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K. Chockalingam, V.G. Kouznetsova, O. van der Sluis, M.G.D. Geers

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2D Phase field modeling of sintering of silver nanoparticles

K. Chockalingam[a], V. G. Kouznetsova[a,*], O. van der Sluis[a,b], M.G.D. Geers[a]

[a]*Department of Mechanical Engineering, Eindhoven University of Technology, 5612 AZ, Eindhoven, The Netherlands*
[b]*Philips Research Laboratories, High Tech Campus 34, 5656 AE Eindhoven, The Netherlands*

Abstract

The sintering mechanism of silver nanoparticles is modelled by incorporating surface, volume and grain boundary diffusion in a phase field model. A direction-dependent tensorial mobility formulation is adopted, capturing the fact that diffusion mainly occurs along the directions tangential to the surface of the particle. A finite element framework is applied to solve the governing equations in a fully coupled implicit manner, and the developed framework is demonstrated for particle sintering of equal and unequal sizes as well as at different temperatures. The obtained results are compared with experimental observations, whereby it is shown that the developed material model adequately describes the sintering mechanism of silver nanoparticles.

Keywords: sintering, Cahn-Hilliard, Allen-Cahn, phase field, silver particles, finite elements, tensorial mobility

Dedicated to Professor Christian Miehe on the occasion of his 60th birthday

As one of the leading scientists in the world in computational mechanics, professor Christian Miehe greatly influenced our work. Many of his contributions to the field are groundbreaking, and of great interest for the entire community. Professor Miehe always showed great interest for multi-scale models, micromechanics and advanced computational approaches for damage and fracture. Among these, he pioneered phase field approaches to fracture. Phase field approaches are intrinsically made to deal with problems characterized by non-convexity or to regularize ill-posed problems. Our contribution focuses on the sintering process, which lends itself excellently to phase field modelling. Moreover, sintering defines the microstructural defects and is therefore determinant for the damage and fracture

*Corresponding author
Email address: v.kouznetsova@tue.nl (V. G. Kouznetsova)