

Advantages of Clustering in the Phase Classification of Hyperspectral Materials Images

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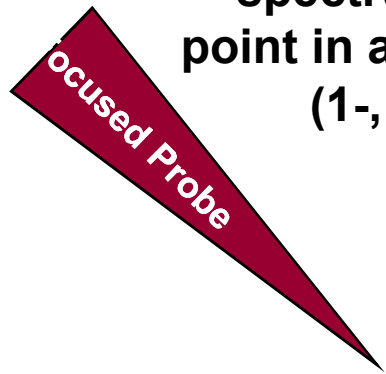


Outline

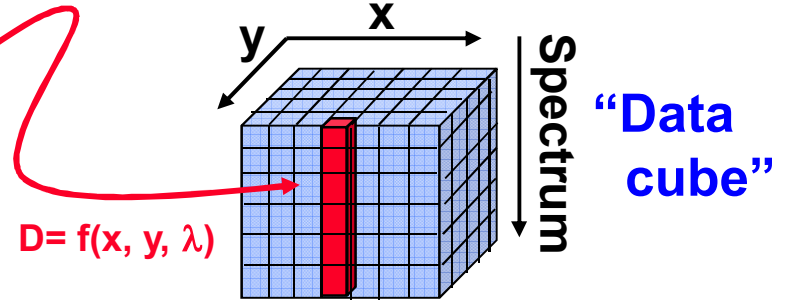
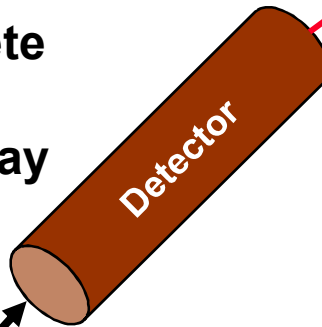
- **Factor analysis (FA) of hyperspectral images**
 - **Can extract spectral and concentration profiles for differentiable chemical species**
 - **Problems in phase classification: number of components cannot exceed chemical rank**
- **Advantages of clustering in phase classification**
 - **Parsimony restriction lifted: number of components can exceed chemical rank of data**
- **Comparison of FA and clustering for two hyperspectral image sets**
 - **Solder bump data set**
 - **Four phase braze interface data set**

Spectral Imaging and Factor Analysis

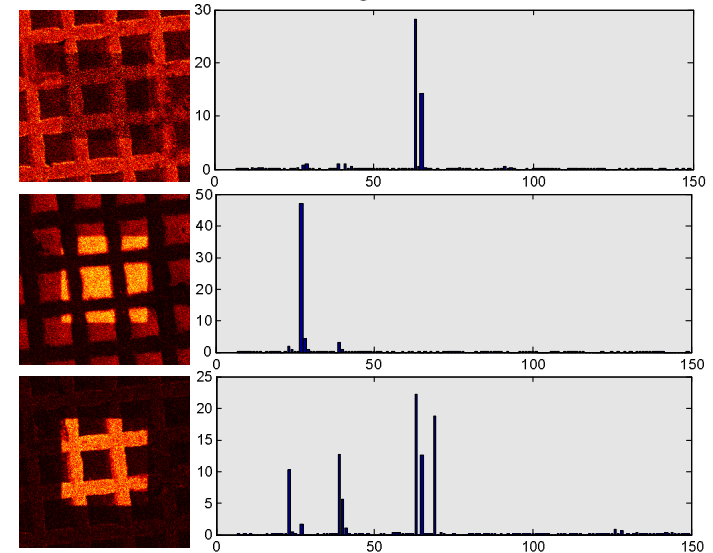
A spectral image
comprises a complete
spectrum at each
point in a spatial array
(1-, 2-, 3-D)



