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Toward few pixel annotations for 3D segmentation of material from electron tomography

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Abstract: Segmentation is a notorious tedious task, especially for 3D volume of material obtained via electron tomography. In this paper, we propose a new method for the segmentation of such data with only few partially labeled slices extracted from the volume. This method handles very restricted training data, and particularly less than a slice of the volume. Moreover, unlabeled data also contributes to the segmentation. To achieve this, a combination of self-supervised and contrastive learning methods are used on top of any 2D segmentation backbone. This method has been evaluated on three real electron tomography volumes.

1 INTRODUCTION

Electron tomography (ET) (Ersen et al., 2007) is a powerful characterization technique for the reconstruction of 3D nanoscale microstructure of material. Volumes are reconstructed from sets of projections from different angles acquired by a Transmission Electron Microscope (TEM) providing a real three-dimensional information at the nanometric scale. The limited number of projections and the difficulty to align them correctly (Frank, 2008) produce noisy data with strong reconstruction artifacts (Figure 1). Standard segmentation approaches generally fail to produce accurate semantic segmentation of this kind of data (Evin et al., 2021), or need intensive expertise of the user (Fernandez, 2012; He et al., 2008; Volkmann, 2010).

Recently, deep learning (DL) based methods have been successfully used in this field (Akers et al., 2021; Khadangi et al., 2021; Genc et al., 2022), inheriting from progresses in 2D or 3D image semantic segmentation (Ronneberger et al., 2015; Çiçek et al., 2016; Milletari et al., 2016; Chen et al., 2018a; Sun et al., 2019). The standard setup is first to train a DL model on a fully labeled dataset, and then use this model on the data at hand. However, this approach requires the availability of a fully segmented set of 3D volumes, which is a tedious preliminary task. In this paper,

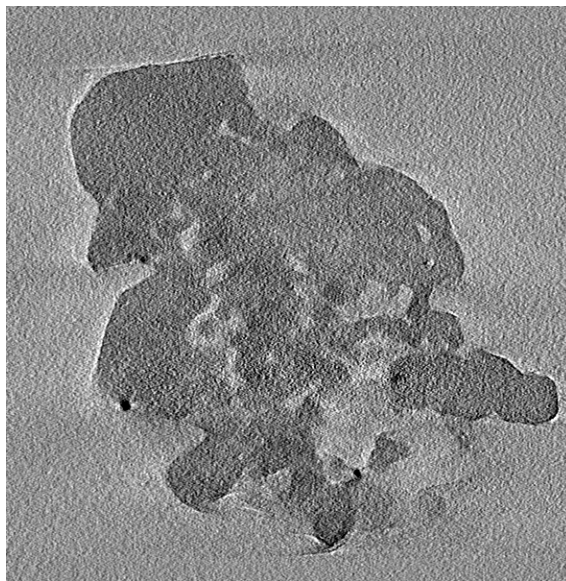


Figure 1: Slice of a volume of zeolite (resolution : 1 nm/voxel). Slices from the volume are noisy and contain artifacts, that make segmentation tasks harder.

we consider a more realistic semi supervised setup. Given a 3D volume, we ask the user to manually segment only a few regions in a few slices (typically a single one or two) of this 3D volume. This small amount of annotated data is then used to train a DL

model, subsequently used to segment the whole 3D volume.

The problem of few available training data is not specific to ET and has been addressed in many computer vision tasks, mainly using transfer learning (Pan and Yang, 2009; Wurm et al., 2019). A promising approach is to rely on contrastive representation learning, whose goal is to learn an embedding space using pairs of positive or negative samples (Hadsell et al., 2006; Dosovitskiy et al., 2014; Zhao et al., 2021). In a supervised setting, mainly used in Siamese networks (Koch et al., 2015), positive pairs are taken from samples of the same class and negative ones are taken from samples of different classes. The unsupervised setting relies on positive pairs obtained from a single sample subject to two independent random perturbations. It was shown to be a powerful self-supervised learning method (Chen et al., 2020; Chen and He, 2021).

