

每个压缩率下算200个样本

## 规模：1000个颗粒

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\*\*制备0.64附近：

1. 从0.1到0.6几全程快速压缩，抑制结晶
2. 最后缓慢压缩确保jam 1e-2 done 5e-3 done 1e-3 done

制备0.65-0.7之间：

1. 先从0.1到0.4快速压缩
2. 然后全程缓慢压缩直到结束 5e-4 done 1e-4 done 5e-5 done 1e-5 done 5e-6 1e-6

## 规模：4N^3: 864

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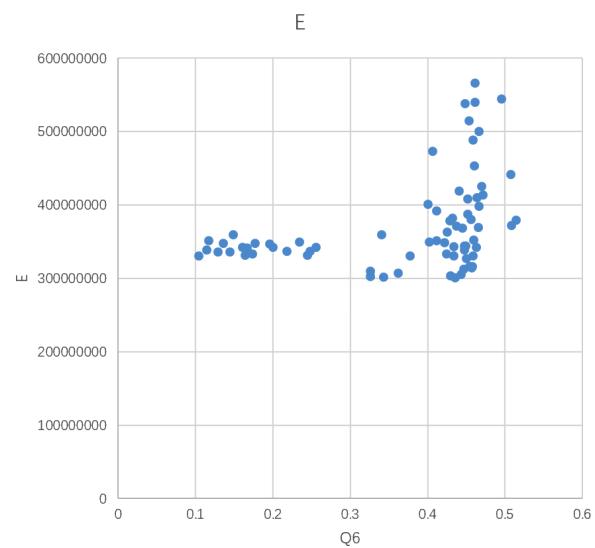
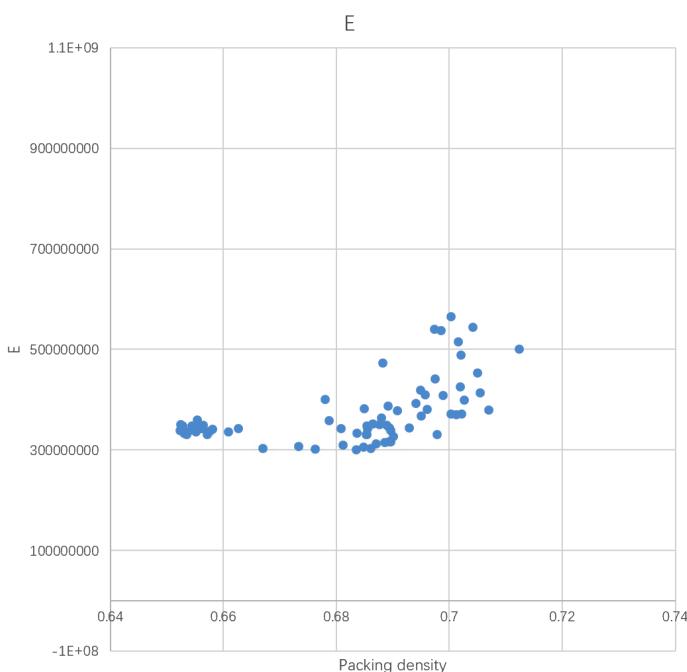
制备0.7-0.74之间：

1. 先从0.1到0.4快速压缩
2. 然后全程缓慢压缩直到结束 5e-4 done 1e-4 done 5e-5 done 1e-5 done 5e-6 1e-6

