Crystalline order on the paraboloid

Luca Giomi

lgiomi@physics.syr.edu

Department of Physics

Syracuse University

Syracuse, NY 13244, USA



Order vs Curvature





- In flat two-dimensional space particles have the natural tendency of packing in a triangular lattice.
- The addition of a non-zero Gaussian curvature gives arise to a different type of crystalline structure due to the competition between order and curvature...





Spherical Crystals



VIPERdb, http://viperdb.scripps.edu



Any triangulation of the sphere must contain at least twelve 5-fold disclinations.

Euler's Theorem

$$V - E + F = \chi$$

Disclination Charge

$$Q = \sum_{i \in \mathbb{S}^2} (6 - c_i) = 6\chi = 12$$



Grain Boundaries "Scars"

In large crystals the presence of additional 5-7 dislocations can lower the elastic stress.

$$R/a \simeq 5$$

R radius, a lattice spacing.

$$N \simeq \frac{4\pi R^2}{\frac{\sqrt{3}}{2}a^2} \simeq 14.51 \left(\frac{R}{a}\right)^2$$
$$\simeq 362$$





Parabolic crystals



Variable Gaussian curvature

$$K(r) = \frac{4\left(\frac{h}{R^2}\right)^2}{\left[1+4\left(\frac{h}{R^2}\right)^2r^2\right]^2}$$
 Boundary, $\chi=1$

$$Q = \sum_{i \in \mathbb{P}^2} (4 - c_i) + \sum_{i \in \mathbb{P}^2} (6 - c_i) = 6\chi = 6$$



A macroscopic model of a parabolic crystal can be obtained in laboratory by assembling a single layer of soap bubbles on the parabolic surface of a rotating liquid...

$$z = \frac{\omega^2}{2g} r^2$$





$$h = \frac{\omega^2}{2g} R^2 = (0 \div 15) \,\mathrm{cm}$$



A dynamical model of a crystal structure

BY SIR LAWRENCE BRAGG, F.R.S. AND J. F. NYE Cavendish Laboratory, University of Cambridge

(Received 9 January 1947-Read 19 June 1947)

[Plates 8 to 21]

The crystal structure of a metal is represented by an assemblage of bubbles, a millimetre of less in diameter, floating on the surface of a soap solution. The bubbles are blown from a fine pipette beneath the surface with a constant air pressure, and are remarkably uniform in size. They are held together by surface tension, either in a single layer on the surface or in a threedimensional mass. An assemblage may contain hundreds of thousands of bubbles and persists for an hour or more. The assemblages show structures which have been supposed to exist in metals, and simulate effects which have been observed, such as grain boundaries, dislocations and other types of fault, slip, recrystallization, annealing, and strains due to 'foreign' atoms.











Defects Phase Diagram

A tentative phase diagram can sketched by using a simple argument based on dislocations screening.

$$K_0 s^2 = \frac{1}{3}$$

with:

$$K_0: \begin{cases} K_{\max} = 4\left(\frac{h}{R^2}\right)^2\\ K_{\min} = \frac{4\left(\frac{h}{R^2}\right)}{\left[1+4\left(\frac{h}{R}\right)^2\right]^2} \end{cases}$$





Numerical simulations

Finding the global minimum of the Riesz energy $E = \sum_{ij}^{1,N} 1/|\mathbf{r}_i - \mathbf{r}_j|^s$ satisfying the non-linear constraint $\mathbf{r}_i \in \mathbb{P}^2$, is a formidable optimization challenge. A combination of the Storn-Price DE algorithm and local minimization methods gave good results for system up to N = 100 particles... larger simulations are running.



N = 40



N = 50





N = 100

Acknowledgements







PHYS. DEP. CMT GROUP

M. Bowick H. Shin C. Thomas

PHYS. DEP. MACHINE SHOP







P. Arnold C. Brown L. Buda



Crystalline order on the paraboloid – p. 11 $\,$