In this article, we propose a new semi-supervised approach to segment a full volume in ET with only few annotated pixels. Our approach fully exploits the labeled as well as the unlabeled pixels of the partially annotated slices to learn a specific pixel-level embedding space relevant for segmentation. More precisely, given a DL model for semantic segmentation, we first reshape the output to define a pixel-level embedding space of dimension D . Then, for training, we rely on contrastive learning and both a weakly-supervised stream for labeled pixels and a self-supervised stream for unlabeled ones (Figure 2). Supervised and self-supervised contrastive learning are used together to fully exploit partially-labeled data (Figure 3). The final segmentation is obtained through a pixel-wise classification layer operating in the embedding space of dimension D .

Our principal contributions are:

- A new semi-supervised learning method for practical 3D image segmentation in ET, which takes advantage of contrastive learning and self learning principles to provide accurate volume segmentation using only few labeled regions of one or two specific 2D slices.
- The model can be easily built on top of any 2D segmentation DL model.
- We provide detailed experimentation on several real ET data, and we show that an accurate segmentation is possible with only one slice and 6% of annotated pixels in this slice.

2 RELATED WORKS

Electron tomography segmentation Due to low SNR and reconstruction artifacts, segmentation of tomograms is a difficult task and manual segmentation still remains the prevalent method (Fernandez, 2012) often used in interaction with the user through visualization tools (He et al., 2008), sometimes combined with various image processing methods as watershed transform (Volkman, 2010). Following the promising development of DL in general semantic segmentation tasks (Ronneberger et al., 2015; Çiçek et al., 2016; Milletari et al., 2016; Chen et al., 2018a; Sun et al., 2019) some recent works have investigated DL based techniques in 2D electron microscopy (Akers et al., 2021; Khadangi et al., 2021). In these works, the bottleneck of the availability of labeled training data is addressed either by a semi-supervised few-shot approach (Akers et al., 2021) or by a scalable DL model, which requires only small- and medium-sized ground-truth datasets (Khadangi et al., 2021). In 3D, we only found a first investigation of U-Net model to multi-class semantic segmentation of a γ -alumina/Pt catalytic material in a class imbalance situation (Genc et al., 2022). In this work, 30 labeled slices and data augmentation are needed to train the model. To the best of our knowledge, our method is the first one providing accurate 3D segmentation with only few annotated pixels in a single slice.

Contrastive Learning Contrastive learning aims to exploit labels better, usually with Siamese networks (Zhao et al., 2021). The goal is to construct a latent space in which objects with the same label are close to each other, and objects with different labels are far from each other. Positive and negative pairs are formed. Positive pairs are composed of two objects of the same class, whereas negative ones are composed of two objects of different classes. A contrastive loss function is used during training to bring positive pairs together and negative pairs far from each other. Contrastive learning has shown excellent results in image classification (Chen et al., 2020; Grill et al., 2020; Khosla et al., 2020; Chen and He, 2021). For semantic segmentation, pairs of pixels can be considered, and these methods can also train a model without labeled data (Chaitanya et al., 2020). When pairs are created without the knowledge of the class, only positive ones can be created. Input images are transformed, and the transformed pixels are compared to their original version. The images, even transformed, represent the same object and a similarity function can be minimized during training.

Semi-supervised methods in semantic segmentation The goal of semi-supervised methods in se-

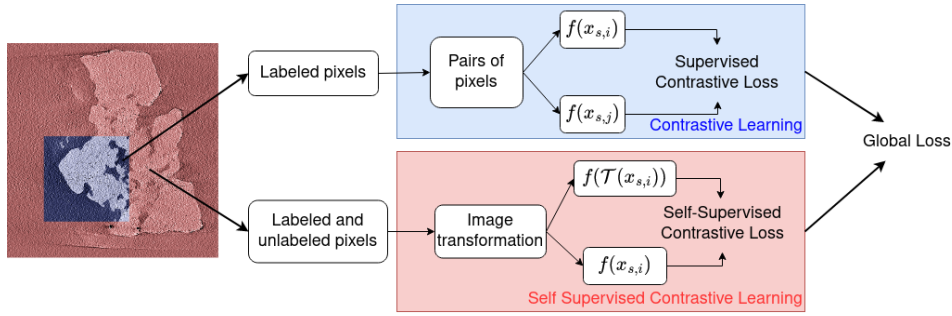


Figure 2: The loss calculation is different depending on pixel labeling. For labeled pixels, pairs of pixels are constructed and are used in a contrastive loss. For labeled and unlabeled pixels, the training image and the transformed version of itself are used as a positive pair in a self-learning contrastive loss. Both contrastive loss and similarity loss are added for the global loss.