Signal



Factor analysis, $D = CS^T$



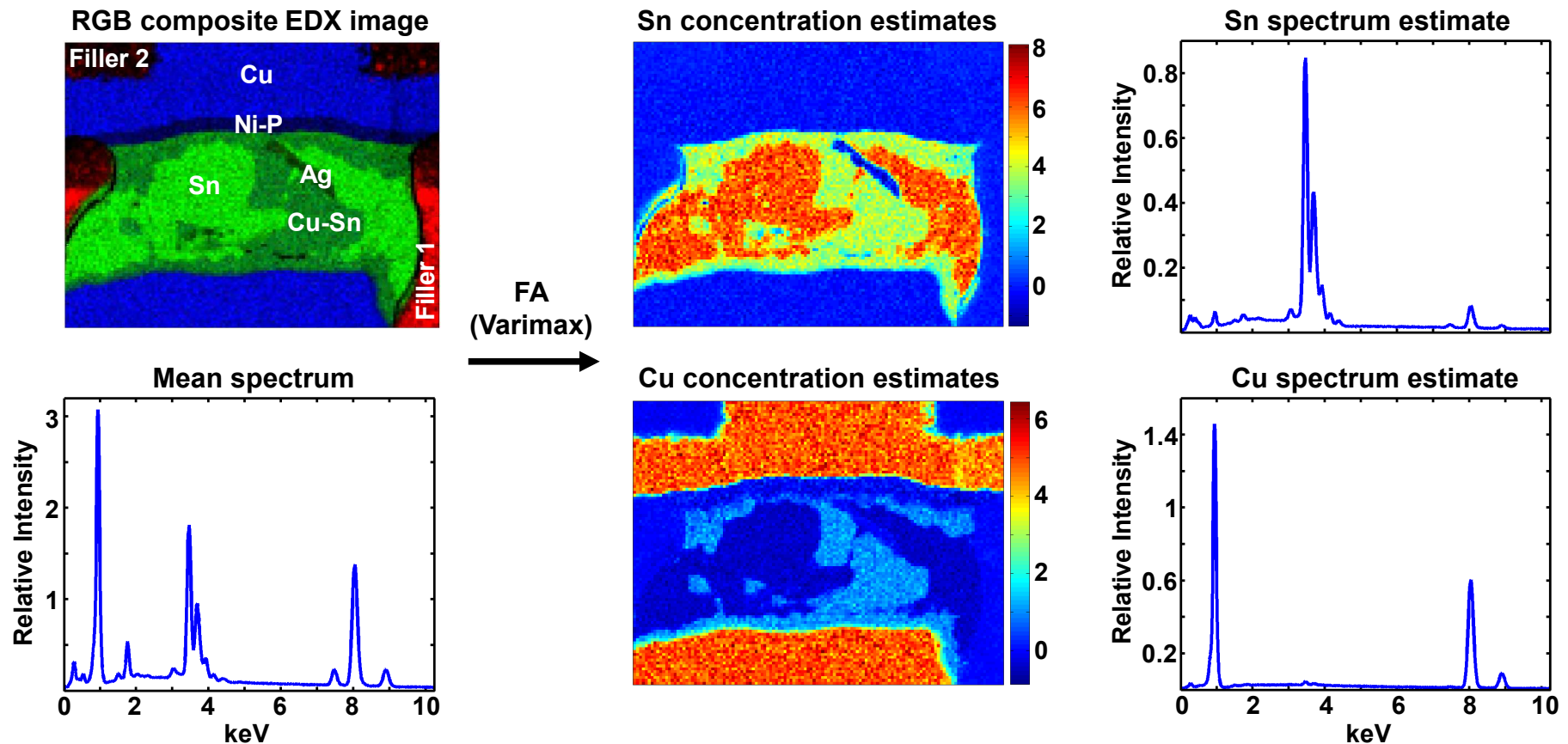
The goal of Factor Analysis is to
estimate:

S, "what is it?"

C, "where is it and how much?"

Limitations of FA for Phase Classification: Solder Bump Data

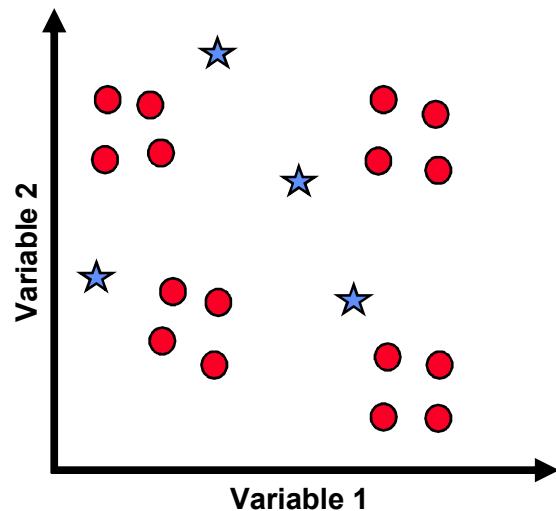
- FA parsimony restriction: number of extracted components cannot exceed chemical rank of data
 - FA fails to identify Cu-Sn intermetallic phase



