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# *Nano*SCULPT: A methodology for generating complex realistic configurations for atomistic simulations

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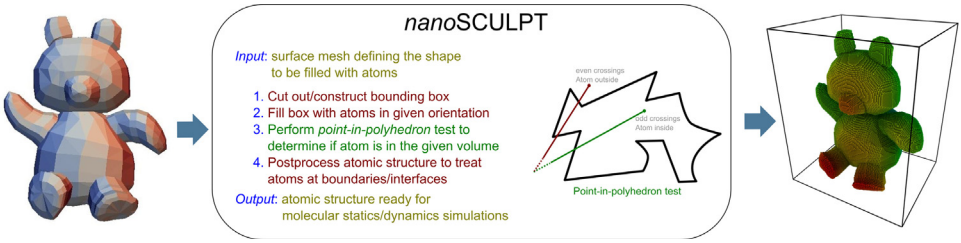
## GRAPHICAL ABSTRACT




## ABSTRACT

Atomistic simulations have now become commonplace in the study of the deformation and failure of materials. Increase in computing power in recent years has made large-scale simulations with billions, or even trillions, of atoms a possibility. Most simulations to-date, however, are still performed with quasi-2D geometries or rather simplistic 3D setups. Although controlled studies on such well-defined structures are often required to obtain quantitative information from atomistic simulations, for qualitative studies focusing on e.g. the identification of mechanisms, researchers would greatly benefit from a methodology that helps realize more realistic configurations. The ideal scenario would be a one-on-one reconstruction of experimentally observed structures. To this end, we propose a new method and software tool called *nano*SCULPT with the following features:

- The method allows for easy sample generation for atomistic simulations from any arbitrarily shaped 3D enclosed volume.

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- The tool can be used to build atomistic samples from artificial geometries, including CAD geometries and structures obtained from simulation methods other than atomistic simulations.
- The tool enables the generation of experimentally informed atomistic samples, by e.g. digitization of micrographs or usage of tomography data.

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## Method details

### *Background*

Large-scale atomistic simulations have now established themselves as a valuable tool in advancing our understanding of the mechanical properties, deformation behavior, and failure of materials. Such simulations have led to unprecedented insights into fundamental deformation mechanisms in metallic materials. Examples include the study of dislocation and grain boundary mediated processes in nanocrystalline metals, investigation of precipitate strengthening, simulation of fracture processes, study of dislocation nucleation controlled plasticity in nano-objects and deformation behavior of nanocontacts.

The determination of quantitative information like obstacle strength or the dislocation drag coefficient requires well-controlled, simplified atomistic simulation setups, which often involve quasi-2D geometries with periodic boundary conditions (PBC) or perfectly planar interfaces. However, the use of overly simplified setups has been shown to artificially suppress important deformation mechanisms. A recent study on curved precipitates in Ni-base superalloys, for instance, revealed interaction mechanisms between matrix dislocations and the misfit dislocation network, which were not observed in prior simulations on planar interfaces [1]. Other examples include the suppression of jogs, kinks or crack front curvature effects in quasi-2D simulations of fracture processes and the suppression of dislocation nucleation at surface steps by using perfectly planar surfaces in the study of nanowires.

Parallel to the increased use of atomistic simulations in materials science, advances in experimental methods like atom probe tomography (APT) [2], automated serial sectioning techniques [3] and 3D X-ray tomographic microscopy [4], which provide high resolution 3D information about the microstructure, have given rise to the emerging field of three-dimensional materials science [5]. Although the 3D information provided by these methods is increasingly used in continuum scale simulation methods like crystal plasticity full-field simulations, the use of experimentally-informed atomistic simulation setups has remained scarce. A primary reason is the lack of resolution of many of these methods, which limits their use in constructing atomistic samples.

A further reason for this near absence of experimentally informed atomistic simulations is simply the lack of a method and a widely available program that can be used to directly construct atomistic samples from 3D data sets. This also explains why mesoscale simulation techniques like phase field models, level-set methods or interface tracking methods are not yet routinely used to provide input structures for atomistic simulations. Most available programs are currently limited to the generation of simple shapes like cylinders, spheres, octahedron and/or other polyhedra [6–8] (see also [9]). The fundamental idea here is to generate a large enough sample, that is generally cuboidal, and "*sculpt*" out the required shape. Although relatively complex shapes can be generated using e.g. series of Boolean operations, the process is, nevertheless, restricted to perfectly geometric shapes and smooth surfaces.

Here we present a methodology and software tool to create *atomistic samples from arbitrarily shaped 3D datasets*, including experimentally obtained data, structures generated from mesoscale simulation methods, and engineering components. This software tool opens up the possibility to make

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