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Mutual dependence between local stress and geometry in two dimensions TAMOGHNA DAS, JACK DOUGLAS, NIST - Natl Inst of Stds Tech — Solids and liquids exhibit a striking change in their resistance to the external stresses associated with the emergence of macroscopic rigidity. While the thermodynamics of the solid-liquid transition is well understood, structural underpinning and dynamics of this transition still remain open. To understand, we simulate a two dimensional Lennard-Jones system in both liquid and crystalline state by varying density at a fixed temperature. The shape of the first coordination shell is quantified and the microscopic density is computed for the generated configurations using standard statistical geometric methods. Next, we attempt to relate these quantities with local virial stress and orientational order using information theoretic measures, namely, Shannon entropy (SE) and mutual information (MI). Interestingly, SE for different stress components shows van der Waals loop like feature with respect to density although they follow distinctly different distributions. MI reveals strong correlation between local geometry and local stress and also captures the transition points. Although the results at the current stage are inadequate to draw any causal connection among the measured quantities, this approach might be useful to understand the emerging rigidity across liquid-solid transition

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