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Statistical Mechanics with Spatial Resolution: a bottom-up approach to nonuniform deformation YING HU, Vanderbilt University — The development of theoretical framework connecting pure atomistic simulations to the constitutive macroscopic behavior of a system undergoing nonuniform deformations has been very challenging. Here I report a new formalism that embeds the traditional principles of statistical mechanics with spatial resolution, applied to deformation of crystals. A "stationary deformation path" is derived for discrete lattice points. This new atomistic representation of deformation is linked to continuum description of deformed crystalline space through a statistical distribution function whose spatial variation obeys a Liouville-like equation. The formulation is applied to describe local/nonuniform deformations. Dislocations are shown to be represented by an independent-acting nonlocal strain field in nonequilibrium conditions. Continuum equations like Kroner's relation for dislocations are rederived. The formulation can be used in analyzing deformation mechanisms associated with defects involving heterogeneous fields at the nanoscale and macroscale, and in studying nanoscale processes where nonlocality is important.

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