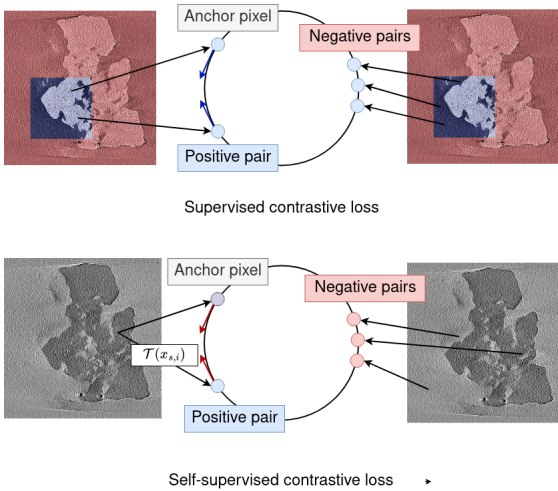


Figure 3: The supervised contrastive loss is computed for each labeled pixels. Given a labeled pixel considered as an anchor pixel, pixels of the same class as this anchor pixel (positive pairs) are pushed together, while pixels of a different class (negative pairs) are pushed aside. The self-supervised loss is computed for both labeled and unlabeled classes. Given an anchor pixel, a single positive pair is obtained by applying a transform to it, while negative pairs are obtained from all other pixels. The anchor pixel and its transformed version are pushed together, while other pixels are pushed aside from the anchor pixel.

semantic segmentation is to optimize how labeled and unlabeled data are exploited together to learn a segmentation task. Transformations can be used in Siamese network to mix a self-supervised loss with a standard supervised methods (Li et al., 2018). Another approach is to apply an adversarial method, where two networks are trained on labeled images. Unlabeled images are fed into both networks and a similarity function is minimized (Peng et al., 2020). In (Ouali et al., 2020), a standard encoder-decoder is used on labeled images. Unlabeled images are fed into several decoders, a slightly modified version of the decoder used for the labeled data. The output

of all the decoders is then compared to the output of the main decoder. In this case, the network is transformed. However, these methods have all their images either fully labeled or fully unlabeled. In our case, images themselves can have unlabeled pixels.

3 PROPOSED METHOD

Our method relies on a 2D representation model trained with contrastive-learning and self-learning principles. This model is used to segment each slice of the volume to provide the final 3D segmentation. Indeed, although several fully 3D convolutional neural networks (CNN) have been proposed (Milletari et al., 2016), they were shown to be more resource intensive than 2D models without providing convincing gains (Kern et al., 2021). The overview of the method is summarized in Figure 2. The whole architecture is composed of an encoder-decoder f used to project pixels of the slice in a pixel level embedding space and a classification layer (a linear model classifier) h providing the semantic segmentation. The representation model f is trained using positive and negative pairs of labeled pixels in the contrastive path, and positive pairs of labeled and unlabeled pixels in the self-supervised path. Note that there is a single embedding space for both labeled and unlabeled pixels. The classification layer is subsequently trained using labeled pixels after freezing the representation model. A standard weighted cross-entropy loss is used to train this classification layer.

3.1 Formalization

The input volume V is a set of S slices $\{X_s\}_{s=1,\dots,S}$ such that each slice $X_s \in \mathbb{R}^{W \times H \times 1}$ where W is its width, H its height and 1 is because the slice is a grayscale image. We denote $x_{s,i}$ the graylevel at pixel

$i \in I$ of slice X_s , I being the image spatial support. We then have $X_s = (x_{s,i})_{i \in I}$. Each slice is processed independently. The output segmentation of slice s is $\hat{Y}_s = h(f(X_s))$. The encoder-decoder f transforms X_s onto $Z_s = (z_{s,i})_{i \in I} = f(X_s) \in \mathbb{R}^{W \times H \times D}$ where D is the dimension of the latent space. The classification layer h performs the pixel-wise class prediction $\hat{Y}_s = h(Z_s)$ such that $\hat{Y}_s \in \mathbb{R}^{W \times H \times C}$, where C is the number of classes.