Clustering: Group Data Points Based on Nearness in Multivariate Space

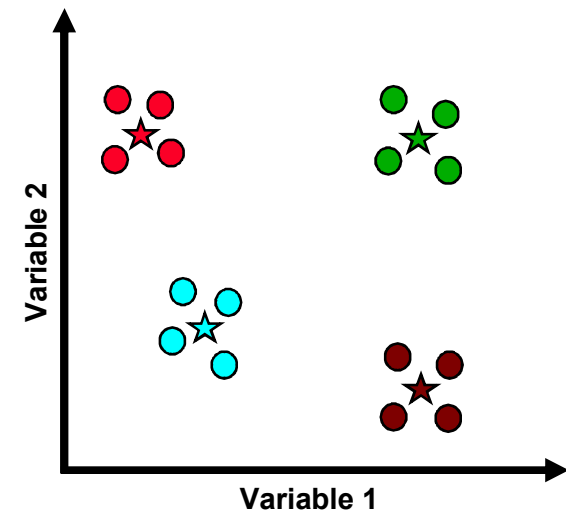
- Partial clustering (fuzzy c-means) requires very limited prior information:
 - Number of clusters in data set
 - Initial set of cluster centers

Four cluster centers (★) initialized



Update cluster centers
and group
assignments until
convergence achieved

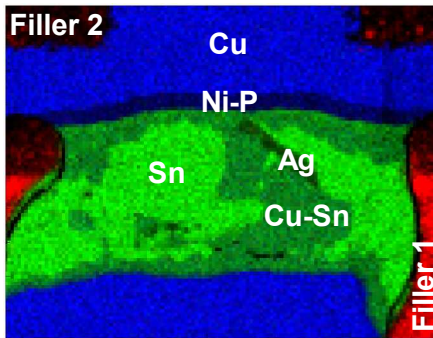
Final cluster assignments



Cu-Sn Intermetallic Phase Identified by Clustering: Solder Bump Data

- Clustering extracts Cu-Sn intermetallic phase: number of phases can exceed chemical rank!

RGB composite EDX image

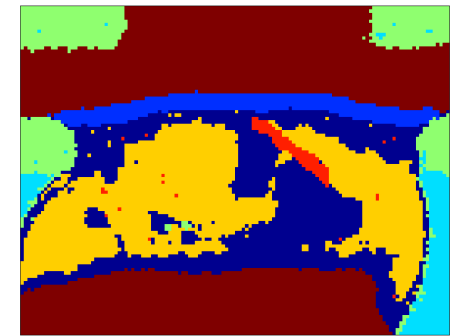


Clustering, $D = CS^T$
(Fuzzy c-means, $m = 1.3$)

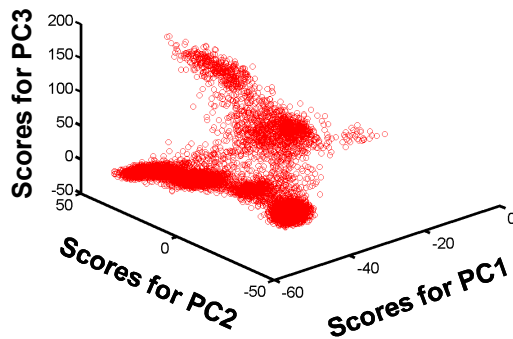
Clustering estimates:

