

Re: ET11862

Quasiperiodic sphere packing generated by random ballistic deposition
model in confined space
by Lin Hao, Ming Yuan, Qi Liu, et al.

Dear Dr. Xia,

The above manuscript has been reviewed by two of our referees. Comments from the reports appear below.

These comments suggest that the present version of the manuscript is not suitable for publication in the Physical Review. However, if you can provide a convincing response to the criticism, we will give further consideration. Please accompany any resubmittal by a summary of the changes made and a brief response to all recommendations and criticisms.

Yours sincerely,

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In this paper, the authors reported a systematic numerical investigation of the packing behaviors of congruent hard spheres in confined quasi-2D domains. The packings were generated via random ballistic deposition (RBD) methods. The authors found that these quasi-2D packings possess characteristics lying between perfect 2D and 3D packing, including long-range correlation and partial geometric frustrations. The authors established scaling relations between the correlation length, order parameter and container width. Importantly, the authors discovered a geometric phase transition as the confinement width varies. The intrinsic non-equilibrium and ergodicity-breaking nature of RBD were also discussed.

This is a very interesting work. This paper is overall well written and easy to follow. The idea of considering confinement as equivalent quasi-dimension is very intriguing. I am happy to recommend its publication in PRE. However, the authors might want to consider addressing the following optional revisions.

It could be helpful if the authors could elaborate a little more on the effects of RBD. It seems that RBD has an intrinsic broken symmetry direction. Would this help select the unique stacking direction of the zig-zag chains? **Would the packing structures and the associated transition behaviors different from the reported results if isotropic packing algorithms were employed**, such as event-driven molecular dynamics (Journal of Computational Physics, 202, 737 (2005)), linear-programming (Physical Review E, 82, 061302 (2010)) or Monte-Carlo methods (Physical Review E, 80, 041104 (2009))?

Another related question is whether the packing states obtained here are generic, similar to RCP or MRJ? These packing states are robust and independent of packing protocols used, but are also ergodicity-breaking and non-equilibrium. It would be interesting to see **whether the unique packing characteristics observed in this work resulted from spatial confinement alone or also strongly depended on the packing protocol**. Either case would be very interesting.

(xcj: 第一位审稿人是觉得工作有趣的，而且他应该是做类似颗粒和玻璃化转变的，所以对这些相关结论比较欣赏。他核心的问题是，现象与制备的方法是否有关。之后应通过文献的对比，加一些尝试性的工作，给出一些定性结论，应该就可以了。)

Report of the Second Referee -- ET11862/Hao

This paper numerically studies packing of spheres in a quasi 2D container generated by a random ballistic deposition (RBD) model. The authors suggest that the system exhibits a geometric phase transition, as they control the short side width w_s by fixing the long side width w_l . The authors suggest that the critical point is located at $w_s=1$, i.e. if three dimensional effects are involved in a system, the system is completely different from a pure 2D system. The order parameter of the phase transition is the probability distribution $p(4)$ of contact number 4, which satisfies $1-p(4) \sim (w_s-1)^{1/2}$ for $w_s < 1.1$ and $(w_s-1)^{1.5}$ for $w_s > 1.1$. The divergence of the correlation function also changes the power law exponent from $\xi \sim (w_s-1)^{-0.47}$ for $w_s < 1.1$ to $(w_s-1)^{-1.7}$ for $w_s > 1.1$. They also found some characteristic behavior of persistent length of quasi-periodic pattern and its characteristic length.

This paper contains some interesting findings from their simulation, but the current version is unreadable, at least, for me. Therefore, I do not recommend the publication of this paper in Phys. Rev. E. If the authors will revise the manuscript completely as a readable form, I will reconsider the possibility of the publication in PRE.

The most frustrated point of this manuscript is that the authors **do not what the geometric phase transition they found is clearly in both the abstract and the conclusion**. It is trivial that any quasi-2D systems differ from pure 2D systems. Probably, one of the most important their findings is **the transition at $w_s=1.1$** , but they do not explain anything what happens at this point. It is interesting that there is no singularity in the behavior of $\langle \Delta_{yz} \rangle$ at $w_s=1.1$, though the authors do not explain anything.

Similarly, the authors just enumerate the results of their simulation without any **theoretical explanations of the obtained results**. Such a paper is not suitable for PRE.

From now on, let me list unsatisfied points.

1. The writing style of this manuscript seems to be one of letters. Because the authors have submitted this paper to PRE, they should rewrite the manuscript following the standard format of PRE, which must have sections.
2. The authors introduce the topological index n , but **the role of the index** is unclear in later discussion.
3. Physical meanings of Eqs. (1) and (2) are unclear.
4. **They should explain the results of $\langle \Delta_{yz} \rangle$ for $w_s > 1.1$** , though the current analysis only contains the results for $w_s < 1.1$.

5. The definition of the persistent length is unclear. It is impossible for followers to reproduce their results only by the first sentence of the last paragraph of p.6 (line 131).
6. The authors suggest that $p(L_p) \sim L_p^{-2}$ but the exponent 2 seems to be too large judging from Fig. 3(b).
7. Are there any relationships between the exponent μ for the characteristic persistent length of pattern and the exponent of $p(L_p)$?
8. Equation (5) contains two z on the left hand side, but the continuous z must be integrated out on the right hand side. So the left hand side should read g_z .
9. The authors **clarify the physical meaning of the singularities at $w_s=1.1$.**
10. The authors need to explain their numerical results by using the theory.

(xcj: 这位审稿人估计是做理论的，比较严格。核心的不足有两个，一个是应该和相变理论联系起来，各个指数之间的关系，这个我要再整理和思考一下。另一个是 $w_s=1.1$ 附近的现象，需要深入研究和解释。)