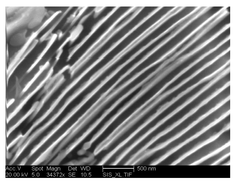
Towards better microstructure representations using deep learning

Avadhut Sardeshmukh, Sreedhar Reddy, BP Gautham (TRDDC, TCS Research, Pune, India)
Pushpak Bhattacharyya (Department of Computer Science and Engineering, IIT Bombay, Mumbai, India)

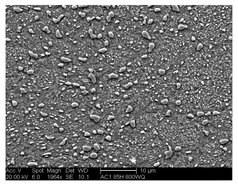
- Process-Structure-Property correlations are central to ICME
- Linking through the space of structures requires good representations of structure
- Need to extract all (and only) the important information from microstructure images
- For example, Ultra-High Carbon Steel[1] microstructures

Pearlite



Features of interest : Lamellar spacing, orientation and so on

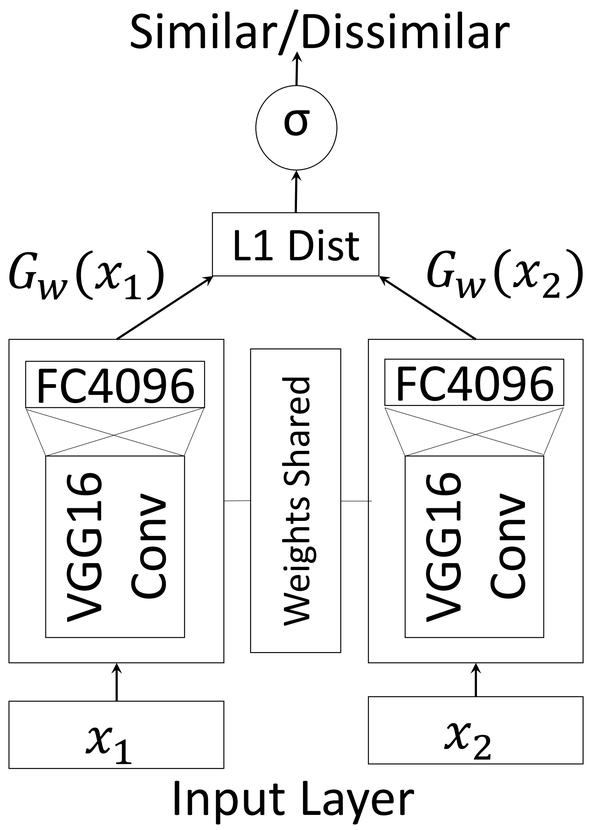
Spheroidite



Features of interest : Grain shape and size distribution, volume fractions and so on

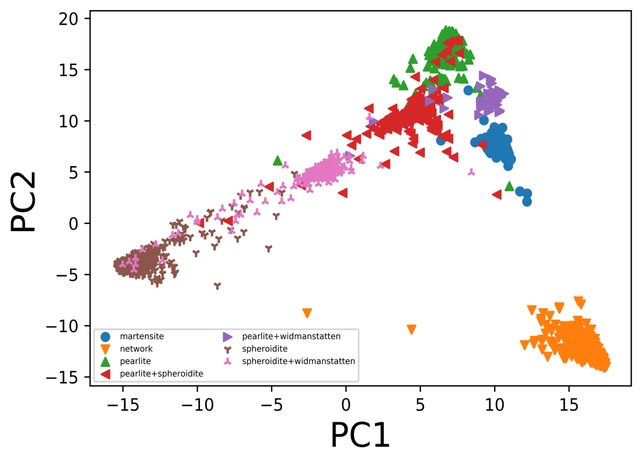
- A major challenge in leveraging deep learning – data sparsity

Reduce data requirement using
- Better learning architectures, hand-crafted for the task at hand; use of transfer learning
- Novel objective functions in neural network optimization



Siamese architecture
- Pair of identical neural networks sharing weights, trained on pairs of inputs
- Trained to minimize distance between similar inputs and maximize distance between dissimilar inputs
- Rather than trying to learn each class, learns the *differences* between classes
- Effective utilization of all available data

- Semantically clustered representation space
- In 2D (using PCA),PC1 seems to correspond to morphology (spherical to needle-like)
- PC2 seems to characterize isotropy, structures with higher values more likely to be anisotropic



- Such a representation could be useful for other downstream tasks such as property prediction
- Indeed, for classification as per processing conditions, better performance than state-of-the-art

Method	3-Phase	7-Phase	Processing Condition
DeCost et al. [1]	96.6	-	88.7
Siamese	98.16	87.5	91.11

[1] Created by DeCost et al.[1], available at https://hdl.handle.net/11256/940 under CC-SA-US3.0 license

[1] B. L. DeCost, M. D. Hecht, T. Francis, B. A. Webler, Y. N. Picard and E. A. Holm: UHCSDB: UltraHigh Carbon Steel Micrograph DataBase. *Integrating Materials and Manufacturing Innovation,* **6**, 197–205 (2017).

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