- **S**, spectrum for each group
- **C**, group assignment for each pixel

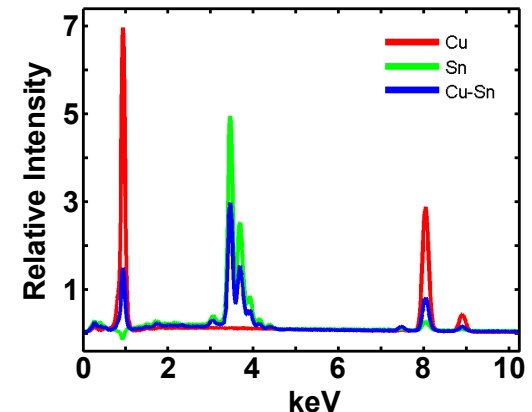
Pixel group assignments



Data points in 3-D PCA scores space



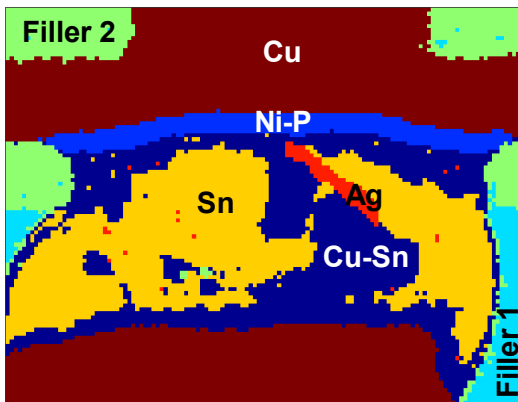
Cu, Sn and Cu-Sn spectra



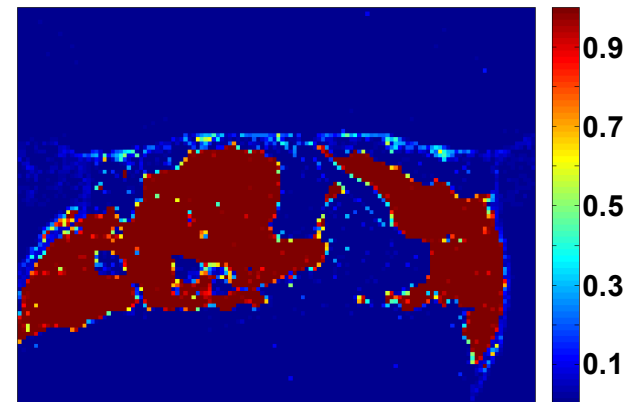
Clustering Applied to Solder Bump Data

- Fuzzy c-means clustering provides for partial group memberships (values lie between 0 and 1)

Crisp pixel group assignments



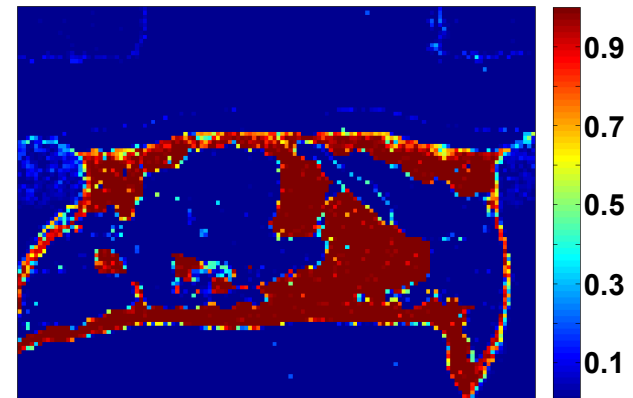
Fuzzy memberships (Sn phase)



Fuzzy memberships (Cu phase)

