ABSTRACT

Non-Fickian Transport in defected Grain Boundaries: Evidence for Fractional Diffusion

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Traditional models of grain boundary (GB) diffusion rely on classical random walk assumptions and Fick's laws, treating transport as local and Gaussian. However, growing experimental evidence shows that this framework breaks down in structurally heterogeneous or defect-rich GBs. In such environments, diffusion becomes anomalous, characterized by non-locality, long-range correlations, and deviations from classical scaling.

This behavior can be effectively described using space-fractional diffusion equations, where atomic displacements follow heavy-tailed distributions rather than normal ones. Rooted in continuous-time random walks and fractional kinetics [1], this framework offers a more accurate description of transport through GBs containing disconnections or percolative transport pathways.

We illustrate this approach with two case studies. In the first, Divinski et al. [2] reported a percolating network of ultrafast transport channels, represented by non-equilibrium GBs, in severely deformed nanocrystalline metals, incompatible with classical diffusion theory. In the second, Sevlikar et al. [3] experimentally validated a fractional diffusion model for Cr diffusion along asymmetrical facet in Ni $\Sigma 11(1\bar{1}3)[110]$ bicrystals under C-type conditions, where GB defects and disconnections produce non-Fickian kinetics.

These findings demonstrate that fractional diffusion is not only a rigorous mathematical tool, but a physically grounded and experimentally supported model for GB transport, at least for defect-rich interfaces. We suggest that such anomalous diffusion behavior may be widespread, and that fractional calculus provides a robust framework for understanding GB-mediated processes in complex materials.

References:

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S. V. (2024). Grain boundary diffusion and segregation of Cr in Ni $\Sigma 11(1\bar{1}3)[110]$ bicrystals: Decoding the role of grain boundary defects. Acta Materialia, 278, 120229.