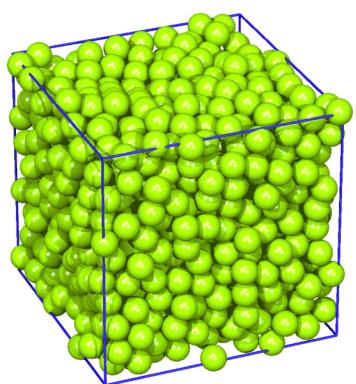
引入defect 集合

对rattler问题要有交代，至少是collectively jammed

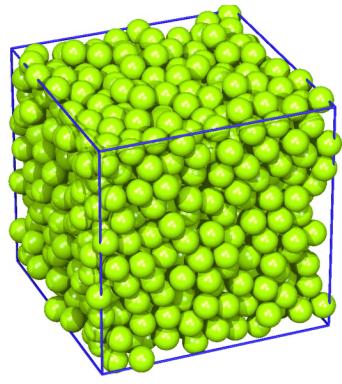
Q6



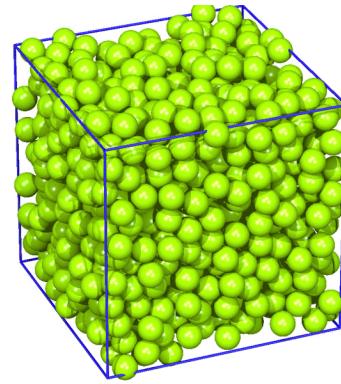
RDF



$\mu=92$   
 $Pd=0.624$   
 $Cn=4.0$   
 $Q6=0.045$



$\mu=0$   
 $Pd=0.6407$   
 $Cn=6.0$   
 $Q6=0.045$



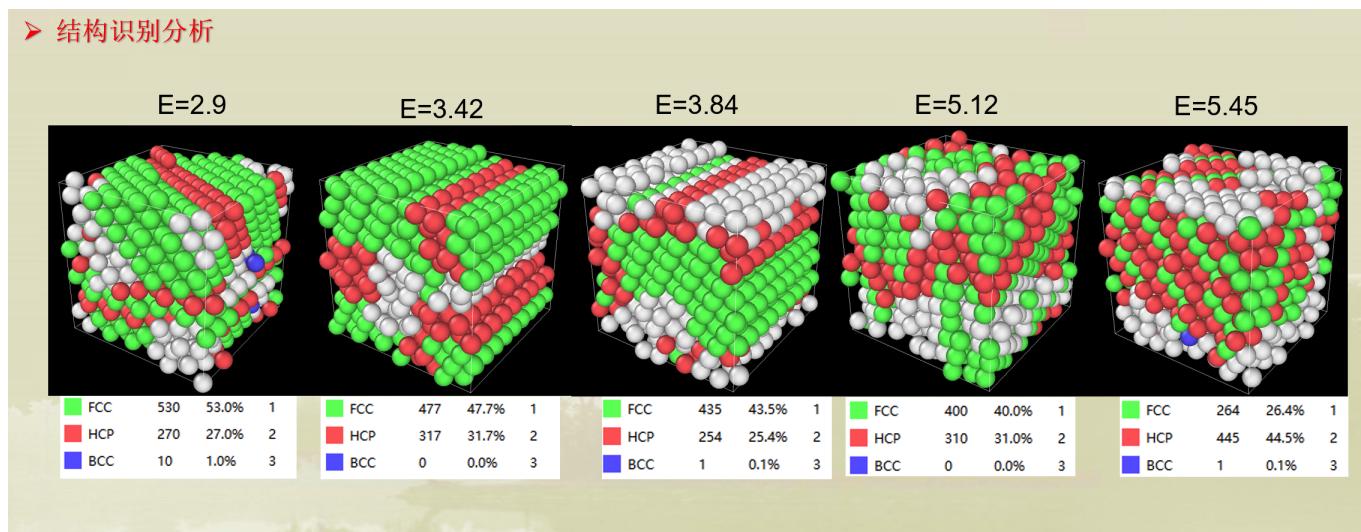
$\mu=92$   
 $Pd=0.568$   
 $Cn=3.8$   
 $Q6=0.045$



Mechanical Characterization of Partially Crystallized Sphere Packings附件里有提到新的RDF计算方法

