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NUMERICAL STUDY OF AMORPHOUS METALS

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Abstract. Amorphous metals, i.e. without defined crystal structure; present many distinguished properties that qualifies them as potential materials for industrial applications. In earlier work, we studied some of their mechanical properties using molecular dynamics (MD) simulations of a CuZr metallic glass. To continue with the understanding of these intrinsic properties we now analyze the behavior of Voronoi cells (polyhedrons generated in a process called Voronoi tessellation), which represent the 3D configuration of an amorphous structure.

According to different indices, such as the number of faces, vertexes, edges among others, we classify these polyhedrons into different categories, whose evolution we can follow throughout the deformation of the sample. The Voronoi tessellation analysis helps us understand the way atoms move respect each other and what kind of local structures most likely appear. This helps us relate the average properties of materials to the atomistic behavior.

Also, combining the data available of the atomic positions in the Voronoi tessellation with the stress tensor calculated with MD, we plot the change of the atomistic strain over time; and we show the nucleation and growth of incipient shear-bands in the sample.