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Measures of Order for Nearly Hexagonal Lattices

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Abstract

Motivated by hexagonal patterns with defects in natural and laboratory systems, we compare quantitative measures of order for nearly hexagonal, planar lattices. These include a spectral measure of order based on the Fourier transform, a geometric measure of order using the Delaunay triangulation, and topological measures of order introduced in this paper. The topological measures are based on a tool from topological data analysis called persistent homology. We contrast these measures of order by comparing their sensitivity to perturbations of Bravais lattices. We then study the imperfect hexagonal arrangements of nanodots produced by numerical simulations of partial differential equations that model the surface of a binary alloy undergoing erosion by a broad ion beam. These numerical experiments further distinguish the various measures of hexagonal order and highlight the role of various model parameters in the formation and elimination of defects. Finally, we quantify the dependence of order on prepatterning the surface to suggest experimental protocols that could lead to improved order in nanodot arrays.

Keywords: Pattern Formation, Nanostructures, Persistent Homology

1. Introduction

A variety of natural systems and laboratory experiments can give rise to patterns. Hexagonal lattices patterns are found, for example, in Rayleigh-Bénard convection experiments [1], the Rosensweig instability in ferrofluids [2], and nanoscale structures formed by bombarding a binary material by a broad ion beam [3, 4, 5, 6]. These patterns are seldom perfect hexagonal lattices. Defects, such as penta-hepta pairs or grain boundaries between regions in which the lattices have different orientations, are common.

The order in a surface pattern can be gauged by a number of time-honored methods. For example, a quantitative measure of the order is obtained by computing the width of the lowest-order peak in the Fourier transform of the surface. A second widely employed method begins with an examination of how the surface's autocorrelation function decays with distance. If it decays exponentially, the characteristic length scale of the decay (the correlation length ξ) gives an estimate of the range over which the order extends. These methods of gauging order can be of limited use in analyzing disordered patterns: For example, the peaks in the Fourier transform may not be separable from the background or from each other, and a region of exponential decay in the autocorrelation function may not be present. Böttger *et al.* [7] computed the correlation length ξ for a series of imperfectly ordered hexagonal arrays of nanodots and showed that it remained nearly constant even as the order increased. Thus, even if ξ can be measured, it can be a less-than-ideal gauge of order.

Over the last decade, a powerful new tool of computational topology called persistent homology (PH) has been developed to characterize the topological properties of a set of points at all length scales [8]. It has quickly become apparent that PH is useful in a wide range of applications. In physics, it has already been employed to characterize the structure of granular media and the force networks in them [9, 10, 11], to study fluid flow [12], to probe the hierarchical structure in glasses [13], and to gauge the order of patterns produced

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