Ovito analysis

## ➤ 结构识别分析



## 不同密度下的最高模量

0.681-3.7

FCC=95

HCP=130

Total=225

0.685-4.09

FCC=157

HCP=61

Total=238

0.690-4.82

FCC=94

HCP=153

Total=247

0.695-5.24

FCC=297

HCP=0

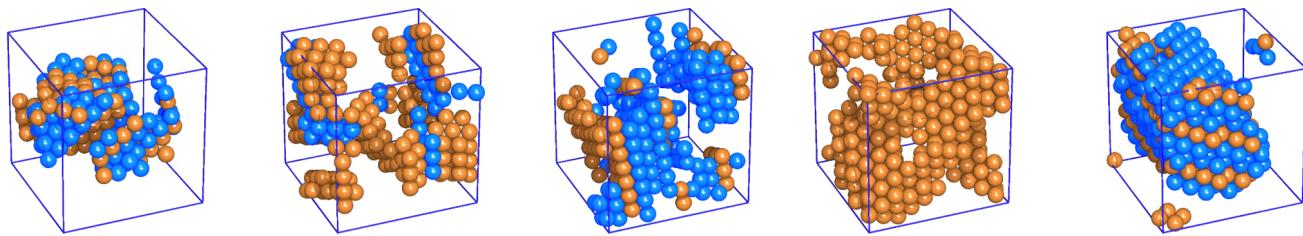
Total=297

0.701-5.45

FCC=183

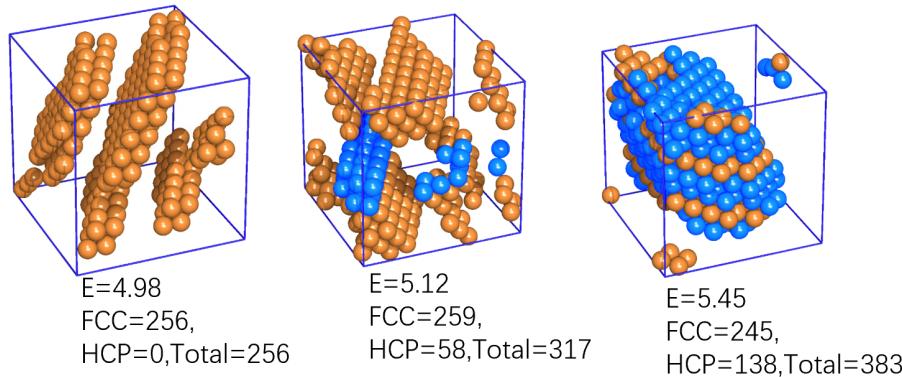
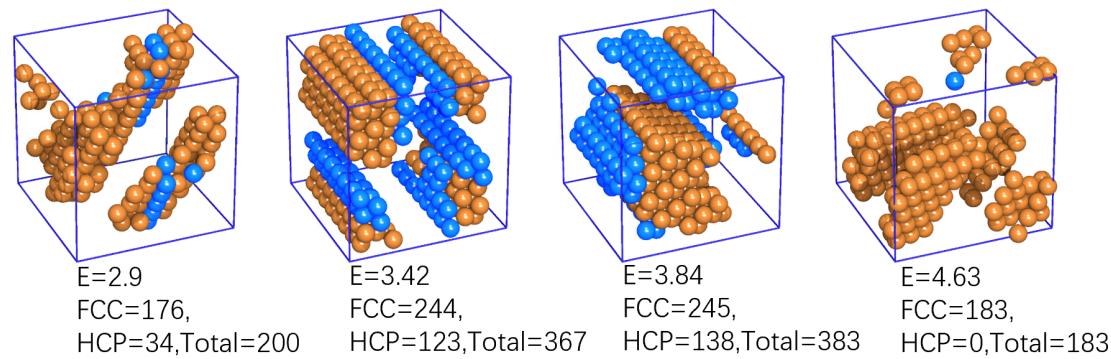
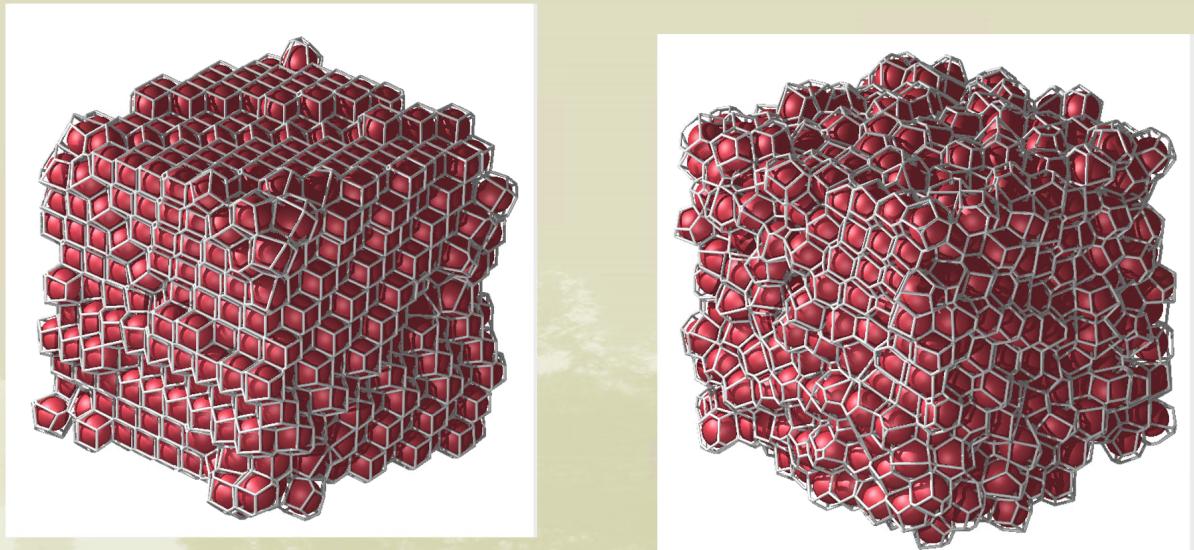
HCP=349

