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Characterizing Atomistic Geometries and Potential Functions Using Strain Functionals EDWARD KOBER, NITHIN MATHEW, SVEN RUDIN, Los Alamos National Laboratory — We demonstrate the use of strain tensor functionals for characterizing arbitrarily ordered atomistic structures. This approach defines a Gaussian-weighted neighborhood around each atom and characterizes that local geometry in terms of n-th order strain tensors, which are equivalent to the n-th order moments/derivatives of the neighborhood. Fourth order expansions can distinguish the cubic structures (and deformations thereof), but sixth order expansions are required to fully characterize hexagonal structures. These functions are continuous and smooth and much less sensitive to thermal fluctuations than other descriptors based on discrete neighborhoods. Reducing these metrics to rotational invariant descriptors allows a large number of defect structures to be readily identified and forms the basis of a classification scheme that allows molecular dynamics simulations to be readily analyzed. Applications to the analysis of shock waves impinging on samples of Cu, Ta and Ti will be presented. The method has been extended to vector fields as well, enabling the local stress to be cast in terms of rotationally invariant functions as well. The stress-strain correlations can then be used as the basis for developing and analyzing potential functions.

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