Lindemann histograms as a new method to analyse nano-patterns and phases

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Bilkent Univ — The detection, observation, and analysis of material phases and atomistic patterns are of great importance for understanding systems exhibiting both equilibrium and far-from-equilibrium dynamics. As such, there is intense research on phase transitions and pattern dynamics in soft matter, statistical and nonlinear physics, and polymer physics. In order to identify phases and nano-patterns, the pair correlation function is commonly used [1]. However, this approach is limited in terms of recognizing competing patterns in dynamic systems, and lacks visualisation capabilities. In order to solve these limitations, we introduce Lindemann histogram quantification as an alternative method to analyse solid, liquid, and gas phases, along with hexagonal, square, and amorphous nano-pattern symmetries. We show that the proposed approach based on Lindemann parameter calculated per particle [2] maps local number densities to material phase or particles pattern. We apply the Lindemann histogram method on dynamical colloidal self-assembly experimental data [3] and identify competing patterns. [1] Veatch, PLoS ONE, 7, 2, 2012. [2] Chakravartya, J. Chem. Phys., 126, 2007. [3] Ilday, MRS Spring, 61, 2016.

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