Total=532



## voronoi分析

## 球填充的Voronoi分析

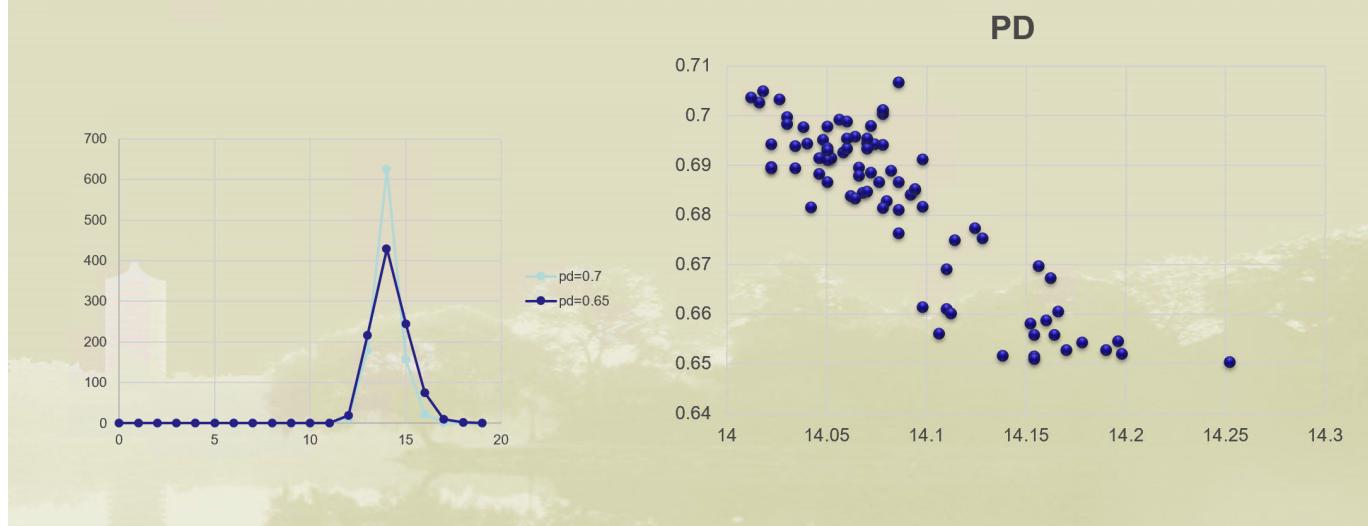


1、结晶数量  
 2、形成2d层状结构

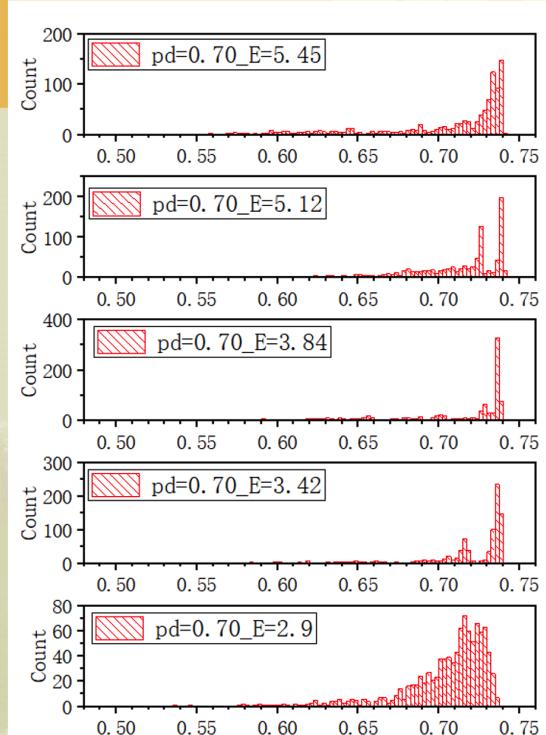
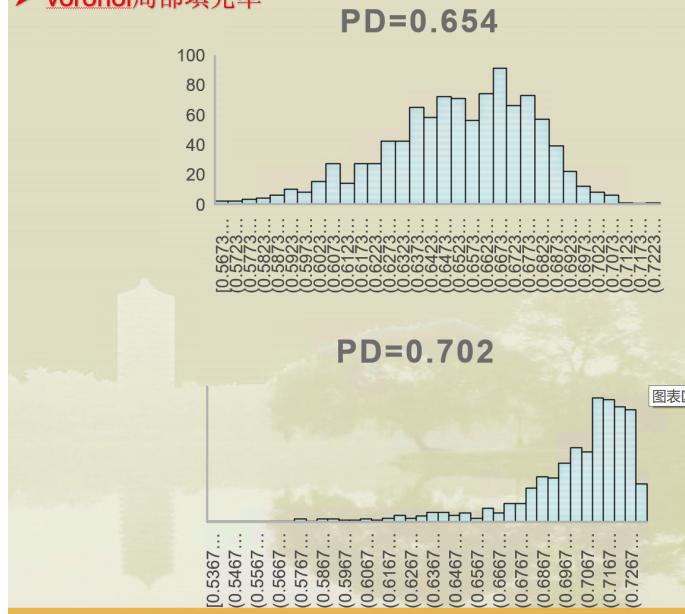
## 配位数

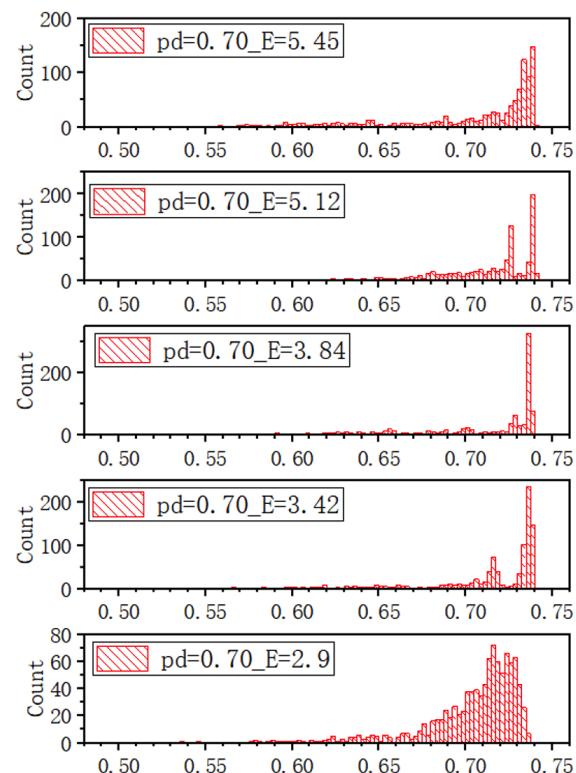
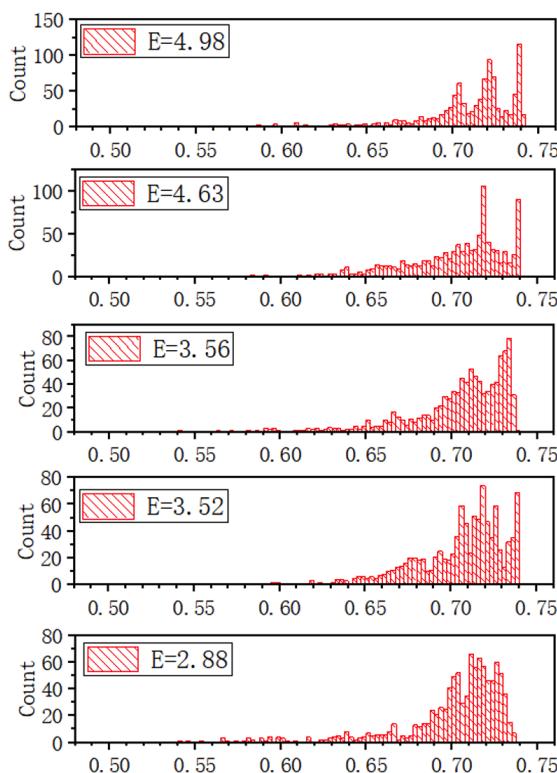
Mechanical Characterization of Partially Crystallized Sphere Packings里的Zg和Zm

