1002
doi:10.1017/S1431927613007009
Microsc. Microanal. 19 (Suppl 2), 2013

An Integrated Data Driven Reconstruction and Molecular Dynamics Simulation for Lattice Structure in Atom Probe Tomography

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Actual Atom Probe Tomography (APT) limits the detection of atoms to around 50%. While there has been some work towards addressing these problems by using better instrumentation, there is another line of thought which has gained more attention and has shown promising results. It involves using the reconstructed data from APT to get an improved reconstruction. For instance Moody *et al* [1], show a reconstruction technique where three independent crystallographic directions must be identified and characterized. Recently Ceguerra *et al* [2], used GM-SRO parameter to give a highly representative description of the atomic scale, which then could be used to generate a lattice based structure. In present work, we propose a method for lattice reconstruction which relaxes some of these requirements and can be applied to regions across grain boundaries or amorphous regions. Motivated for the idea of improve the existing techniques for the reconstruction of the sample, we introduce in this work a simple methodology that consist of four steps: (i) the use of an initial structure which is provided by Atom Probe Tomography IVAS Software [3]; (ii) the elimination of overlapping atoms; (iii) detection of atomic vacancies [4] with the incorporation of missed atoms; (iv) and finally the use of classical molecular dynamics [5] methods. This technique doesn't require or assume crystallographic information and the only parameter used in the atomic vacancies detection algorithm corresponds to the first neighbor distance of the crystal.

As an example, we show a tungsten sample structure with 303,859 atoms, see figure 1, where the atomic position of the detected atoms (x, y, and z) is taken from IVAS software as an *initial input* used in the proposed reconstruction process. This structure is used as a template, and the procedure can be applied to different materials. Once we have the structure, we analyze it using the Radial Distribution Function (RDF) to remove the overlapped atoms. We can observe in figure 2, that there are atoms with a distance less than 1.93 Å (calculated atomic radius of tungsten[6]), suggesting that they are extremely close to each other (overlapped or duplicated: note that the first maximum is located at $r < 1$ Å). Then, we proceed to remove the atoms with ~~a~~ inter atomic distance less than 1.93 Å, and use atomic vacancies detection algorithms to relocate them and fill the missed atoms from the raw data. This particular feature is very helpful to identify zones where the atoms are not well distributed, like grain boundary regions.

Once the atoms are relocated in the structure, a classical molecular dynamics is carried out in order to improve the atomic structure, shape, and morphology of the data. The simulation was realized using a modern classical metallic potential for Tungsten [7], using the Finnis-Sinclair formalism, and simulated in micro-canonical ensemble (NVE) at room conditions during a time of 5ps and using a time step of 0.1 fs. After the process, characterization of the structure and comparison with the initial structure is carried out to show the principal advantages and disadvantages related to the proposed methodology. For

comparison we use RDF, angular distribution function, coordination number, and common neighbor analysis.

In conclusion, we observe not only an improvement in the atomic distribution of the initial structure, but also a sample with a relaxed structure which can be an useful input for complex analysis or simulations[8], provided mostly by an experimental procedure, and only with one structural parameter required to build. Presentation will focus on procedure, application and comparison with existing techniques, and some of the challenges and future possibilities in this direction[9].

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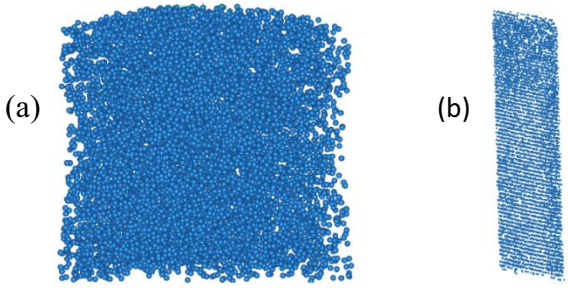

Figure 1: A representation of the Tungsten sample obtained from IVAS Software. (a) correspond to the full sample and (b) a region of interest of the sample.

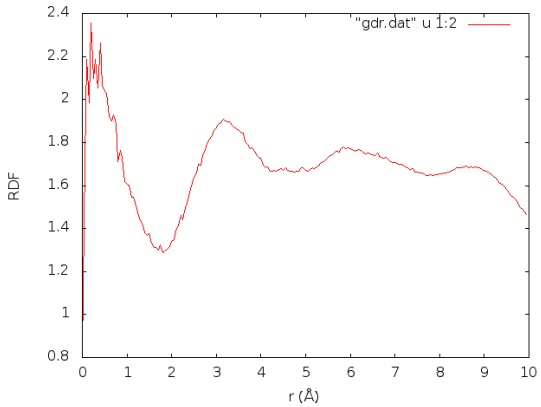

Figure 2: Radial distribution function of Tungsten atoms evaluated on the initial structure of the sample.

https://doi.org/10.1017/S1431927613007009 Published online by Cambridge University Press