Each voxel of the volume is either labeled or unlabeled. Let Y_s be the pixel-wise class label map of the slice s , then $Y_s = (y_{s,i})_{i \in I}$ with $y_{s,i} \in \{\emptyset, 1, 2, \dots, C\}$ where $1, 2, \dots, C$ are the labeled classes and \emptyset represents unlabeled pixels. We note \mathcal{L}_s the set of labeled pixels and \mathcal{U}_s the set of unlabeled pixels:

$$\mathcal{L}_s = \{i \in I, y_{s,i} \neq \emptyset\}, \quad \mathcal{U}_s = \{i \in I, y_{s,i} = \emptyset\} \quad (1)$$

The loss function is computed differently if the pixel is labeled or unlabeled. Pixels in \mathcal{L}_s follow the contrastive path, whereas pixels in \mathcal{L}_s and \mathcal{U}_s follow the self-learning path. For sake of simplicity, in the following subsections, we will consider the case of a single labeled slice X_s for training, but it can be easily generalized to any number of training slices by summing the corresponding losses.

3.2 Contrastive Loss

A contrastive loss is computed for labeled pixels (Khosla et al., 2020). This loss aims to learn a representation space where pixels from the same label are close to each other in that space, while pixels from different labels are far from each other in that space. The contrastive loss is relevant in our case because the model can be fed with only a few number of labeled pixels and the contrastive loss can fully exploit each pixel by forming positive and negative pairs. For each labeled pixel $x_{s,i}$, $i \in \mathcal{L}_s$, positive pairs $\mathcal{P}_{s,i}^+$ and negative pairs $\mathcal{P}_{s,i}^-$ are constructed. As the label is known for this kind of pixels, given an anchor pixel, positives pairs are built by choosing pixels of the same class as this anchor pixel, whereas negatives pairs are composed of pixels of a different class (Figure 3). We have:

$$\mathcal{P}_{s,i}^+ = \{j \in \mathcal{L}_s, i \neq j, y_{s,i} = y_{s,j}\} \quad (2)$$

$$\mathcal{P}_{s,i}^- = \{j \in \mathcal{L}_s, i \neq j, y_{s,i} \neq y_{s,j}\} \quad (3)$$

Let $\mathcal{P}_{s,i} = \mathcal{P}_{s,i}^+ \cup \mathcal{P}_{s,i}^-$ be the set of pairs that are formed for each pixel $x_{s,i}$. To balance positive and negative pairs and limit the computational complexity, we randomly choose an equal number of positive and negative pairs such that the total number of pairs per pixel is a given constant value N_p .

The supervised contrastive loss (Khosla et al., 2020) associated to one labeled slice is defined as:

$$L_1(Z_s) = \frac{-1}{N_{\mathcal{L}_s}} \sum_{i \in \mathcal{L}_s} \frac{1}{N_p} \sum_{j \in \mathcal{P}_{s,i}^+} \log \frac{\exp(\text{sim}(z_{s,i}, z_{s,j}))}{\sum_{k \in \mathcal{P}_{s,i}^-} \exp(\text{sim}(z_{s,i}, z_{s,k}))} \quad (4)$$

with $N_{\mathcal{L}_s}$ the number of pixels in \mathcal{L}_s and sim is the cosine similarity, defined as:

$$\text{sim}(u, v) = \frac{u \cdot v}{\|u\| \cdot \|v\|} \quad (5)$$

3.3 Self-Supervised Contrastive Loss

A self-supervised method is used for labeled and unlabeled pixels. It is especially useful for unlabeled data, as the information on labels is unknown. To train without labels, the training slice is transformed, and a self-supervised contrastive loss is computed between each transformed image (Chen et al., 2020). The corresponding pixels, even from slightly transformed images, should have their feature vector close to each other in the representation space. These two pixels are considered as a positive pair. All other combinations are considered as negative pairs (Figure 3). Let \mathcal{T} be a random transformation of the pixels of the original slice $x_{s,i}$, $i \in I$. The output Z_s of the original slice and the output of its transformed version $\tilde{Z}_s = f(\mathcal{T}(X_s)) = (\tilde{z}_{s,i})_{i \in I}$ are compared.