## ➤ voronoi配位数

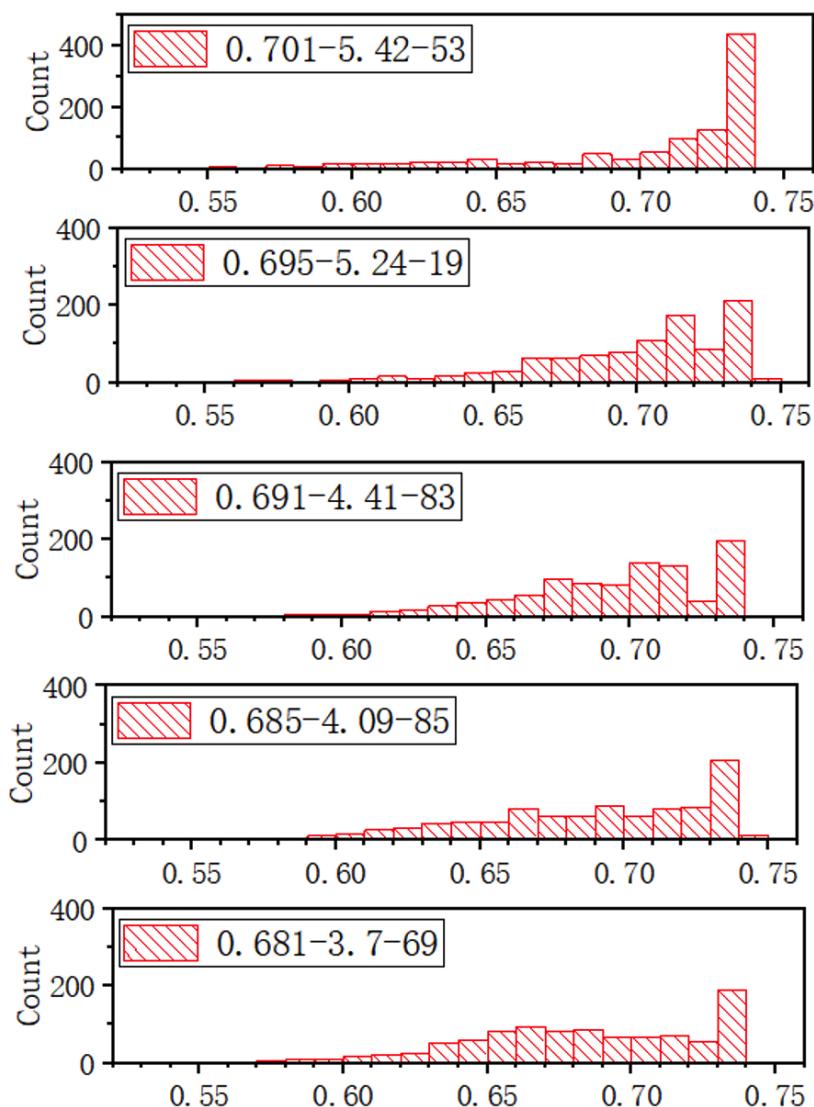


## ➤ voronoi局部填充率

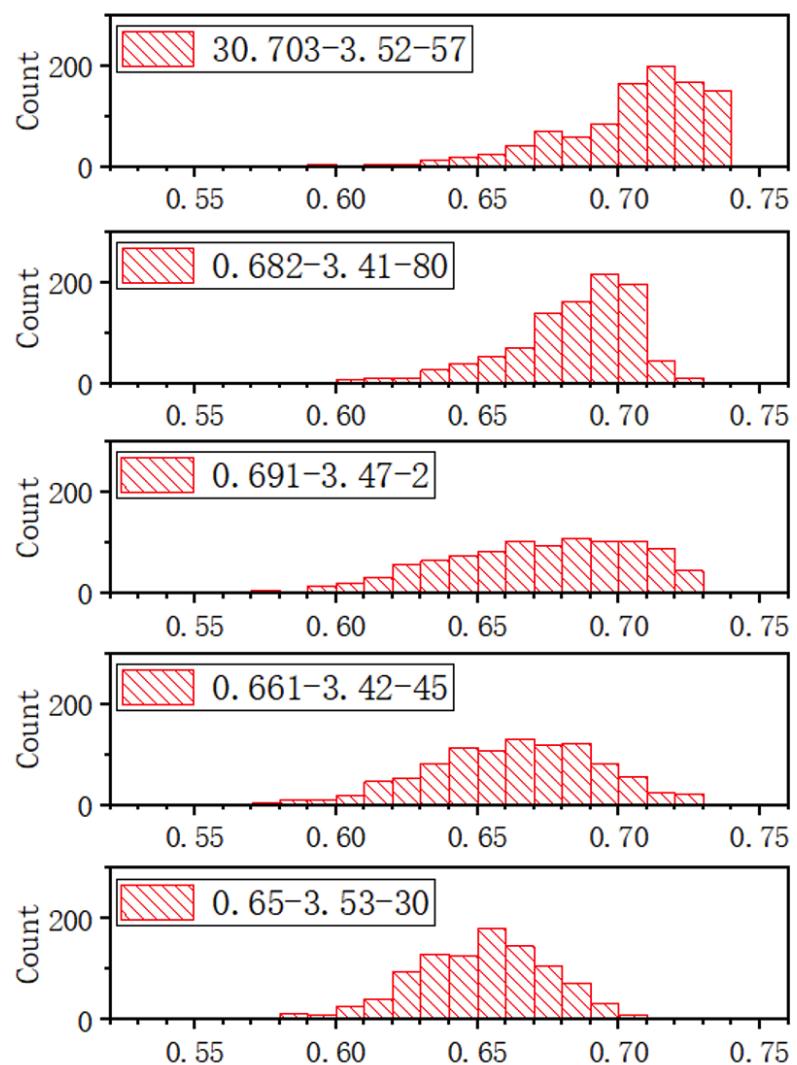




