Materials Theory

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Characterization of dislocation ensembles: measures and complexity

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When dislocations were first proposed at the beginning of the twentieth century to explain basic facts in metallurgy (Orowan 1934; Taylor 1934), the primary hypothesis was that they behave similarly to point particles, forming a liquid at larger scales in analogy to other excitations identified in physics (Anderson 1972). However, as characterization techniques improved, it became clear that dislocations do not obey the physics of point-like particles, but rather behave like the twigs of a bird's nest (Cottrell 1953). They bend and exhibit long-range interactions leading to complex topologies as their density increases with increasing deformation. While dislocation density has long been used as an internal variable governing important aspects of mechanical behavior, it has been recently understood that the complete characterization of dislocations in a material requires more specific tools and measures. Developing and exploiting such measures can be instrumental towards fostering further advances in metallurgy and materials science, especially in regimes where materials are required to withstand extreme conditions.

Among other crystal defects, the dominant role of dislocations emerges in crystals under mechanical loads. Their loop topology and capacity for multiplication lead to immense defect configurational complexity, typically manifesting in patterning at finite strains, and control key mechanical properties such as yield strength, work hardening, ductile fracture toughness, high-stress creep rate, and resistance to fatigue crack initiation. The characterization of the dislocation ensembles' complexity has long been under development, with a common tool being Nye's dislocation density tensor (Nye 1953) and its spatial correlations. However, upon zooming into a dislocation network it becomes clear that there is additional complexity which goes beyond the average behavior and global correlations embedded in these classical density metrics. Such multiscale complexity manifests itself through features ranging from the scale of individual dislocations, which may develop complex and jerky line shapes, over the local topology of the dislocation network configuration, to the overall evolution of the network's emerging patterns with increasing deformation.

The advances presented in this Special collection explore all aspects of the emerging features in dislocation complexity. As far as single dislocations are concerned, Bertin and colleagues achieved a practical advance where dislocations and their slip trajectories can

be dynamically visualized in simulations as atomic positions change with time. Péterffy and colleagues demonstrated that single dislocations in the important material class of solid solutions, which includes steels and high entropy alloys, display irregular and jerky line shapes from the nanoscale up to a quite large spatial correlation length (> 100 nm) that actually diverges when stress pushes dislocations towards yield. As dislocations form complex networks, interactions within the network lead to correlations, as well as dislocation junctions that locally re-structure the network topology. On the former aspect, Hochrainer and colleagues present how dislocation correlations require notions and show characteristics which are unprecedented in systems of point particles, while Anderson and El-Azab developed a new way of coarse-graining dislocation networks to account more efficiently for mutual dislocation interactions. On the latter, Akhondzadeh and colleagues demonstrated how topological changes in binary junctions drive significant dislocation multiplication on inactive slip systems, while producing a network topology that is more complex than previous theories suggest. At higher length scales, dislocation networks often exhibit a patterned, cellular morphology which is known to strongly influence mechanical properties (Xia and El-Azab 2015; Zaiser 2006). On this aspect, Wu and Zaiser achieved a further step in the path of coarse-graining and modeling the formation and evolution of dislocation cells. Finally, it is clear that the complexity and variety of dislocation networks requires machine-based tools for classification and understanding of the vast range of possible mechanical responses. On this feature, Salmenjoki and colleagues demonstrated that the complexity encoded in dislocation networks can be captured through machine learning in the case of a transition that takes place in materials with increasing amounts of precipitates.

Beyond steel and other traditional metals, these works represent a contribution within a wider effort to advance materials by design and to identify novel material classes and chemical compositions that display improved properties and manufacturability. A systematic path to these advances requires proper classification measures as a fundamental prerequisite for the design of microstructures that achieve superior mechanical responses. The results presented in this Special collection will certainly contribute positively in this direction.

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Authors' contributions
The author(s) read and approved the final manuscript.

Competing interests
The authors declare that they have no competing interests.

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