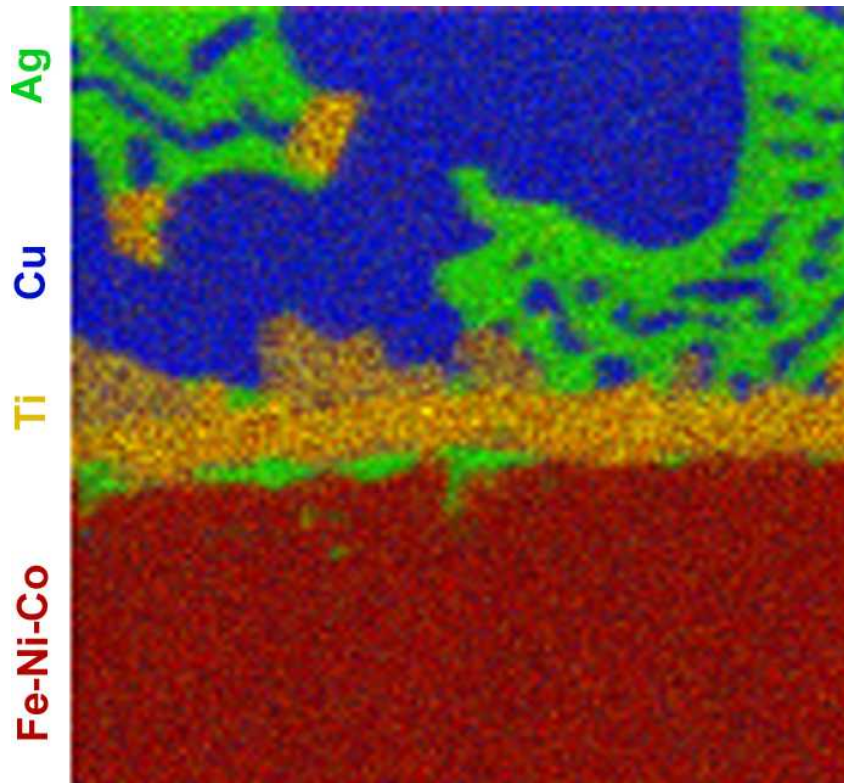


Fuzzy memberships (Cu-Sn phase)

