VIDEO ARTICLE
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Structure – Dynamics – Property Relationships in Hierarchical Nanoscale and Disordered Materials

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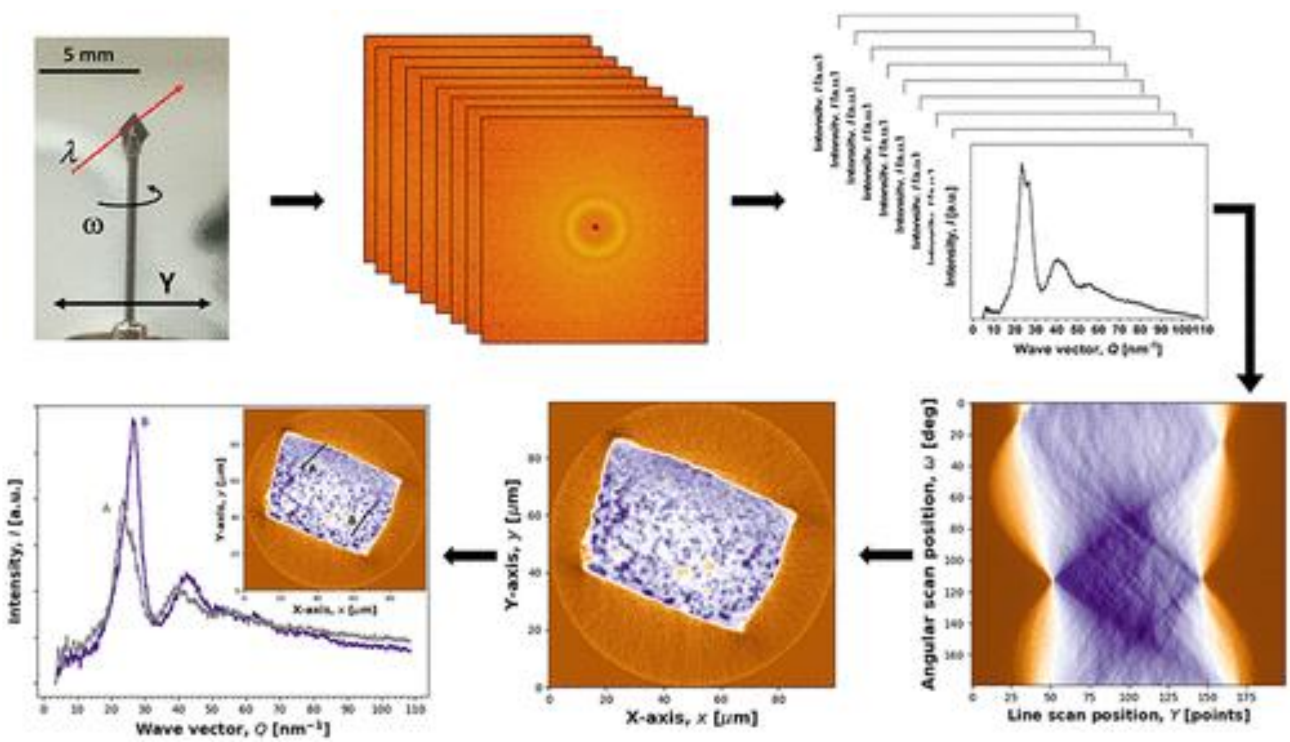
Graphical Abstract



Abstract

Metallic materials with tailored properties are crucially important for a variety of structural and functional applications. There is a strong need not only for successful development of new high-performance alloys but also for elaborating suitable processing routes and characterization techniques enabling phase and microstructure selection and control, necessary for optimization of the related physical and mechanical properties. This talk explores the structural diversity and characteristic structure features of nanostructured and disordered systems elucidating the role of modern characterization techniques including synchrotron radiation, electron microscopy and ultrafast scanning calorimetry for unravelling detailed structure-property correlations.

