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Deep Data Analysis of Atomic Level Structure-Property Relationship in an Iron Superconductor $Fe_{1.05}Te_{0.75}Se_{0.25}$

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Understanding the underlying physics of superconducting materials can be greatly facilitated by establishing a relationship between atomic structure and electronic properties at the nanoscale. We obtain the structural data through high-resolution scanning tunneling microscopy (STM), whereas scanning tunneling spectroscopy (STS) mapping of the same area provides information on the local electronic properties such as band structure and, in our case, the superconductive gap. We explore the electronic interactions via the multivariate statistical methods such as Principle Component Analysis (PCA) [1,2] and Bayesian Statistics [3,4] to analyze the data structure and reveal the correlations between structure and functionality. This approach is applied to chemically phase separated $Fe_{1.05}Te_{0.75}Se_{0.25}$ superconductor, to identify effects of local phase separation, structural defects, and magnetic impurities on superconductive behavior.

A low temperature STM was used to acquire atomically resolved images and perform STS on the same region. We then identify all the atoms in the 25x25 nm area shown in Fig. 1 and correlate topographic features with the spectral response by transforming two data sets to lie on identical imaging axis and then identify atoms with a multitude of structural and electronic variables through the local and spectral analysis. Atoms shown in Fig. 2(a) are clustered by their imaged height and spectra associated with those points are averaged together and plotted in Fig.2(b) using the same color code. We test our hypothesis of correlating height to band gap size Fig.2(c), where the band gap was found using similar fitting procedures as in [5].

The procedure outlined in the previous paragraph is also performed for the other types of structural data. The result is two separate arrays of structural and spectral variables on identical imaging axis. Figure 2(d) shows the correlation coefficient for each of the 25 spectral variables and 25 structural variables. For example, pixel (1,1) is the correlation coefficient of atom height to atom gap size and pixel (7,1) corresponds to the first principle component of the spectral response of the atom to the height of the identified atom. In this approach, the statistically significant atomic configurations are established and further used as an input into first principle modeling. Thus, the determined electronic structure is then compared to the local tunneling spectra.

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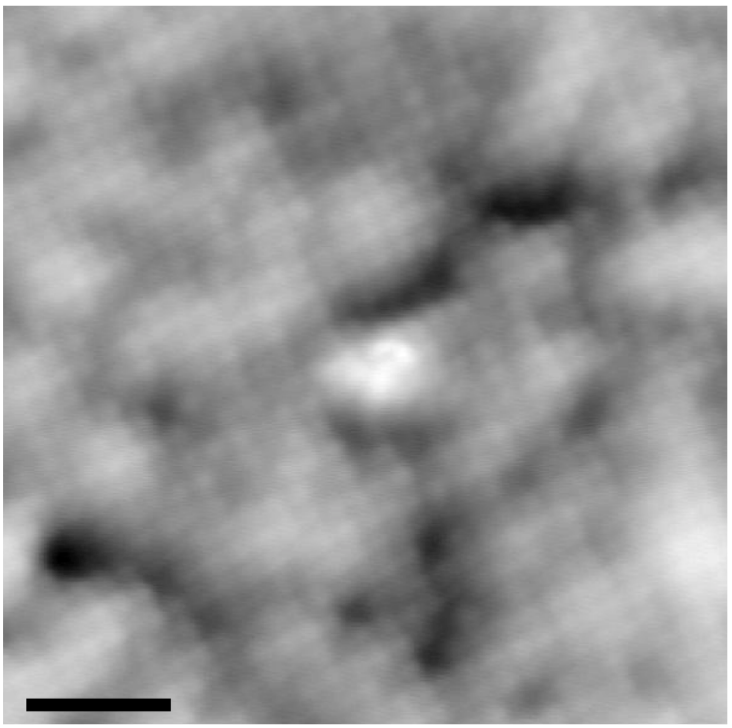

Figure 1 Topographic scan of FeTeSe surface cleaved at Low Temperature. Scale bar = 5 nm

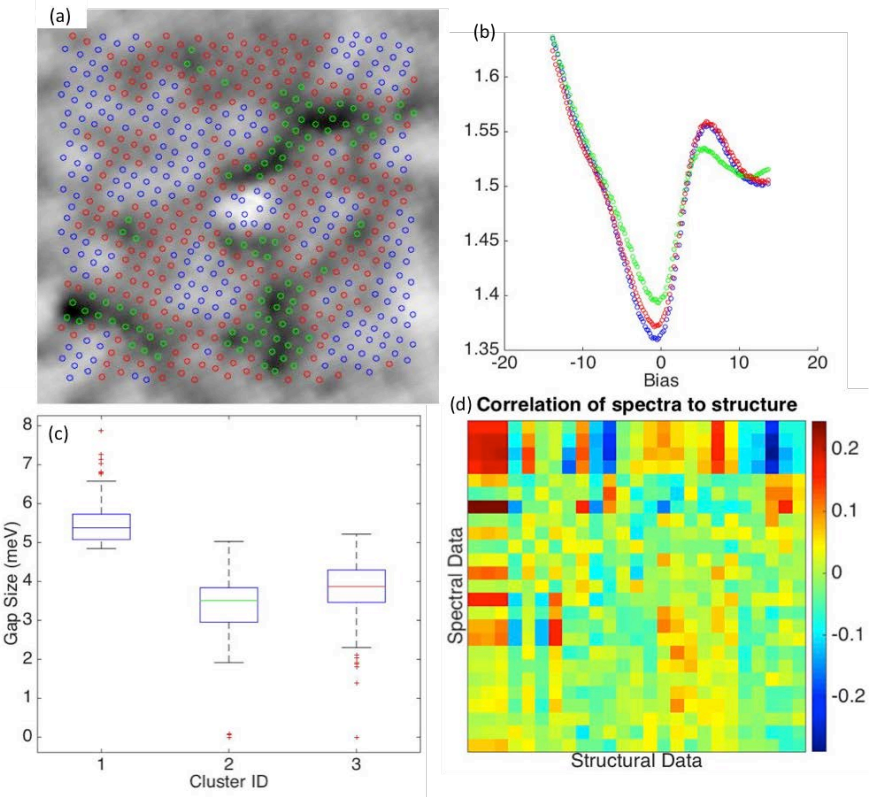

Figure 2 a) Atomic Resolved Image with atoms located. b) Mean spectra associated with the color coded atoms. c) Gap Fit for those spectra. Colors correspond to spectra and atoms. d) Correlation coefficients of different structural and spectral information associated with each atom.

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