

EVALUATION OF SOME METHODS FOR ESTIMATING THE COMPOSITIONS OF FINE PRECIPITATES

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The ability to estimate the composition of ultrafine particles is one of the unique features of atom probe tomography. Methods such as selected volume analysis and concentration profiles have been used to estimate the composition of particles. However, these manual methods are time consuming and prone to user bias. In addition, the multimillion atom datasets generated with the three-dimensional atom probe and the local electrode atom probe in particular, make these simple methods impractical for routine use. Therefore, some alternative automated methods have been developed.

Key considerations in some of these automated methods are the assignment of the atoms between the particle and the matrix and their efficiency. One effective method where there is a significant difference in the solute content of the matrix and the particle is the maximum separation method developed by Hyde. This method is based on the principle that the solute atoms are closer together in a solute-enriched particle than in the solute-depleted matrix. Therefore, a maximum separation distance between one or more solute atoms can be selected to assign the solute atoms to the particle or the matrix. Once these solute atoms are assigned, parameters such as the center of mass, radius of gyration, Guinier radius and radial concentration profiles for the center of the particle can be calculated. In order to determine the composition of each particle, an interface between the particle and the matrix has to be defined so that the numbers of the other atoms in the particle can be estimated. The precise location of this interface is critical for small precipitates as a high proportion of atoms lie at the surface of the particle. The interface may be defined by placing a three-dimensional grid through the data as in the envelope method, applying a second maximum separation distance, or with an adaptive marching cube algorithm. A comparison of the parameters and the effectiveness of these approaches will be discussed. In all of these methods, the composition of small particles was found to depend on the precise definition of the interface.

Alternative methods that do not require the precise position of the interface to be established have also been developed. For example, the tracer method can be used to estimate the composition of particles and the extent and level of solute segregation to dislocations and interfaces. In this method, the three-dimensional data are divided into a regular array of voxels (volume elements). The composition at each voxel is determined based on the number of atoms of each type in the voxel. The voxel with the maximum (or minimum) concentration of one or more solutes in each column of voxels along one of the orthogonal (or an arbitrary) directions is then determined. These voxels are used to generate a two-dimensional contour map of the concentration for each solute.

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