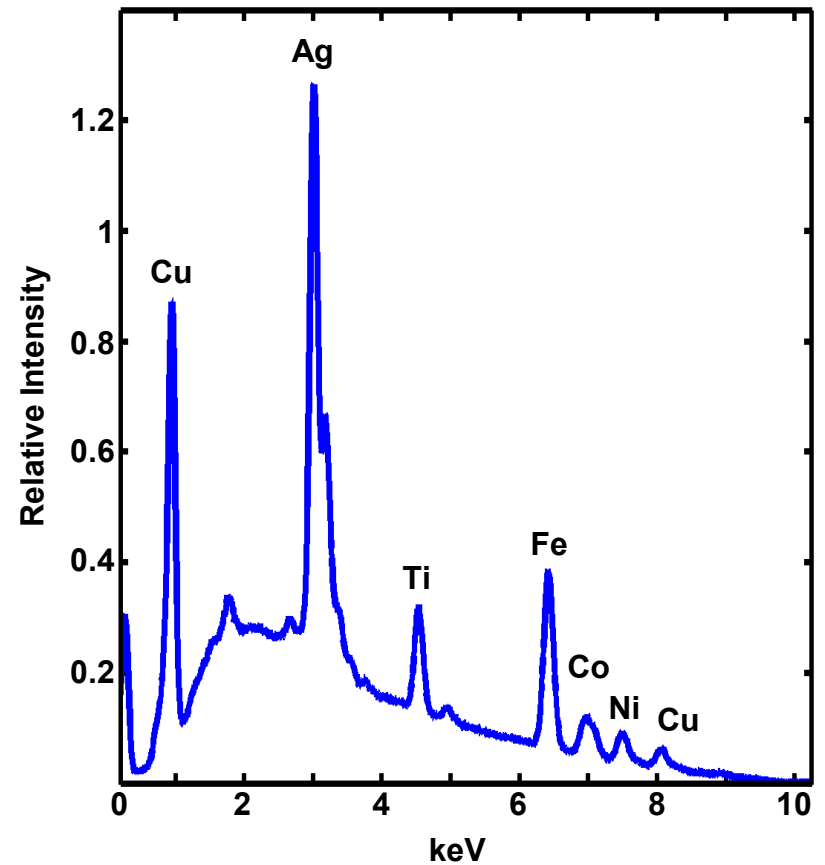


Braze Interface Data

RGB composite EDX image



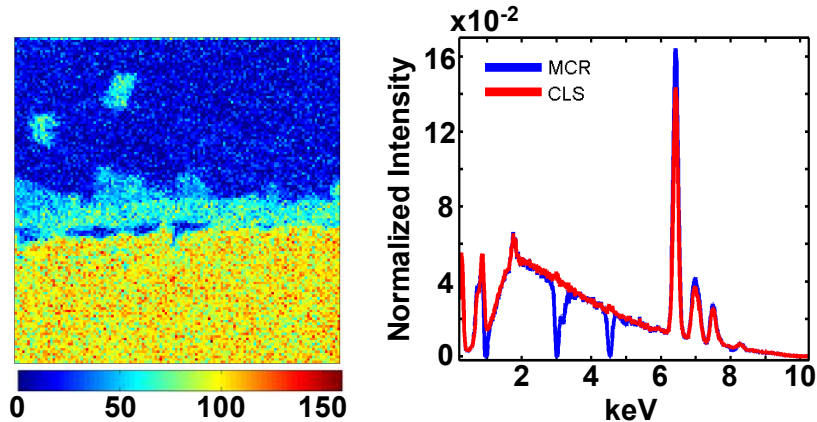
Mean spectrum



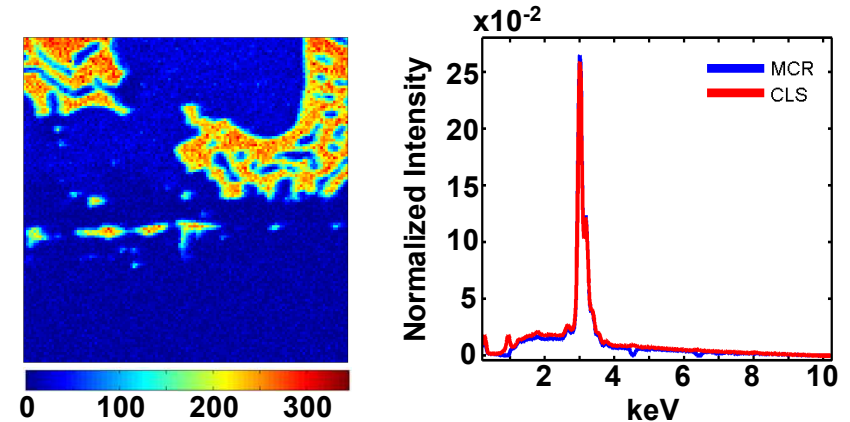
Braze Interface Data: Factor Analysis (Non-Negativity Constrained MCR)

- Biased phase estimates obtained using FA:

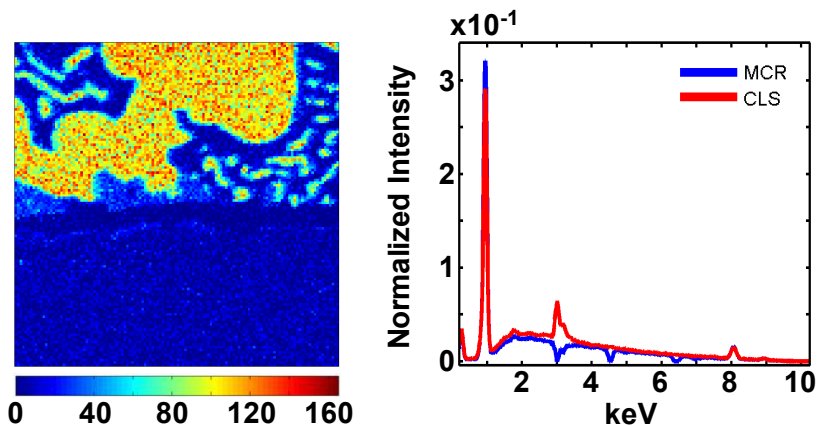
Fe-Ni-Co phase



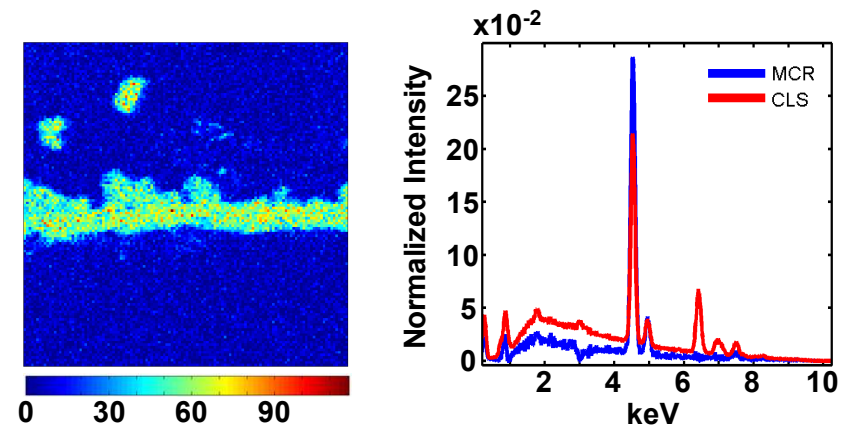
Ag phase



Cu phase



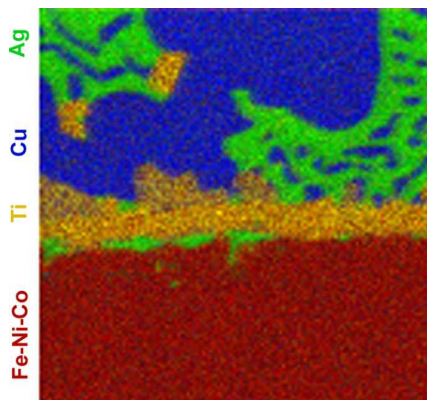
Ti phase



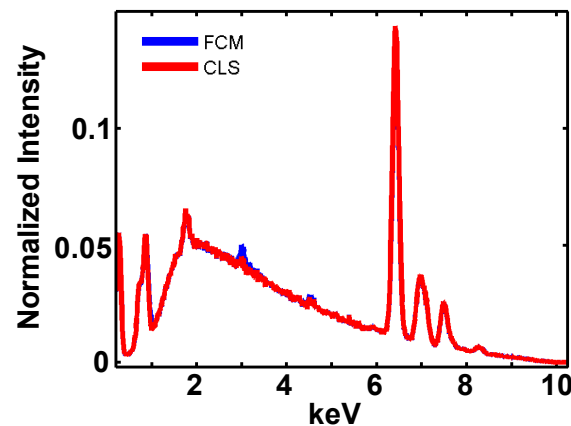
Braze Interface Data: Clustering

- Superior phase classification results obtained using clustering (fuzzy c-means, $m = 2$):

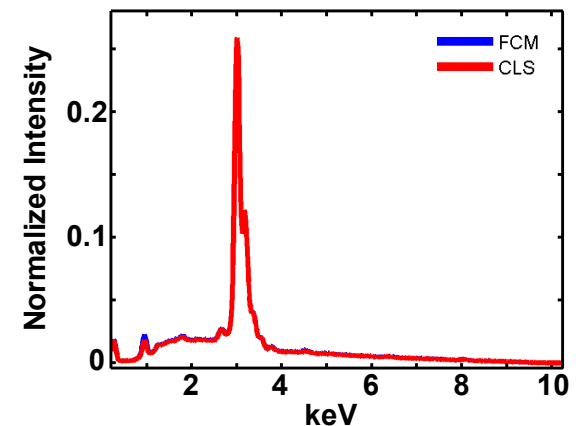
RGB composite EDX image



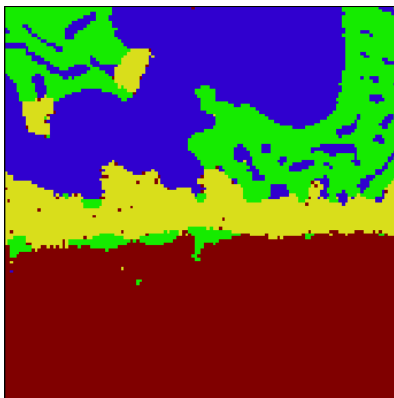
Fe-Ni-Co spectra (FCM vs. CLS)



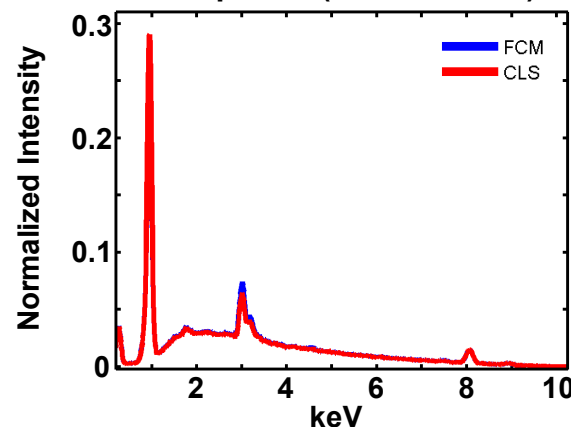
Ag spectra (FCM vs. CLS)



