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Mesh Generation from Energy Dispersive Spectroscopy Data of Multiphase Microstructures

by Efraín Hernández-Rivera, S. Gary Hirsch, and Brady Butler

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DEVCOM Army Research Laboratory

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14. ABSTRACT
Achieving performance of materials when subjected to extreme environments necessitates advanced materials or processing techniques. Bonding of dissimilar materials via brazing is a promising route, but results in complex microstructures with multiple intermetallic phases that are challenging to model. This work presents a methodology for generating digital twins from energy dispersive spectroscopy (EDS) data, enabling accurate numerical simulations of material behavior within the FEniCS framework. The process involves phase identification and clustering from EDS elemental maps, followed by a novel microstructure cleansing approach using a Potts-like Monte Carlo model to smooth interfaces and remove spurious features. Finally, the cleansed microstructure is converted into a suitable computational mesh. This workflow provides a cost-effective and efficient means of predicting material response, supporting the development of advanced materials for demanding applications.

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bonding, brazing, digital twin, dissimilar material, energy dispersive spectroscopy, finite element, intermetallic, mesh, Sciences of Extreme Materials

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1. Introduction

Material properties are often one of the limiting factors in achieving increased performance or performing under extreme environments (e.g., hypersonic vehicles). To mitigate the material limitations, two general paths can be employed: synthesizing exotic materials (e.g., high entropy alloys) and novel processing technique (e.g., dissimilar materials bonding). While the former aims at developing new materials, the latter seeks to leverage well-understood materials and determine the ideal processing conditions conducive to the development of a high-performing metamaterial.

An important aspect to consider is that depending on the processing methodology, the resulting metamaterial could result in complicated microstructural features. This is especially true when brazing, where multiple phases could be formed in the bonding of the dissimilar systems. For instance, it is known that brazing leads to intermetallic compounds, which will critically influence the processed material.[1]

Therefore, tools that can predict the material behavior under a wide range of application and environments is essential. These could be done by high-throughput experimentation, but these can be challenging to scale and are expensive. This is especially true when operating under extreme environments like hypersonic vehicles, which experience very high temperatures. Since these novel processing techniques result in complex microstructural features, it is crucial to properly characterize them. Traditionally, scanning electron microscopy (SEM) has been used to get different microstructural level features, like grain or pore size and distribution. However, multiple compounds are formed when brazing, each possibly having very different material properties. To qualitatively characterize these microstructural differences, energy dispersive spectroscopy (EDS) can be employed, which analyzes surface structures and yields an elemental composition map. These maps can be used to determine where unique phases are present, which is crucial to understand how the material performs (e.g., when subjected to an external load).

Once the microstructure is analyzed, numerical methods like finite element (FE) can be used to predict how the material will respond to different stimuli. However, going from a pixelated image to an FE mesh is a nontrivial task. This is a drawback of FE where the quality of the mesh strongly influences the accuracy and reliability of the predicted results. This is especially true for microstructures with complex geometries, as is expected of intermetallic compounds, which can play a significant

role on the material's strength and thermal resistance.

In this report, we demonstrate a methodology to generate digital twins from EDS data that can be used within the FEniCS framework.[2] For clarity, EDS data will be described for a complex (eight-element system), which results in multiple intermetallic compounds, and a brief exploration into clustering will be discussed. Finally, a strategy to cleanse the resulting microstructure will be presented.

2. Experimental Data Generation

Our aim is to join two dissimilar materials: SiC and Ti-6Al-4V. One challenge to joining ceramics and metals is their inherent differences in material properties, i.e., disparate coefficients of thermal expansion (CTEs) that can induce weak bonds. To mitigate this, the brazing of a Ti-6Al-4 alloy to Saint-Gobain SiC was carried out using InCuSil ABA, a low-temperature active brazing alloy. Specimens were heated to 725 °C under an inert atmosphere to promote wetting and bonding at the metal–ceramic interface. This results in a complex microstructure with multiple intermetallic compounds, as shown in Figure 1.

EDS is a characterization technique where electrons are used to excite a samples atoms, which go on to emit X-rays. These X-rays are emitted at a given energy characteristic to specific atoms (e.g., Si Kα $\sim$ 1.74 keV). The EDS detector then measures all the emitted X-ray data and generates a spectrum, providing a qualitative representation of the elemental components present in the sample. More importantly, the technique provides an elemental map (i.e., atomic content per pixel), which can be used to generate digital twins of the microstructure's phases.