The self-supervised contrastive loss associated to slice X_s is defined as:

$$L_2(Z_s) = \frac{-1}{N_I} \sum_{i \in I} \log \frac{\exp(\text{sim}(z_{s,i}, \tilde{z}_{s,i}))}{\sum_{j \in I, i \neq j} \exp(\text{sim}(z_{s,i}, z_{s,j}))} \quad (6)$$

where N_I is the number of pixels in I .

The final loss is a combination of both losses :

$$L(Z_s) = L_1(Z_s) + L_2(Z_s) \quad (7)$$

4 EXPERIMENTS AND RESULTS

4.1 Implementation Details

For the encoder-decoder f , a U-Net like model is used to project pixels in the embedding space (Figure 4). The encoder is composed of three downsampling steps. A downsampling step is composed of two 3×3 convolution layers followed by a ReLU layer and a 2×2 Max Pooling layer with a stride 2 for downsampling. The input image resolution is halved

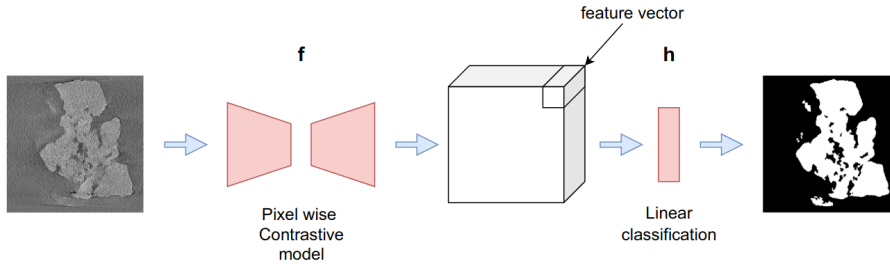


Figure 4: Our model is based on U-Net, with three stages. The output is the projection for each pixel in the embedding space. A classification layer is trained to transform the feature vectors into a segmentation map.

and the number of channels is doubled for each down-sampling step. The decoder is also composed of three steps, with an upsampling layer followed by a 2×2 convolution layer that halves the number of channels, a concatenation with the corresponding feature map from the encoder and two 3×3 convolution layers followed by a ReLU. As a result, the number of filters for each layer of the encoder is 16, 32 and 64. For each layer of the decoder, the image resolution is doubled and the number of channels is halved. The resulting number of layers are 64, 32 and 16. At the end of the network, a feature map at the size of the input is obtained. A 1×1 convolutional layer is applied with 16 filters to project the result in the embedding space. The loss function is computed, depending upon the fact that the pixel is labeled or unlabeled. To compute the final segmentation result, a pixel-wise classification layer h is trained on the output of the training data. This layer is composed of a single convolutional layer with a kernel of size 1×1 . The classification layer is trained with a weighted standard cross-entropy loss, where unlabeled pixels' weight is set to 0 (Çiçek et al., 2016).

For each labeled pixel, 10 positive pairs and 10 negative pairs are made, and thus $N_p = 20$.

Table 1 details the random transformation used on the training slice in order to compute the self-supervised loss, as well as their probability of occurring and their respective parameters. As each pixel is associated to a corresponding transformed pixel, only transformations that do not change the structure of the slice are chosen. The parameters are chosen so that the resulting image corresponds visually to a realistic image.

The Intersection over Union (IOU) is computed on the whole volume V to assess our results :

$$IOU(V) = \frac{\sum_{s=1}^S \hat{Y}_s \cap Y_s}{\sum_{s=1}^S \hat{Y}_s \cup Y_s} \quad (8)$$

The closer the IOU to 1, the better the 3D semantic segmentation result.

