterises a different aspect of the shape of $K$; for example, the moment tensor $W_0^{2.0}$ is an integral measure of the distribution of mass of the solid cell, $W_1^{2.0}$ of the same distribution of the hollow cell and $W_1^{0.2}$ of the orientational distribution of facet directions (see ref. [14] for an interpretation of the remaining tensors). A simple way for reducing these tensorial measures into scalar shape measures is the ratio $\beta_V^{\nu, s} = e_{\min}/e_{\max}$ of the smallest eigenvalue $e_{\min}$ of $W_V^{\nu, s}$ to the largest eigenvalue $e_{\max}$, although other invariants could also be used [5, 17]. An object $K$ with $\beta_V^{\nu, s} = 1$ is said to be isotropic with respect to the Minkowski tensor $W_V^{\nu, s}$, and smaller values than 1 correspond to anisotropy or elongation. Note that this notion of isotropy is not a measure of deviations from a sphere (in contrast to the concept of asphericity [18]), but a measure of elongation; a cube, all regular polyhedra, the Voronoi cells of hcp and fcc closest packings of spheres all have $\beta_V^{\nu, s} = 1$, for all six tensors.

Our previous analysis [11] of Voronoi cell shapes in monodisperse static disordered sphere packs below packing fractions of 64% has demonstrated:

(a) The average Voronoi cell anisotropy ($\beta_V^{\nu, s}$) appears to be largely protocol-independent. The Voronoi cells become on average more isotropic as the packing fraction increases. See Fig. 2(a).

(b) The fraction of isotropic cells with $\beta_V^{\nu, s} = 1$ vanishes for packings below $\approx 64\%$, cf. Fig. 2(b) and ref [13].

(c) Changes in anisotropy are qualitatively the same, regardless of the morphological aspect (i.e. which of the six Minkowski tensors) is used to characterise it.

(d) Larger cells are less isotropic than smaller ones, with an approximate linear relationship between the average $\beta_0^{2,0}$ and the local packing fraction, see Fig. 6 in ref. [11].

(e) In Lubachevsky Stilling simulations where configurations below and above $\phi_{BEP}$ can be obtained, a change in the distribution and averages of cell anisotropies $\beta_V^{\nu, s}$ is observed, reflecting the onset of local crystalline domains. See Fig. 2(a) and also ref. [13].

(f) Non-static or unjammed disordered sphere configurations are more isotropic than jammed disordered packings at the same density, at least those obtained from random local distortions of slightly eroded jammed pack-
Bravais lattice given by three lattice vectors translational unit cell. These are obtained by testing if a bead, i.e. all beads (and also their Voronoi cells) are decorating the points of a Bravais lattice with a single the same hemisphere), and any bead is connected to any tact with at least 4 other spheres (which may not all be in finite set of non-overlapping monodisperse spheres ar-

ing or as non-terminal configurations with finite pressure in the Lubachevsky Stilinger algorithm.

We here present an analysis of \( \beta^C \) for the Voronoi cells of crystalline bead packs. This analysis provides a reference for the interpretation of Voronoi cell anisotropy values in disordered packings. In addition, this analysis is also motivated by the following question, related to point (i) above and indeed posed to us by an anonymous referee: At a fixed volume fraction below \( \phi_{RCP} \approx 64\% \), are there any ordered crystalline static bead packs whose Voronoi cells are less isotropic (i.e. smaller values of \( \beta^C \)) than the jammed disordered structures?

For our purposes, a crystalline bead packing is an infinite set of non-overlapping monodisperse spheres arranged on a periodic lattice with 3 independent lattice vectors. To ensure staticity, each sphere must be in contact with at least 4 other spheres (which may not all be in the same hemisphere), and any bead is connected to any other via a chain of sphere-sphere contact points.

We specifically study periodic bead packs obtained by decorating the points of a Bravais lattice with a single bead, i.e. all beads (and also their Voronoi cells) are symmetrically equivalent and there is only one bead per translational unit cell. These are obtained by testing if a Bravais lattice given by three lattice vectors \( \mathbf{a}, \mathbf{b}, \mathbf{c} \), all of unit length \( |\mathbf{a}| = |\mathbf{b}| = |\mathbf{c}| = 1 \) represents a valid static sphere pack, as defined above, for spheres of diameter 1.