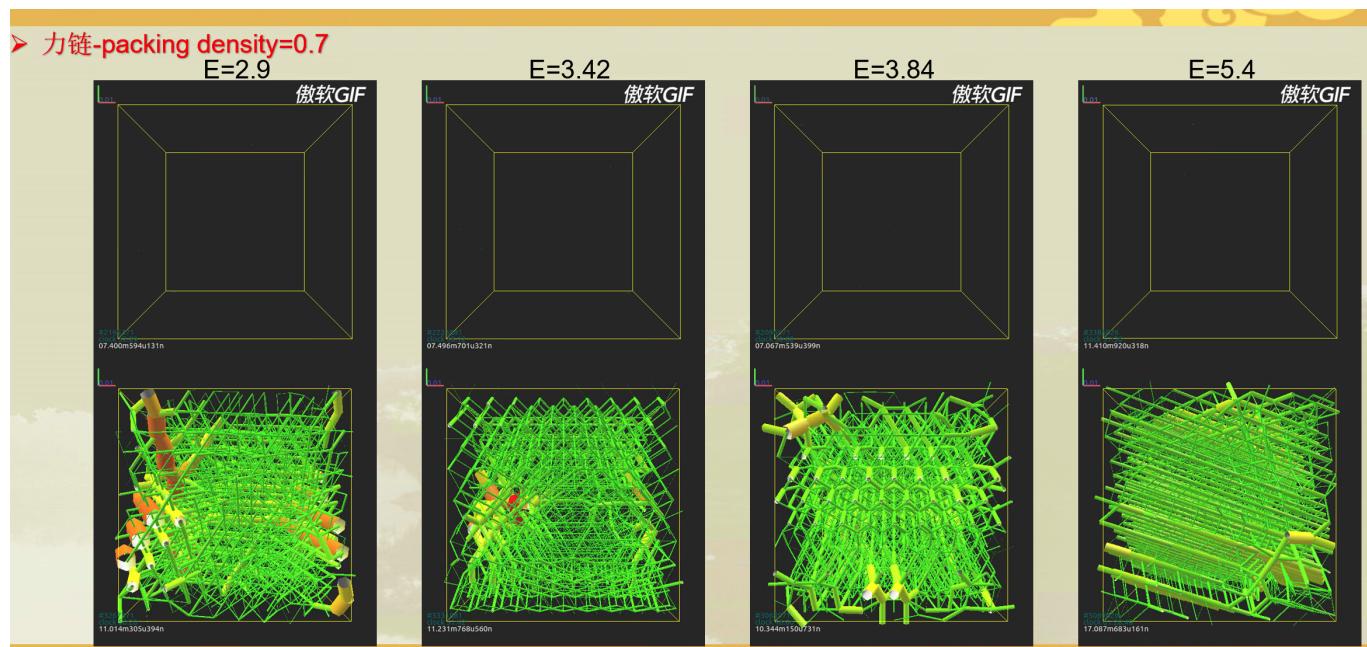
## 不同密度下的最高模量



## 不同密度的最低模量

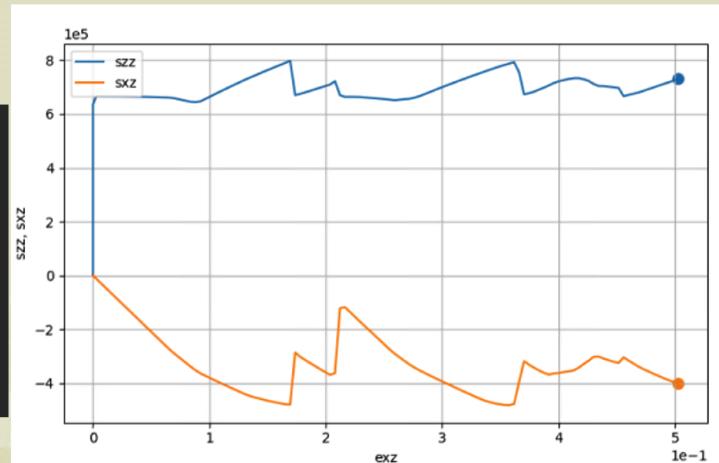
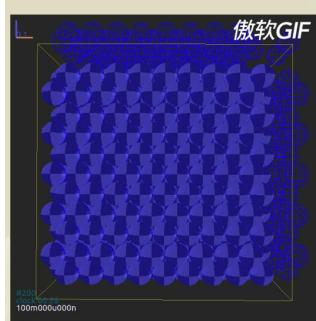


