Ben-Gurion University of the Negev Blaustein Institutes for Desert Research The Swiss Institute for Dryland Environmental and Energy Research Alexandre Yersin Department of Solar Energy and Environmental Physics

## <u>Title:</u>

## Mapping Structural Heterogeneity at the Nanoscale with Scanning Nano-structure Electron Microscopy (SNEM)



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> Zoom Meeting link: https://us02web.zoom.us/j/83451185771

## Abstract:

In recent years, Electron Diffraction, and especially the 4D-STEM [1] is growingly becoming a routine part of structural characterizations of materials at the nano-scale. Its un-matched spatial resolution (down to sub-nm) enables the exploration of local variations within a sample, which alternatively is averaged over the entire irradiated samples area, when explored, for example, by x-rays. As often shown in electron-microscope, samples are often heterogeneous, and consequently, their local properties, which then reflect on the average behavior of the material, composite, or device. In this study, we explore how far we can take electron diffraction when the interest is in the evolution of materials.

We challenge ourselves with mapping the local structure in a composite of crystalline Ni and amorphous Zr-Cu-Ni-Al Bulk Metallic Glass (BMG) fused into a composite via hot-rolling [2]. We use scanning precession electron diffraction to captured 4D-STEM data with 3 nm step size from a FIB-fabricated Ni/BMG/Ni laminate. Using an automated data reduction and analysis pipelines, (including: distortion correction, auto-masking, azimuthal-integration, Fourier-transformation, least-square function fitting, and Non-Negative-Matrix factorization) we get structurally meaningful features, which we generalize as Quantities of Interest (QoI). Using both the 2D diffraction patterns and the reduced 1D-electron Pair Distribution Functions (ePDFs), we generalize the concept of mapping structurally-significant QoI's derived from a spatially-correlated diffraction pattern as scanning nano-structure electron microscopy (SNEM).

Date & Location:Tuesday, October 19, 2021, 16:00Zoom meeting: <a href="https://us02web.zoom.us/j/83451185771">https://us02web.zoom.us/j/83451185771</a>

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We find clear variations in structural features across the Ni/BMG interface, as well as within the BGM itself, which indicate the presence of nano-crystalline inclusions with higher structural correlation length, and evidence for variations in the degree of clustering of alike atoms (e.g., Zr-Zr) in the BMG, which indicate a varying short-range chemical order. We could also extract the distribution of atomic pairs, exposed the BMG/Ni inter-diffusion front, and estimate the effective local structure in different regions of the sample. Augmenting these results with atomic composition EELS maps correlations we found that correlations with local composition do exist, such as the fact that nano-crystalline inclusions within the BMG are located in Cu-deficient regions, but may diverge from structural correlations in different regions of the sample with identical stoichiometry.

These results are an example of the richness SNEM can provide, and with the assistance of automated (and in the future - autonomated) pipelines, bring us closer to exposing (and potentially controlling) the history of heterogeneity in evolving systems.

- Xiaoke Mu, Andrey Mazilkin, Christian Sprau, Alexander Colsmann, Christian Kübel, (2019). Microscopy. 3554, 301
- [2] Sina Shahrezaei, Douglas C. Hofmann, Suveen N. Mathaudhu (2019). JOM. 71, 2

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