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An Integrated Data Driven Reconstruction and Molecular Dynamics Simulation for Lattice Structure in Atom Probe Tomography JOAQUIN PERALTA, Departamento de Física, Universidad Andrés Bello, República 220, Santiago, Chile, KAUSTUBH KALUSKAR, Embryyo Innovations, 100, NCL Innovation Park, Maharashtra, India, CLAUDIA LOYOLA, Departamento de Física, Universidad Andrés Bello, República 220, Santiago, Chile, KRISHNA RAJAN, Department of Materials Science and Engineering, Iowa State University, 2220 Hoover Hall, Ames, Iowa, USA — Atom Probe Tomography (APT) is an experimental technique that gives 3D atomistic spatial resolution of a material specimen. Actual APT limits the detection of atoms around 50%. In this work, we propose a new reconstruction methodology, which relaxes some requirements of the actual procedures, and can be applied to regions across grain boundaries or amorphous regions. This methodology consist of four main steps: (i) the use of an initial structure which is provided by APT IVAS Software; (ii) the elimination of overlapping atoms; (iii) the detection of atomic vacancies with the incorporation of missed atoms; and (iv) the use of classical molecular dynamic (MD). As a bed-test, we show a tungsten sample structure. We analyze it using structural properties, as Radial Distribution function, to detect overlapped atoms. The vacancies detection algorithm is used to identify atomic vacancies in a crystalline or amorphous region. This particular feature is very helpful to identify zones like grain boundary regions. Once the atoms are relocated in the structure, a classical MD is carried out in order to improve the atomic structure, shape and morphology of the data. The final result, provided by the MD simulation, is characterized and compared with the initial structure.

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