Contribution ID: **90** Type: **3. Oral presentation**

Atomistic Stress Analysis during Nanoparticle Sintering: Molecular Dynamics Insights Beyond Continuum TheoryAtomistic Stress Analysis during Nanoparticle Sintering: Molecular Dynamics Insights Beyond Continuum Theory

Stress development at particle contacts during sintering plays a critical role in microstructural evolution and mechanical performance. While molecular dynamics (MD) simulations have been widely used to elucidate atomistic sintering mechanisms such as surface and grain-boundary diffusion, stress analysis has largely relied on classical continuum theories, which describe densification using an effective normal sintering stress acting only at the neck region. In this work, MD simulations combined with an ultrafast quenching–long-time averaging (UQ-LTA) approach are employed to resolve the full stress tensor during nanoparticle sintering. By removing thermal fluctuations through ultrafast quenching followed by long-time stress averaging at cryogenic temperature, UQ-LTA enables extraction of mechanically meaningful stress fields both within and beyond the neck region, including non-hydrostatic components not resolved in continuum descriptions. Geometrically constrained models with fixed grain boundaries are used to examine how grain-boundary mismatch and dislocation activity influence stress localization. The MD-resolved stress fields are compared with classical continuum descriptions, revealing both similarities and fundamental differences in stress evolution. The proposed MD–UQ-LTA framework is general, with silver nanoparticles used as a representative example. This study provides atomistic insight into stress-driven phenomena that are inaccessible to conventional theories.

Professional Status of the Speaker

Doctoral or Master Student

Interest in submitting a paper in a special issue of

Journal of the European Ceramic Society (Elsevier)

Invitation letter for visa

Yes

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Session Classification: Modelling and simulation of sintering at multiple scales

Track Classification: Group 1: Modelling and simulation of sintering at multiple scales