## 力链分析



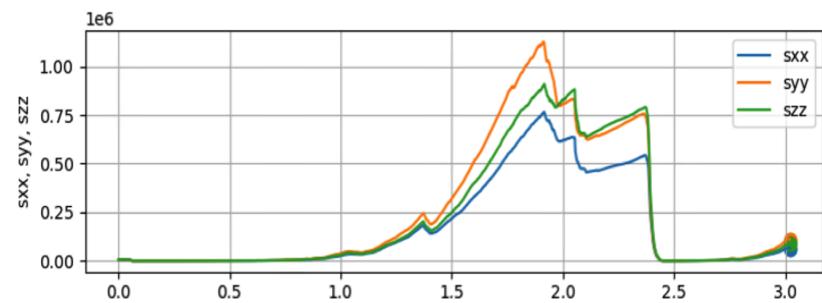
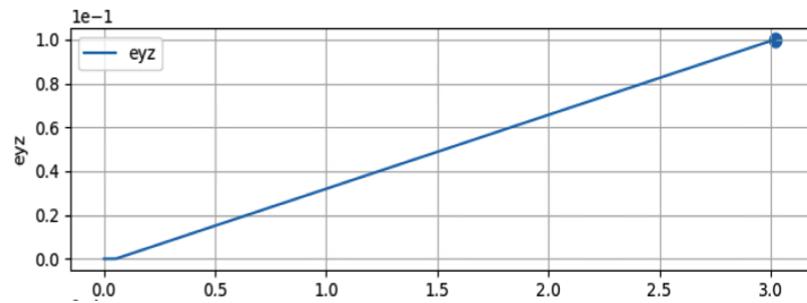
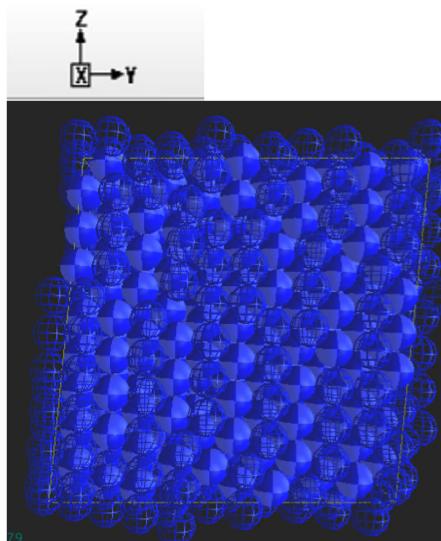
## 剪切

## ➤ 剪切过程



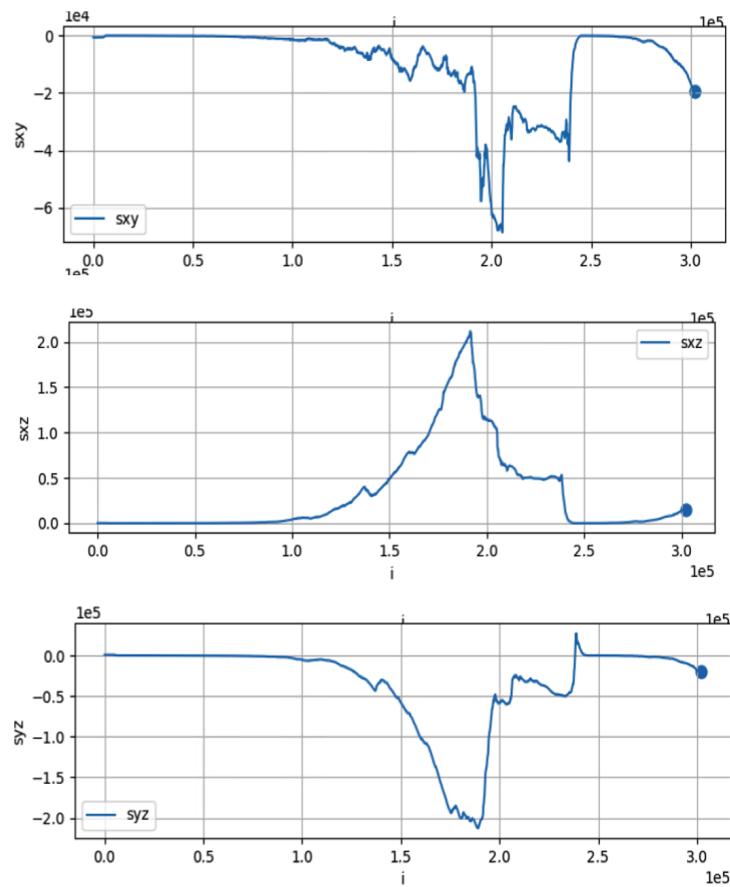
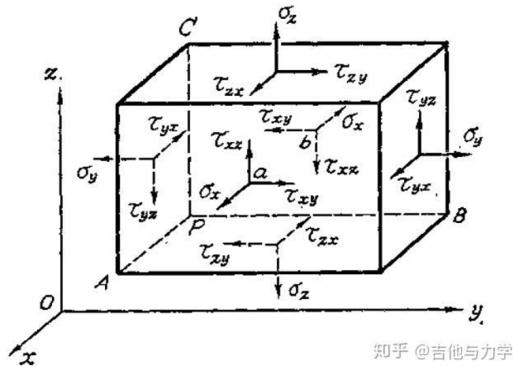
## 剪切