Transformation	Probability	Parameters
Gaussian noise	1	$\mathcal{N}(0, [0.01; 0.06])$
Gray level shift	0.5	$[-0.01; 0.01]$
Gaussian blur	0.5	$\sigma = [0.5 - 1.5]$

Table 1: Random transformations used to compute the self-supervised loss.

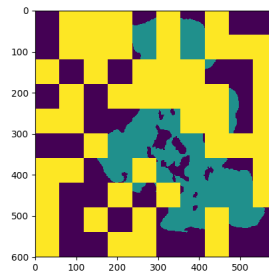


Figure 5: Example of a partially labeled slice ($r = 0.5$) used to train the model. Blue pixels represent the object, purple pixels, the background and yellow pixel are unlabeled data.

4.2 Data

Zeolites are used in several chemical processes in the energy field (Flores et al., 2019) and are composed of nanoscale cavities that are challenging to segment properly (Figure 1). Our methodology is illustrated on ET volume of hierarchical zeolite, NaX Siliporite G5 from Ceca-Arkema (Medeiros-Costa et al., 2019). The size of the volume is $592 \times 600 \times 623$. 10 slices are selected as the pool of possible training slices. A 5-fold cross validation is used, where 1 slice for training and 1 for validation are chosen for each fold. All other slices of the volume are used for test. The annotation for the training slice is artificially hidden to provide partially labeled data to the network. Each slice is divided into 100 equally sized patches. A random number of patches are set to be hidden. At least one patch with object pixels and one patch with background pixels are selected to ensure that positive pairs

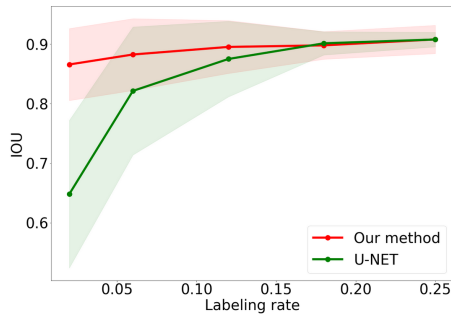


Figure 6: Mean IOU of our method (red) and U-Net (green) when reconstructing the segmentation mask for the volume with one partially labeled training slice for different labeling rate. The green and red areas represent the standard deviation of the results with U-Net and with our method (each experiment is a 5-fold cross validation, repeated 5 times).

r	0.02	0.06	0.12	0.18	0.25
U-Net	0.648	0.821	0.875	0.902	0.908
Ours	0.866	0.883	0.895	0.898	0.908

Table 2: Comparison of IOU between our method with both loss combined and a U-Net architecture.

and negative pairs can be created. An example of a partially annotated slice can be seen in Figure 5. The number of hidden patches depends on a labeling rate denoted r .

4.3 Results

Study of parameter r We compare our method with U-Net as a reference for different labeling rates to illustrate the benefit of learning an embedding space. In addition to the 5-fold cross validation, each experiment is repeated 5 times, resulting in a total of 25 realizations by experiment. The mean and standard deviation are computed across these realizations. The U-Net network is modified in order to make it compatible with partially labeled data like in Çiçek *et al.*'s work (Çiçek *et al.*, 2016) where a weighted cross-entropy is used and unlabeled pixels' weights are set to 0. The results are shown in Figure 6 and in Table 2. Our method performs significantly better than U-Net for small labeling rates, and has similar performance for higher learning rate. The results are already pertinent, only using 2% of one labeled slice for training.

Comparison study between supervised and self-supervised losses An ablation study was made to study, for each labeling rate r the effect of activating either the supervised or the self-supervised loss alone or the combination of both. As shown in Table 3, when only the self-supervised loss is used, the results are good even for a small labelling rate: the latent space is well learned with only few anno-

r	0.06	0.12	0.18	1.00
Self-Supervised	0.907	0.869	0.891	0.916
Supervised	0.773	0.875	0.861	0.926
Combined	0.883	0.895	0.898	0.927

Table 3: Comparison of obtained mean IOU for independent trainings by activating either the self-supervised, the supervised or both losses (each experiment is a 5-fold cross validation, repeated 5 times and the average is reported in the table). Note that the classification layer h is always trained with supervision.

