

## Creating Isoconcentration Surfaces in Low-Chemical-Partitioning, High Solute-Containing Alloys

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The proximity histogram or proxigram has become a prevalent means of quantifying chemical partitioning in atom probe data sets. The proxigram is generated by the creation of an isoconcentration or isodensity surface around a cluster or precipitate from which the composition normal to the interface (both into and out of the surface) is measured [1]. The advantage of the proxigram is the ability to obtain compositional data normal to this surface even if the surface is anisotropic or has a varying radius of curvature. These surfaces also provide clear visual representation of precipitate features that can allow direct comparison to other microscopy techniques, such as transmission electron microscopy.

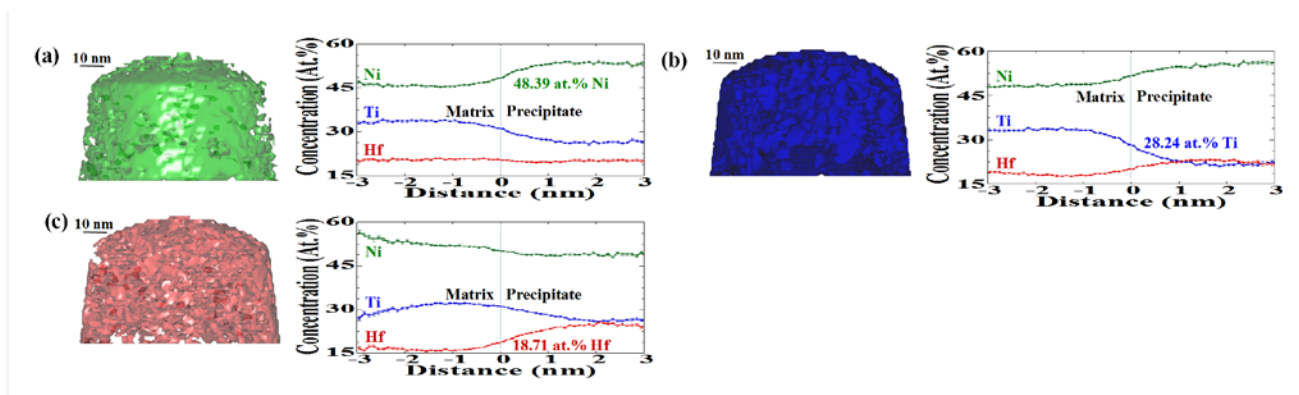
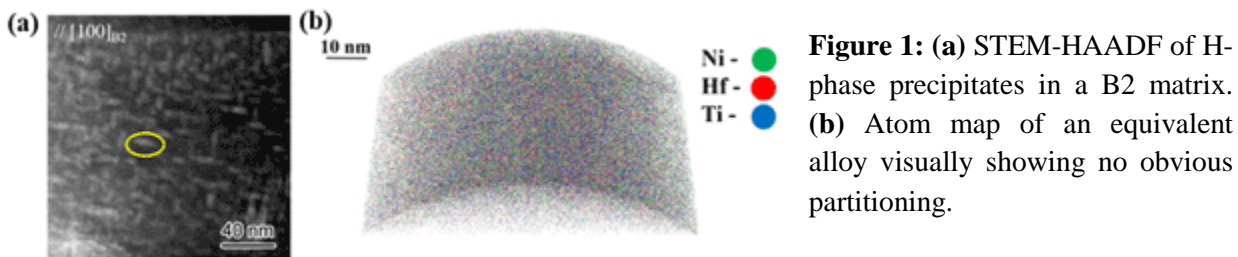
In high chemical partitioning systems, the atom map is usually sufficient for the user to identify the element that should be used to create the isosurface. In cases where chemical partitioning is weak in the atom map, selection of which species and its corresponding isoconcentration value can be difficult to determine, see Figure 1. For low solute systems (<~10 at.%), various clustering algorithms can be used to identify the partitioned species from which the proxigram can be created. Unfortunately, for high-solute alloys, the clustering algorithms are not as robust because the probability that the first, second and so forth nearest neighbor is the solute atom itself is quite high making statistical distinction for cluster identification difficult.