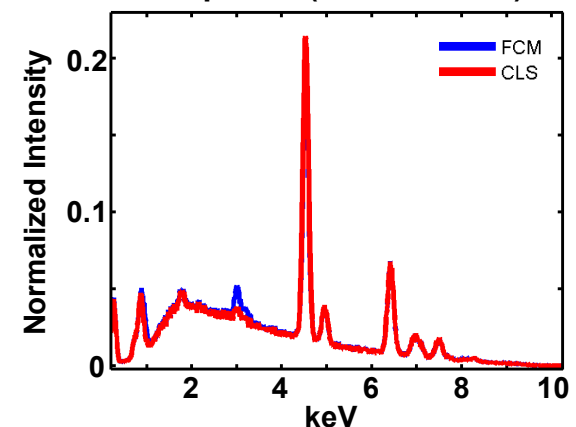
Crisp pixel assignments



Cu spectra (FCM vs. CLS)



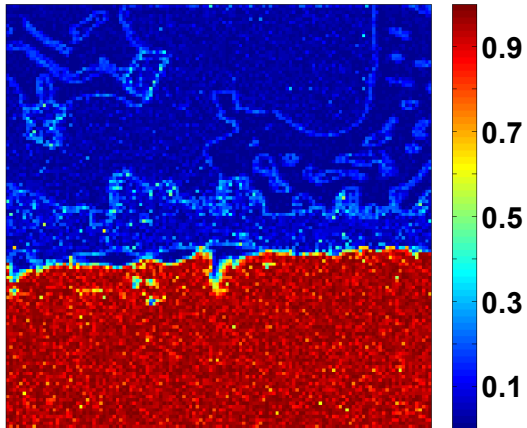
Ti spectra (FCM vs. CLS)



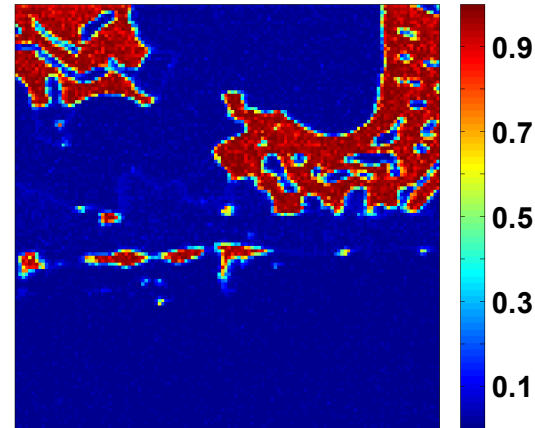
Braze Interface Data: Clustering

- Fuzzy membership images match expectations:

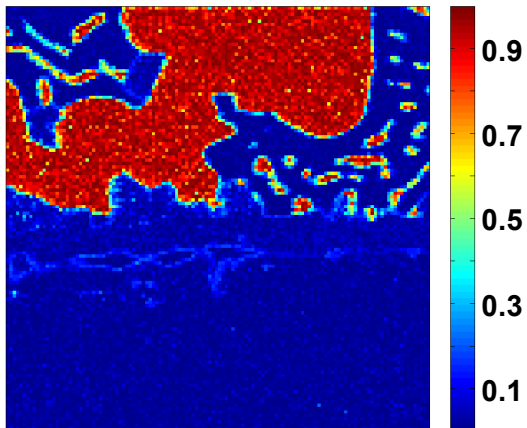
Fe-Ni-Co phase



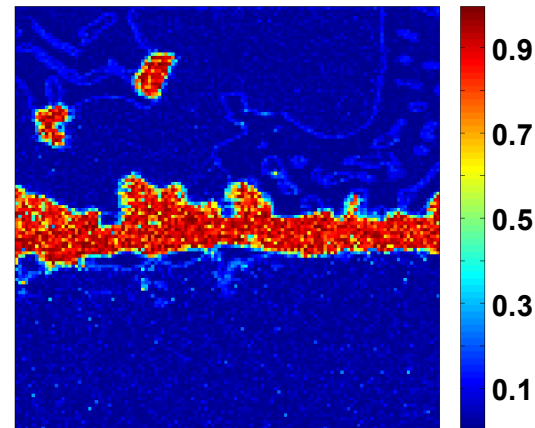
Ag phase



Cu phase



Ti phase





Conclusions

- **Clustering can solve phase problems which are intractable using FA (e.g., solder bump data)**
 - **In FA, number of phases cannot exceed chemical rank of data**
 - **In clustering, number of phases cannot exceed the number of pixels in image**
- **Braze interface data demonstrates that clustering can avoid bias problems encountered using FA**