In practise, we parametrise the vectors by the three crystallographic angles between them, \( \gamma = \angle(\mathbf{a}, \mathbf{b}), \alpha = \angle(\mathbf{b}, \mathbf{c}) \) and \( \beta = \angle(\mathbf{c}, \mathbf{a}) \), and scan the representative range of \( \alpha, \beta, \gamma \in [0, \pi] \) by even discretisation in intervals of \( 10^{-3} \). For each set of values, we test for particle overlap with an absolute tolerance of \( 10^{-4} \) (for particles of diameter 1) and for particle neighbourhood with an absolute tolerance of \( 10^{-4} \).

Figure 3 shows the results of the analysis of the Voronoi cell anisotropies of these crystalline packings. Each diagram is a scatter plot, where each point represents one of the generated packings. The color coding provides additional information about the kissing number (coordination), i.e. the number of neighbour spheres in contact with the sphere. Noteworthy results are

(a) As expected, the simple cubic packing with \( \phi = \pi/6 \approx 0.52 \), the bcc packing with \( \phi = \sqrt{3}\pi/8 \approx 0.68 \) as well as the fcc and hcp packings with \( \phi = \pi/\sqrt{18} \approx 0.74 \) are isotropic w.r.t. all tensors, i.e. \( \beta_{ij}^C = 1 \).

(b) With respect to the tensors \( W_{0,0}^2, W_{2,0}^2, W_{0,2}^2, W_{2,2}^2 \) and \( W_{1,1}^0 \), the sc, bcc, fcc and hcp packings are the only ones with isotropic Voronoi cells. However, for the interface tensor \( W_{1,0}^1 \), an additional isotropic case exists, namely the hexagonal AAA stacking at \( \phi = \pi/(3\sqrt{3}) \approx 0.60 \) (see Fig. 1). In terms of the mass distribution this
Voronoi cell is not isotropic, but in terms of the surface normal distribution it is.

(c) The hexagonal AAA stacking (see Fig. 1) is maximally isotropic w.r.t. interface tensor $W_{1}^{2,0}$ and it is more isotropic w.r.t. the moment tensor $W_{0}^{2,0}$ than any of the other crystalline packings with the same packing fraction $\phi$. However, w.r.t. the tensors $W_{3}^{2,0}$ and $W_{4}^{2,0}$ the AAA structure is the least isotropic one out of all crystalline packings analysed here. See Fig. 3.

(d) There is no universal correlation between kissing number (coordination) and Voronoi cell anisotropy. For example, with respect to the moment tensor $W_{0}^{2,0}$, the kissing number can increase (see the arrow marked “B” in Fig. 3a) or decrease (A) with increasing anisotropy.

(e) For all packing fractions below $\phi \approx 0.61$, marked as point C in Fig. 3(a), none of the sphere packings described above has Voronoi cells that are more anisotropic (i.e. with smaller values of $B^2_0$) than the average anisotropy of the jammed disordered structures studied in ref. [11]. In particular in terms of the facet orientational distribution ($W_{0}^{2,0}$) all crystalline Voronoi cells are significantly more isotropic than the jammed disordered ones. However, with respect to $B^2_0$ there are crystalline Voronoi cells in the range $\phi > 0.61$ that are less isotropic than the average jammed disordered ones.

Note that sphere packs with $|a| \neq 1$, or $|b| \neq 1$ or $|c| \neq 1$ exist, but are excluded from this analysis since an efficient search through the then six-dimensional configuration space is hard (For a more systematic approach, the enumeration of crystalline sphere packs by Koch and Fischer [23] appears as a good starting point). A preliminary generation of some packings with $|a| \neq 1$, or $|b| \neq 1$ and $|c| \neq 1$ has yielded the following result, that requires confirmation. For all resulting such packings that have $\phi > \pi/6 \approx 0.524$, the cell anisotropies are between the minimal and maximal anisotropies found for packings with unit length lattice vectors, for all tensors.

The seemingly well-defined and smooth curves representing the minimally and maximally observed anisotropies in Fig. 3 are an indication that analytic expressions for these envelopes could be determined. For this purpose, existing knowledge (see the table on p. 112 of ref. [24]) of possible Voronoi cell structures for crystalline lattice configurations may be helpful.

It appears that local structure analyses based on shape characterisation of Voronoi cells is a useful approach for granular systems. Compared to standard approaches by using the nearest neighbour bond network, this approach has two significant advantages. First, it is a more geometric method and avoids the problems associated with the discrete nature of the changes of neighbourhood [5]; whereas a neighbour bond abruptly ceases to exist, the Voronoi cell shape changes continuously. Second, the method generalises more readily to configurations of spherical particles where the notion of a bond network is even more ambiguous. Spherical bead packs are an important model for this method, and the crystalline configurations provide reference values.

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