This poster presents a methodology to identify the correct species and isoconcentration value when low chemical partitioning and a high solute content exists in an alloy. We have used the 50.3Ni-29.7Ti-20Hf (at.%) alloy as our case study. Upon solutionizing, water quenching and aging, the alloy precipitates the H-phase from a B2 matrix [2]. These precipitates are visible in the (S)TEM-HAADF image, Figure 1(a), but the atom map, Figure 1(b), does not delineate the precipitate and matrix based on any of the chemical species' partitioning behavior.

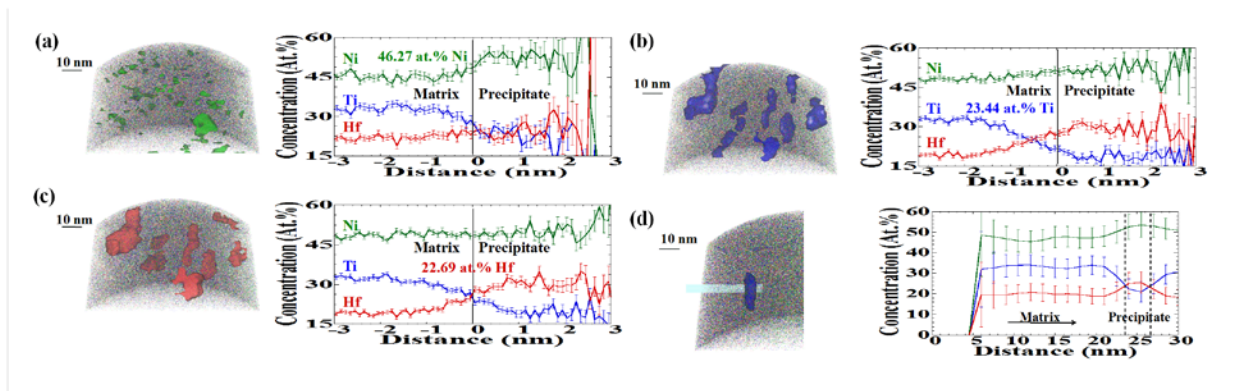
To identify the H-phase precipitates, the following procedure was developed and is general in its application. (1) Select the bulk composition as the starting values for each species' isoconcentration value. This will likely be incorrect as it does not account for partitioning between the matrix and precipitate but provides for a common reference. (2) Based on the definition of the proxigram, the user-defined isoconcentration value must coincide with the composition at the interface (0 on the x-axis) of the proxigram. Through user-defined iterations of isoconcentration values, these isoconcentration values will eventually converge to the outputted isoconcentration value at the interface, Figure 2. From those proxigrams, the specific composition for each respective species within each phase can now be extracted, *i.e.* the Ni composition is found from the created Ni isoconcentration proxigram, the Ti composition from the Ti isoconcentration created proxigram, and so forth. (3) Using those values for the phase compositions, a new isoconcentration surface is generated, Figure 3, that delineates the phases. (4) By placing a 1D profile through each phase, one can determine which species enrich each phase. In our case study, one must select either Ni, Ti, or Hf as the final rendered proxigram. The proxigram that shows agreement with the 1D profile identifies this correct species, which in this example was Ti.

**References:**

- [1] O.C. Hellman, *et al. Microscopy and Microanalysis* **6** (2000) 437.
- [2] F. Yang, *et al. Acta Materialia* **61** (2013) 3335.
- [3] The authors gratefully acknowledge funding from NASA grant NNX09AO61A



**Figure 2:** (a) Ni isoconcentration surface and proxigram at 48.39 at.%. (b) Ti isoconcentration surface and proxigram at 28.24 at.%. (c) Hf isoconcentration surface and proxigram at 18.71 at.%. The circle denotes the isoconcentration value at the interface for that species and is in agreement with the user-selected isoconcentration value used to create the corresponding surface. Unfortunately, these isosurfaces do not clearly represent the visual delineation of the precipitate and matrix noted in Figure 1(a). Figure 3 describes the creation of the correct isoconcentration species and value to generate the correct rendering.



**Figure 3:** The isoconcentration surfaces whose value matches the precipitate compositions determined in the proxigrams of Figure 2 for each species. (a) Ni isoconcentration surface and proxigram at 46.27 at.%. (b) Ti isoconcentration surface and proxigram at 23.44 at.%. (c) Hf isoconcentration surface and proxigram at 22.69 at.%. (d) 1D profile which shows agreement with the Ti isosurface and proximity which indicated that Ti was the correct species and isoconcentration value to use for reporting final phase compositions.