Figure 2 shows a representative sketch (for a three-element material system) and a dataset extracted from the EDS detector. The spectrum shown in Figure 2a is a representative sketch of a three-element material as detected by the experimental equipment. It is clear that the collected X-rays corresponding to elements 0 and 2 overlap due to the close energy at which they are emitted, which causes peak broadening and requiring care when identifying elements. The tabulated data (Figure 2a) provides the number of X-rays counted by the detector determined to correspond to a specific element, with each row corresponding to a specific pixel/location on the sample surface. The relative count of each X-ray can be used to qualitatively describe the elemental composition of a sample.

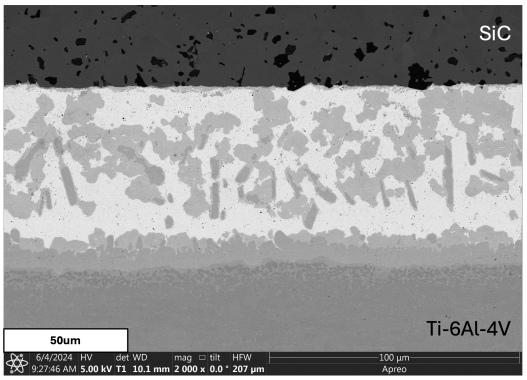
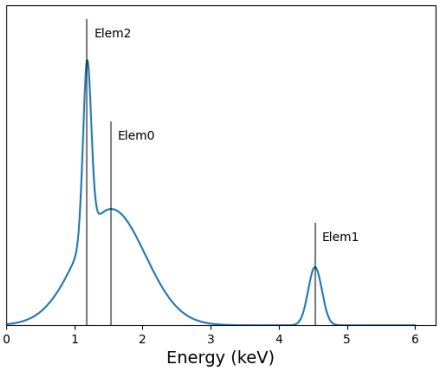


Figure 1. Backscatter SEM showing the dissimilar materials, as well as the intermetallic phases developed during processing.

a) b)



	InL	AgL	AlK	SiK	C K	CuK	TiK	V K	CPS	Field
0	83	338	4	17	33	15	6	13	13	13
1	99	318	14	13	33	16	6	9	9	9
2	76	297	14	13	41	18	13	8	8	8
3	71	295	12	14	24	11	13	12	12	12
4	79	339	4	15	28	22	15	5	5	5
...	...	...	...	...	...	...	...	...	...	...
204795	82	112	12	3	8	53	39	7	7	7
204796	54	94	11	2	3	57	52	11	11	11
204797	61	94	8	12	6	53	36	16	16	16
204798	50	96	9	6	9	51	24	9	9	9
204799	42	100	10	10	12	46	31	9	9	9

204800 rows × 10 columns

Figure 2. Raw count data collected by the EDS detector, a) sketch of a hypothetical spectrum and b) the experimentally collected dataset used in this work.

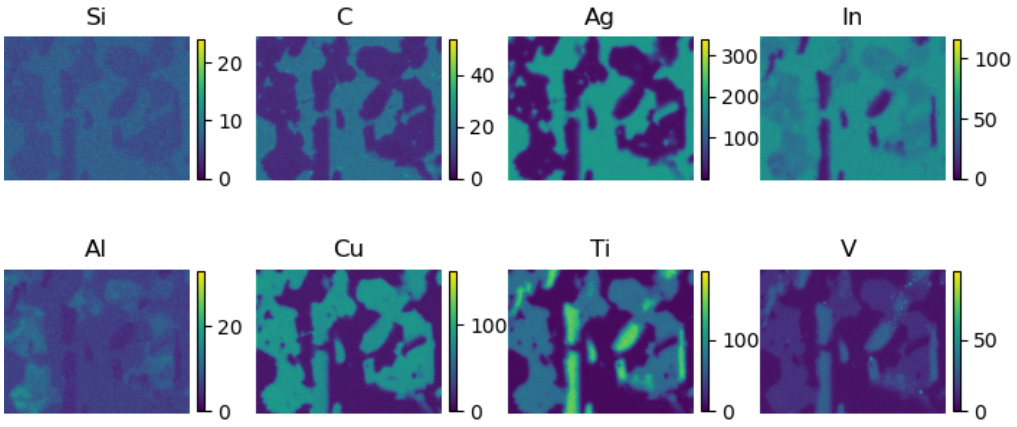


Figure 3. Elemental map for a brazed sample. The scale bars correspond to counts.