The structure of matter at the nanoscale, in particular that of amorphous metallic alloys, is of vital importance for functionalization. With the availability of synchrotron radiation, it is now possible to visualize the internal features of metallic samples without physically destroying them. Methods based on computed tomography have recently been employed to explore the local features. Tomographic reconstruction, while it is relatively uncomplicated for crystalline materials, may generate undesired artefacts when applied to featureless amorphous or nanostructured metallic alloys. However, X-ray diffraction computed nanotomography can provide accurate details of the internal structure of a metallic glass. The power of this method will be demonstrated by applying it to hierarchically phase-separated amorphous material with a small volume fraction of crystalline inclusions, focusing the X-ray beam to 500 nm and ensuring a submicrometer 2D resolution via the number of scans.

In general, metallic glasses as characteristic disordered solids are materials with outstanding strength and elastic properties that make them tantalizing for engineering applications. Yet the poor understanding of how their amorphous atomic arrangements control their broader mechanical properties (hardness, wear, fracture, etc.) impedes the ability to apply materials science principles in their design. Hence, uncovering the hierarchical structure that exists in metallic glasses across the nano- to microscale is of utmost importance. Nanobeam electron diffraction experiments reveal that the local hardness of microscale domains decreases with increasing size and volume fraction of atomic clusters with higher local medium range order (MRO). This allows to propose a model of ductile phase softening that will enable the future design of metallic glasses with optimized properties by tuning the MRO size and distribution in the nanostructure.

Finally, the atomistic mechanisms governing aging and rejuvenation in glasses are still unclear. In-situ X-ray diffraction allows to investigate the structural rearrangements during annealing from 77 K up to crystallization in Cu-Zr-Al-Hf-Co bulk metallic glass, rejuvenated by high pressure torsion at cryogenic and room temperature. The configurational entropy calculated from X-ray pair correlation functions gives a structural footprint of deformation-induced rejuvenation. With synchrotron radiation, temperature and time resolutions comparable to calorimetry are possible, allowing to correlate changes in atomic configuration to calorimetric signals and to attribute those to changes of dynamic and vibrational α-, β- and γ-relaxations. The results suggest that the structural footprint of the β-transition is related to entropic relaxation with first-order characteristics. Dynamic mechanical analysis reveals that non-reversible structural rearrangements are preferentially activated throughout the β-transition. The low-temperature γ-transition mostly triggers reversible deformations with a change of slope in the entropic footprint suggesting second-order characteristics.

Altogether, these examples show how modern structure characterization techniques allow deep insights into the atomic structure and the underlying mechanisms determining physical and mechanical properties, thus providing guidelines for optimized alloy design and tailoring of properties.

Keywords: X-ray diffraction, computed nanotomography, nanobeam electron diffaction, nanostructured and disordered systems, hierarchical structures, structure-property correlations.

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Biography of Presenting Author

Jürgen Eckert is Director of the Erich Schmid Institute (ESI) of Materials Science of the Austrian Academy of Sciences and Chair Professor of Materials Physics at Montanuniversität Leoben, Austria. His main research interests are materials physics, metastable materials as well as design and synthesis of advanced high performance nanostructured and disordered materials for structural and functional applications. He is co-author of more than 1250 scientific papers and holds 24 patents in the areas of materials science and processing technology. He serves on the editorial board of several journals in the area of materials physics, including International Journal of Materials Research, Powder Metallurgy, Metals, Material Design & Processing Communications, Materials Today Advances, SN Applied Sciences, Nanomaterials, etc. He received several honors and awards such as the Gottfried Wilhelm Leibniz Award of the German Research Foundation, an ERC-Advanced Grant and a Proof-of-Concept Grant of the European Research Council, the ISMANAM Senior Scientist Award, the Hsun Lee Lecture Award of the Chinese Academy of Sciences, the DGM Georg-Sachs-Prize, the THERMEC 2021 Distinguished Award and the IAAM Advanced Materials Award etc. He is a Member of the Austrian Academy of Sciences, Fellow of the Materials Research Society (MRS), Honorary Member of the Indian Institute of Metals, Member of the Saxon Academy of Sciences and Humanities at Leipzig, Germany, Foreign Fellow of the Indian National Academy of Engineering, and elected IAAM Fellow.

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