Progressive pearl necklace collapse mechanism for Cerato-Ulmin aggregation film

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Objective

Hierarchical process:
from monomers towards necklace chains and than compact monolayer

Atomic Force Microscopy Imaging

Worm Like Chain model
Semiflexible Polymer Collapse
Dutch Elm Disease

A devastating event in the history of tree diseases.
It is caused by the fungus *Ophiostoma novo-ulmi* and vectored by bark beetles
First observation in Netherlands 1921

8-kDa
75 a.a
phytotoxic class II hydrophobin
Hydrophobin

- 75-100 a.a.
- Secreted by filamentous fungi
- Tendency to self-assembly as an amphipathic film at hydrophylic/hydrophobic interfaces
- Presence of eight cysteine with disulfide bridges
- Hydropathy pattern

Class I
Rodlet like surface pattern

Class II
Planar compact pattern

Schizophyllum commune
**Cerato-Ulmin**

- Interaction between fungi and other host organism
- Coating hypha fungal surface
- Contributes to the hydrophobicity of hypha surfaces
- Promotes aerial hypha formation
AFM images

Stirring of water protein solution

Deposition on mica

Distribution of Height

H=1.8nm

Zoom on the film

Zoom on the chain

Zoom on the "pearl" unit
AFM images

Chain Bridges

Islands

Rapid stirring

Progressive necklace collapse

Balancing stirring

Intermediate stage of aggregation
AFM Chain analysis

The chain will come close to form an approximate ring
Evaluate the radius of the best ring overlapping the chain

Assume a semiflexible chain
Calculate the probability that the polymer has to close up in a ring of assigned radius $R$
Worm Like Chain Model

Polymer as a semi-flexible filament

Persistence length
End to end distance

$\mathbf{R}$ the total end to end vector of an ideal chain

End to end distance probability distribution for the collapse of a semiflexible polymer
Assumptions

- The process of successive aggregation results in long 1D chains
- 1D chains described by worm like chain model with a persistence length $L_p$
- If chain of length $L$, than there will be a finite probability that two edges of the chain will come close to form a ring: $R=L/2\pi$
- A ring is formed when the distance between two edge smaller than $\sigma$

\[
P(R/l_p) = \frac{2\kappa \sigma^2}{Nk_BT} \left(\frac{\sigma}{L}\right)^3 \sum_{j=1}^{\infty} j^2 (-1)^{j+1} \exp \left(-\frac{\kappa}{k_BT} \frac{\sigma^2}{2} j^2\right) \left[ \frac{\exp(\alpha_j)}{\alpha_j} \left( 1 - \frac{2}{\alpha_j} + \frac{2}{\alpha_j^2} \right) - \frac{2}{\alpha_j^3} \right]
\]
Match

![Graph showing the relationship between P(R/Lp) and R/Lp, with experimental data and theory curves.](image-url)
Conclusions

• A model to interpret the precursor stage of the assembly aggregation process

• In the intermediate stage of the aggregation the protein behaviour described as a semi-flexible polymer
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