A series of spectra are generated for each pixelated location, which then get indexed to identify corresponding elements. Therefore, these can be rearranged into maps that accurately describe the surface morphology, as shown in Figure 3. Given that the materials being bonded are SiC and Ti-6Al-4V (Ti64), and the brazing material is InCuSiI, we can readily map based on the expected atomic constituents. The color differences show the relative intensity (X-ray count) detected from each element for the scanned surface, which brighter (green) and darker (purple) colors representing a qualitative lower and higher composition, respectively. A useful feature is how these maps show "clustering" of specific elements. These are due to the presence of intermetallics that have nucleated and formed as the samples cool and the bond is formed. An alternative visualization of the data is performing a correlation analysis on the raw data (see Figure 4). This shows that there are several clusters, indicating the presence of different elemental compositions "cluster" and helping narrow the search when determining the number of unique phases. The clustering is usually a multi-step process of dimensionality reduction (e.g., principal component analysis [PCA]) and grouping of similar PCAs (e.g., K-means clustering). There is clustering of the Cu, Ti, V, and Al (to a lesser extent). This is reflected in three specific Ti-phases present, α-Ti (Al rich), β-Ti (V rich), and a Ti-Cu intermetallic compound. Other clustering data shows that Ag, In, and C tend to cluster. The low energy C peaks may have overlap with other nonmetallic interstitials (e.g., oxygen) leading to erroneous clustering results. However, there is a stable Ag-In phase expected in this particular low-temperature brazing alloy.

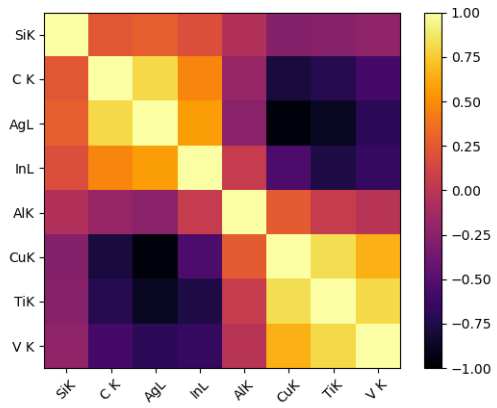


Figure 4. Pearson correlation of the raw count data.

3. Digital Twin Generation and Meshing

While the raw EDS data can yield a general description of the microstructural features (e.g., different phases), the phase-clustered microstructures often result in rough interfaces. This can be seen in Figure 5 (as clustered) where the interfaces between the differently colored phases are jagged. Furthermore, there are regions with large amount of randomness (see red circle), which are not conducive to stable numerical analysis. To mitigate this, a simple Potts-like Monte Carlo model[3,4] was implemented where pixels are allowed to flip positions, but no state changes are allowed. This phase-conserving model basically results in a type of surface energy minimization by reducing the "jaggedness" of the original images (i.e., reducing the interface between unlike phases). Similar approaches have been implemented to simulate surface migration during sintering[5] and pore migration.[6] This algorithm results in the random walk of single-pixel phases that cluster into precipitate-like phases once they come into contact (as highlighted on the blue circle). These phases are not representative of the original microstructure; therefore, they are removed by changing their state to be that of the larger surrounding phase (i.e., nonconserved event). This final step, shown in Figure 5 (right), results in a digital twin with smoother interfaces that is free of any single-pixel phases.

Once a suitable digital twin microstructure is generated, it needs to be converted into a mesh that can be read into a FE solver. For our purposes, we are focusing on a conversion to a FEniCS friendly mesh, but there are other tools that have been