	Zeolite 1	Zeolite 2	Alumina
U-Net $r = 0.06$	0.821	0.219	0.128
Ours $r = 0.06$	0.883	0.443	0.533
U-Net $r = 0.25$	0.908	0.392	0.196
Ours $r = 0.25$	0.908	0.595	0.729

Table 4: Results of our method for several volumes.

tated pixels. As the labelling rate grows, only the classification layer benefits from the supplementary data. This results in little improvement as the labelling rate increases. The contrastive loss does not perform well when only few data are provided, but as there are more labelled data, the supervised loss performs better due to more diverse pairs of pixels. When combining both supervised and self-supervised loss, good results are obtained with a small labelling rate, while performing better as the amount of labelled data raises. Both supervised and self-supervised contrastive loss are required to obtain the best segmentation. The whole reconstructed volume with both losses combined can be seen in Figure 7.

Generalization to other volumes Another volume of the same kind of zeolite (size $512 \times 512 \times 100$) and a volume of γ -alumina (Gay *et al.*, 2016) (size $592 \times 840 \times 296$) have also been segmented with our approach. The results can be seen in Table 4. We compared our method with both losses combined against a U-Net like network. Our model performs better than U-Net in most cases. Moreover, our method reaches maximum values at a smaller labelling rate than U-Net, and performs better than U-Net with very small values of r . The reconstruction of the segmentation of the volume can be seen in Figure 7.

5 CONCLUSION

In this paper, we introduce a new semi-supervised learning method for 3D image segmentation in electron tomography. Our model can achieve accurate segmentation of electron tomography volumes with only less than a slice for training data by using both

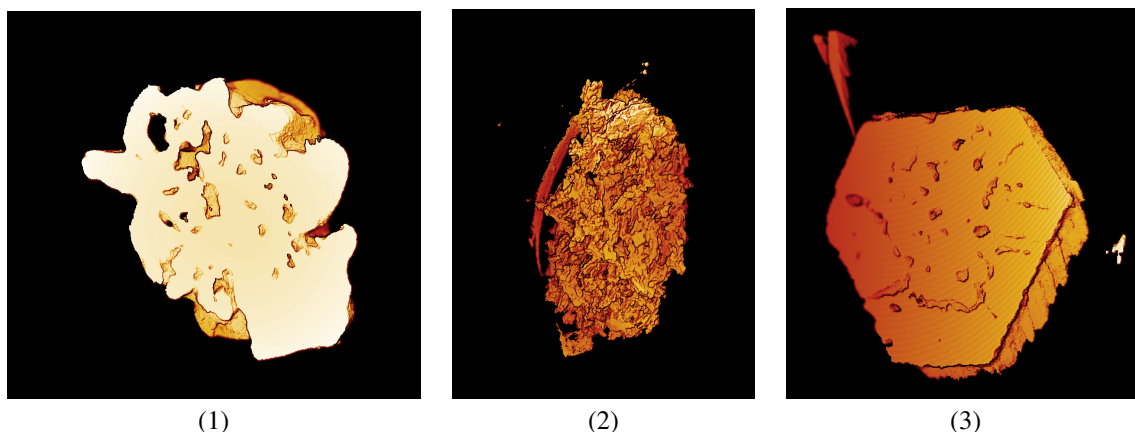


Figure 7: 3D reconstructions of the segmentation map of zeolites (1) (2) and γ -alumina (3). The volume (1) is cut to render the inner structure of the volume. 6% of one slice has been taken to train the model used for each volume.

labeled and unlabeled data. Specifically, we combine a contrastive path for labeled voxels and a self-supervised path for unlabeled ones. This strategy tends to maximize the possible use of all the information available from the data. As the model can be built on any 2D segmentation DL model, more modern architecture such as DeepLabV3+ (Chen et al., 2018b) or UNet++ (Zhou et al., 2018) can be investigated for future work. We have illustrated our strategy on electron tomography volume of material, but it is not limited to this type of data and acquisition, and could be used in other fields as well, such as medical applications.

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