Escape from frustration and yielding of frustration-controlled assembly: particle design rules for self-limiting ribbons and rings

Douglas M. Hall*, Mark J. Stevens*, and Gregory M. Grason

1University of Massachusetts, Amherst, MA  and 2Sandia National Laboratories, Albuquerque, NM

• IRG-1 aims to design self-assembly with well-defined dimensions much larger than the building blocks
• We develop a new coarse-grained model to connect particle design to self-limitation and escape behaviors
• We connect continuum theory of frustrated assembly to features of discrete particles and their interactions

How can we design particles to extend self-limiting assembly size?

Theory of frustrated ribbon morphologies and escape to tubules by flattening

Continuum ribbon elastic energy + line tension: \( F = E + 2AL \)

- IRG-1 aims to design self-assembly with well-defined dimensions much larger than the building blocks
- We develop a new coarse-grained model to connect particle design to self-limitation and escape behaviors
- We connect continuum theory of frustrated assembly to features of discrete particles and their interactions

Discrete particle model with tunable frustration

Yielded bonds allow hierarchical assembly and imply lower limit to frustration-controlled assembly

Role of bending stiffness anisotropy and strain softening in escape by flattening

- Upper limit to self-limiting assembly sizes connected to particle geometry, distinct bending modes, and range of interaction
- Self-limiting structure may form hierarchical assembly
- Lower size limit from the interaction range, limit to strain that can be supported in assembly before yield

Funded by NSF DMR-1608862
NSF MRSEC DMR-1420382
work done at DOE CINT User facility

Self-limiting ribbons and escape in amphiphile and nanoparticle assembly

Serafin Nat. Com. (2021)
Ziserman, PRL (2011)

How can we design particles to extend self-limiting assembly size?

Theory of frustrated ribbon morphologies and escape to tubules by flattening

Continuum ribbon elastic energy + line tension: \( F = E + 2AL \)

- IRG-1 aims to design self-assembly with well-defined dimensions much larger than the building blocks
- We develop a new coarse-grained model to connect particle design to self-limitation and escape behaviors
- We connect continuum theory of frustrated assembly to features of discrete particles and their interactions

Discrete particle model with tunable frustration

Yielded bonds allow hierarchical assembly and imply lower limit to frustration-controlled assembly

Role of bending stiffness anisotropy and strain softening in escape by flattening

- Upper limit to self-limiting assembly sizes connected to particle geometry, distinct bending modes, and range of interaction
- Self-limiting structure may form hierarchical assembly
- Lower size limit from the interaction range, limit to strain that can be supported in assembly before yield

Funded by NSF DMR-1608862
NSF MRSEC DMR-1420382
work done at DOE CINT User facility

Self-limiting ribbons and escape in amphiphile and nanoparticle assembly

Serafin Nat. Com. (2021)
Ziserman, PRL (2011)