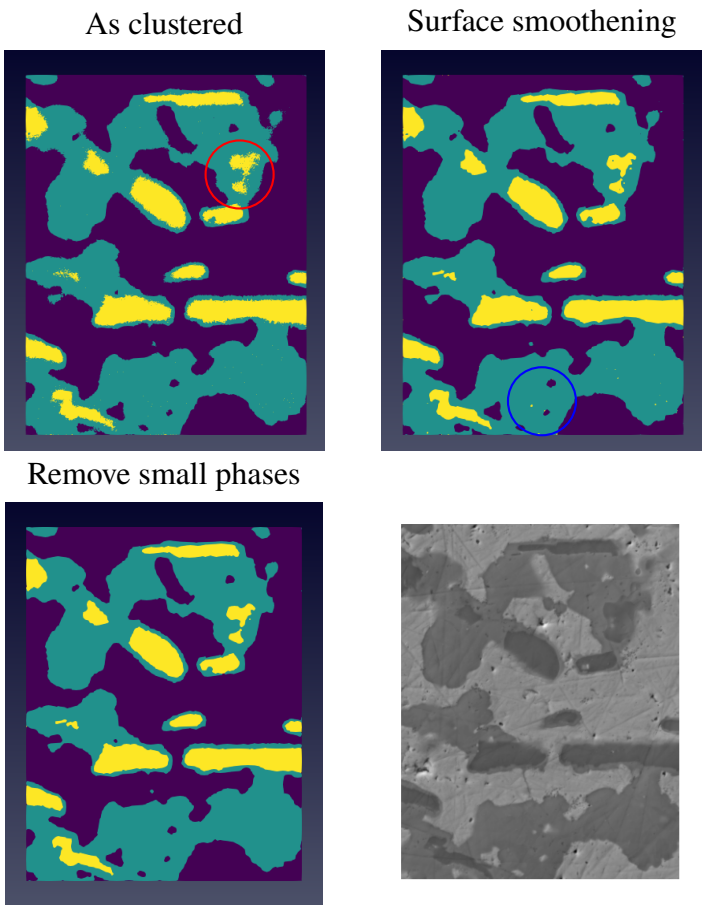


Figure 5. Digital twin generated from the EDS data.

Table 1. Code snippet to initialize mesh values.

```
1    p = Function(V)
2    p.vector().set_local(phase[dof_to_vertex_map(V)])
3    f_out = XDMFFile('FEniCS_mesh.xdmf')
4    f_out.write_checkpoint(p, "phases", 0, XDMFFile.Encoding
        .HDF5, False)
```

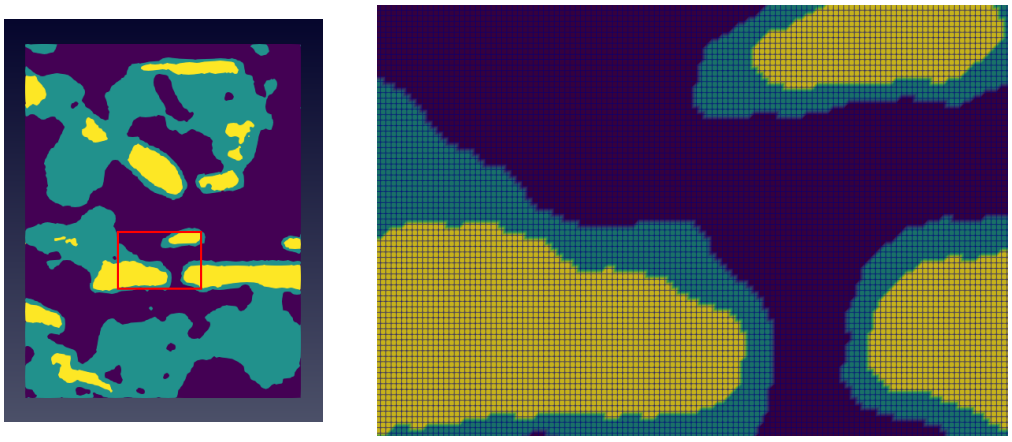


Figure 6. Meshed digital twin using legacy FEniCS's XDMF format.

used to generate more exotic meshes.[7] A typical FE mesh is defined from nodal positions, which are then used to define elements via connectivities. Hence, this pixel level information needs to be mapped into the nodal positions. This is done with FEniCS native functions, which allow for the building of a quadrilateral mesh from a `FunctionSpace` V. As outlined in Table 1, a `phase` array can be mapped to the function V's nodal points (degrees of freedom) straightforwardly (line 2). Once the nodal values have been defined, these can be written into an an eXtensible Data Model and Format (`XDMF`) mesh, which can be readily used by FEniCS, as shown in Figure 6.

4. Summary

This report outlines a method for creating digital twins of complex material microstructures created through brazing, which is used to bond materials with dissimilar properties (e.g., CTE). Brazing results in intricate microstructures of intermetallic compounds whose interaction and behavior are difficult to analyze and predict.

This work demonstrates how multiphase complex microstructures, characterized via EDS, can be used to generate digital twins that are subsequently used to generate FEniCS readable meshes. These meshes can ultimately be used to predict the mechanics response of the resulting material. To generate the digital twin, a Potts-like model was used to minimize interfacial energy on the experimental data. The resulting microstructure was then postprocessed to remove small phases, and this cleaned microstructure was used to initialize the nodal values on an FEniCS XDMF mesh.

The ultimate goal is to be able to accurately predict how these materials behave under processing conditions, without needing extensive and expensive physical testing. With the meshed digital twins and corresponding physical models, it is possible to simulate microstructural evolution during operating conditions. This approach supports initiatives focused on efficient materials development and is particularly relevant for applications requiring materials that can withstand extreme conditions.

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List of Symbols, Abbreviations, and Acronyms

CTE	coefficient of thermal expansion
EDS	energy dispersive spectroscopy
FE	finite element
PCA	principal component analysis
SEM	scanning electron microscopy
XDMF	eXtensible Data Model and Format

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