Using Machine Learning Techniques to Identify Soft Spots in Amorphous Materials

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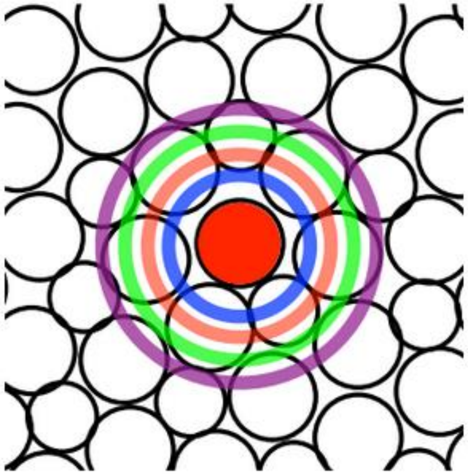
Localized areas of rearrangement

Crystals have defects
Amorphous materials have soft spots

Identify soft spots

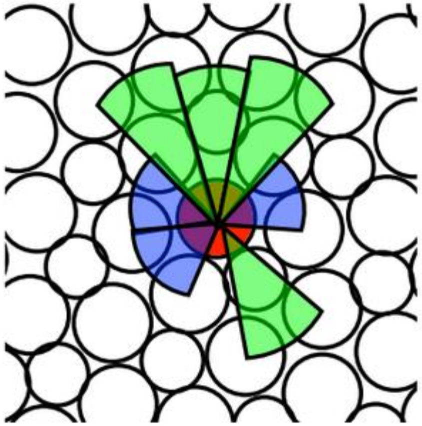
Use geometrical descriptors
Angular and radial

Radial descriptor



$$S(i; r, \sigma) = \sum_j e^{-(R_{ij}-r)^2/\sigma^2}$$

Angular descriptor



$$Q(i;\xi,\lambda,\zeta) = \sum_{j,k} e^{-(R_{ij}^2+R_{ik}^2+R_{jk}^2)/\xi}(1+\lambda\cos\theta_{ijk})^{\zeta}$$

Begin with a training set

A set of particles
Know which are hard/soft

Calculate the n-descriptors

Determine angular and radial quantities for the set

Summarize n-descriptors

Plot each particle in n-dimensional space
Each axis represents one of the n-descriptors

Construct a hyperplane

Separate hard and soft particles

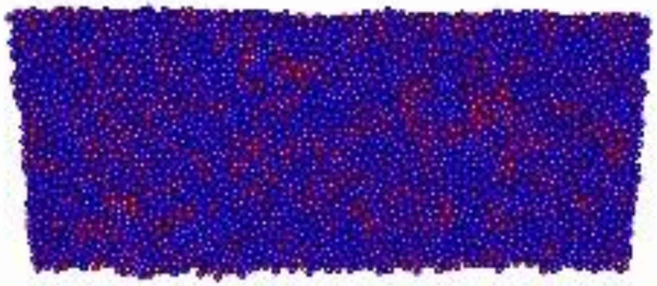
Analyze new data

Plot data in the hyperplane
Calculate softness field

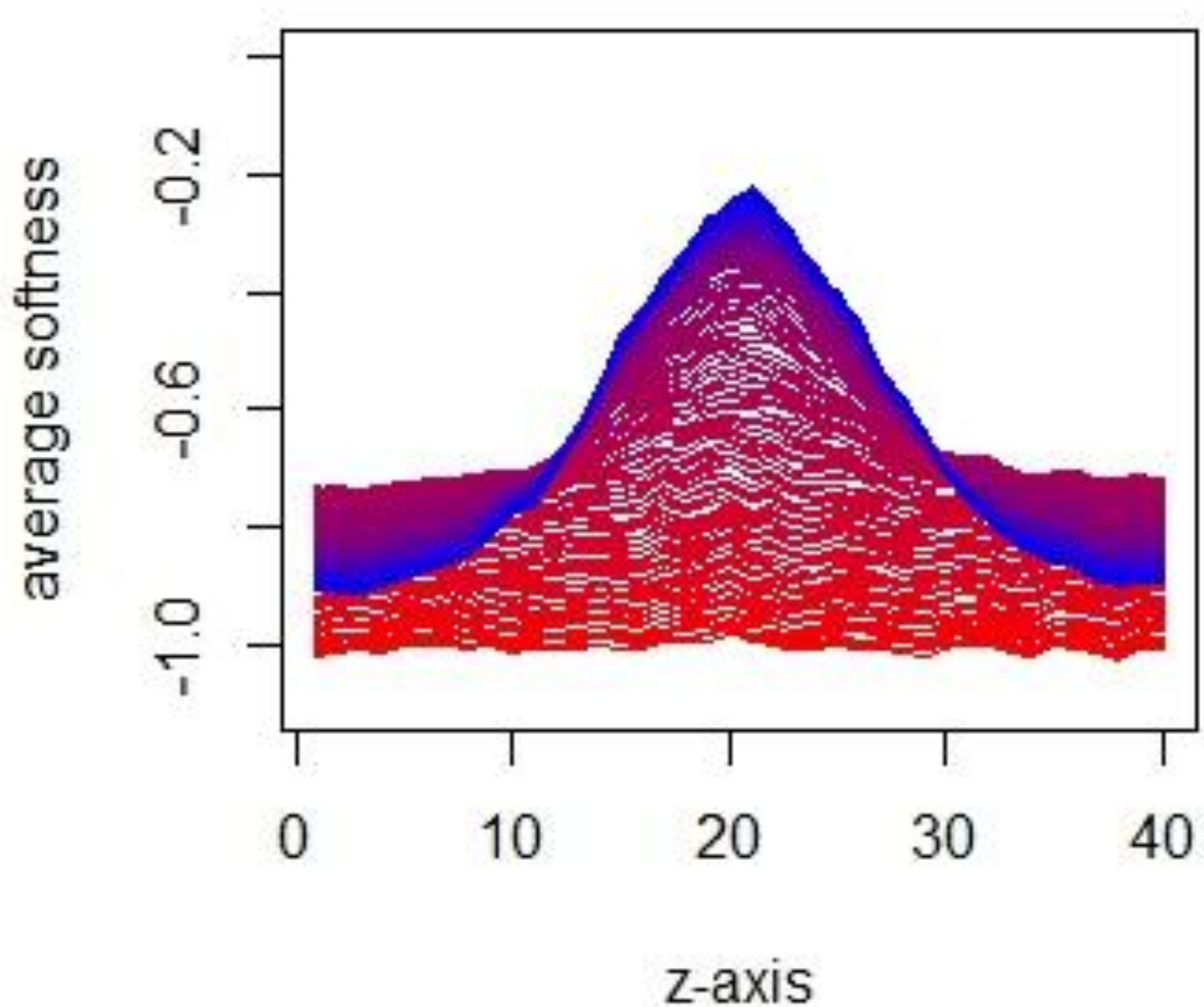
Our system

Pillar with aspect ratio of 2
42410 particles
5mers (polymer chains)
Strained at a constant rate

Our system



Softness vs Z (average of 63 pillars)



Further research

Look at radius as a function of the length of the pillar
Analyze the fast cooled pillars and the isoconfigurational ensemble