Development of Software for Characterization of Local Atomic Structures in Amorphous Metals Via Weighted Voronoi Diagrams

Zachary E. Markow

Washington University in St Louis

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Metallic glasses have unique properties that hold great promise for engineering applications. To harness this potential, it is critical to advance the understanding of the links between metallic glasses’ volume properties and nanoscale atomic structures. However, the characterization of these structures is not straightforward; the atomic configurations of metallic glasses are disordered or amorphous compared with the regular atomic structures of crystals, which possess long-range periodicity. A weighted Voronoi diagram (abbr. WVD) is a descriptive, chemically specific, precise tool available for characterizing short-range atomic configurations in amorphous materials. Mathematically, an unweighted Voronoi diagram (abbr. UVD) is the set of minimum-volume polyhedra whose faces are formed by the perpendicular bisector planes between pairs of atoms. Each type of WVD that we use is essentially a UVD in which these planes are shifted to adjust the volume and shape of each polyhedron according to the size of the enclosed atom. Unfortunately, current approaches that construct Voronoi diagrams are insufficient for our needs. For this reason, we have developed our own program to study the local atomic structures of metallic glasses via WVDs. This program was tested extensively on crystalline lattices with known structures, and the expected output data were produced. Presently, our program is being tested on previously studied amorphous materials, and the preliminary results from these tests suggest that our program will likely soon be ready to analyze never-before-studied metallic liquid and glass samples.