应变与正应力



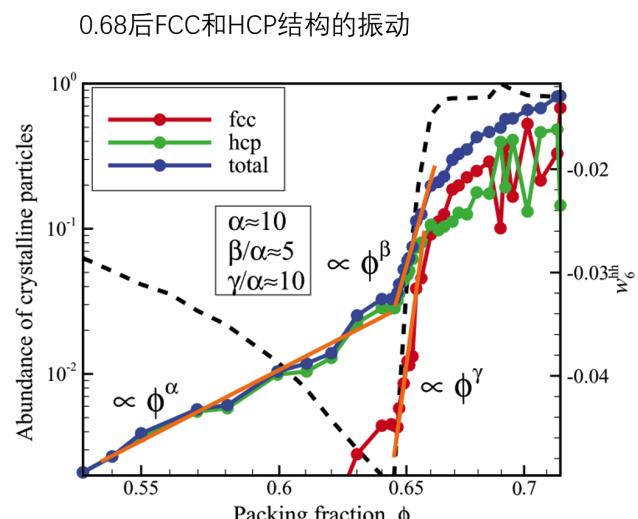
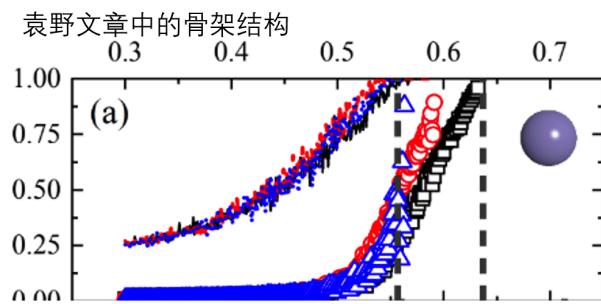
# 剪切

## 切向应力

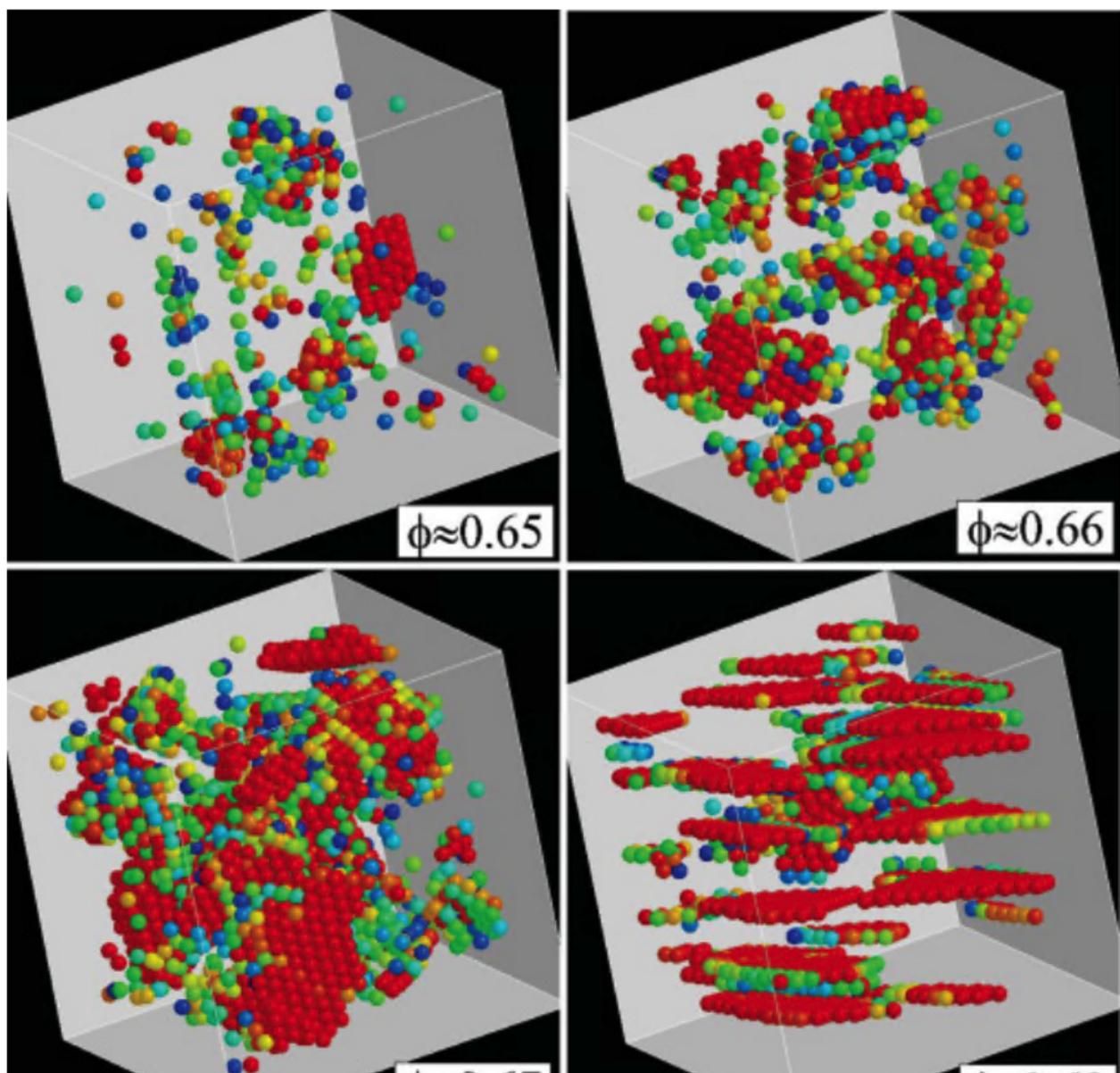


这里的本构和dem怎么建模，可以参考Mechanical Characterization of Partially Crystallized Sphere Packings。

其他可借鉴



## 3D结构转化为2D结构



$\phi \approx 0.67$  $\phi \approx 0.68$ 

# Structural properties of dense hard sphere packings (2011)

有篇名为structural and mechanical characteristics of sphere packings near the jamming transition值得看一下。