INL/MIS-19-54969-Revision-0

Modeling Sintering Processes of Nanoparticle Inks

Austin Robert Biaggne, Michael D McMurtrey, Joseph Louis Bass, Larry K Aagesen Jr

August 2019

The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

INL/MIS-19-54969-Revision-0

Modeling Sintering Processes of Nanoparticle Inks

Austin Robert Biaggne, Michael D McMurtrey, Joseph Louis Bass, Larry K Aagesen Jr

August 2019

Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy

Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

In-Pile Instrumentation Program: Advanced Manufacturing

Modeling Sintering Processes of Nanoparticle Inks

Austin Biaggne[1,2], Michael McMurtrey[2], Joseph Bass[2], Larry Aagesen[2]

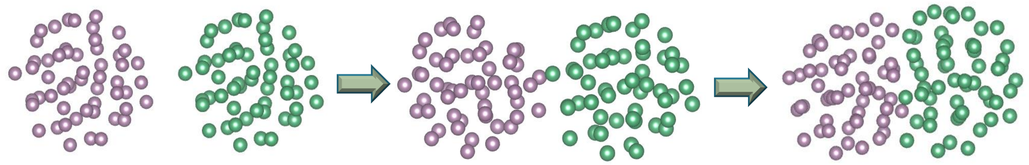
[1]Boise State University [2]Idaho National Laboratory

Objective: Determine optimal processing parameters for sintering and substrate adhesion of printed sensors.

Background / Significance

The In-Pile Instrumentation program conducts research needed to develop and deploy unique instruments to characterize the behavior of fuels and materials during experiments inside of nuclear test reactors. Work is being performed to explore advanced manufacturing techniques to create novel sensor designs that would not be possible with traditional methods. One such technique is direct ink writing, a form of material jetting that puts down inks made up of a liquid carrier and nanoparticles. The particles must be sintered in such a way so that they result in continuous lines or films, not discrete nanoparticles. Adhesion to the substrate is also important so that the sensors are robust and don't fail mid-test in a reactor.

Previous work on sintering mechanisms has been done using atomistic scale modeling (shown below for Mo and Nb nanoparticles with 1 nm diameters). It was found that, while necking and diffusion occur within the structures, the scale is too small to analyze sufficiently. Due to the small scale of the atomistic models, phase field was viewed as a more favorable option as it can be scaled up significantly to include larger nanoparticles and a substrate.



Methods

The phase field sintering model was built on an existing model implemented in the MOOSE framework which utilizes a grand-potential functional that considers an Allen-Cahn equation and generalized diffusion. Chemical potential is the "evolved" variable.

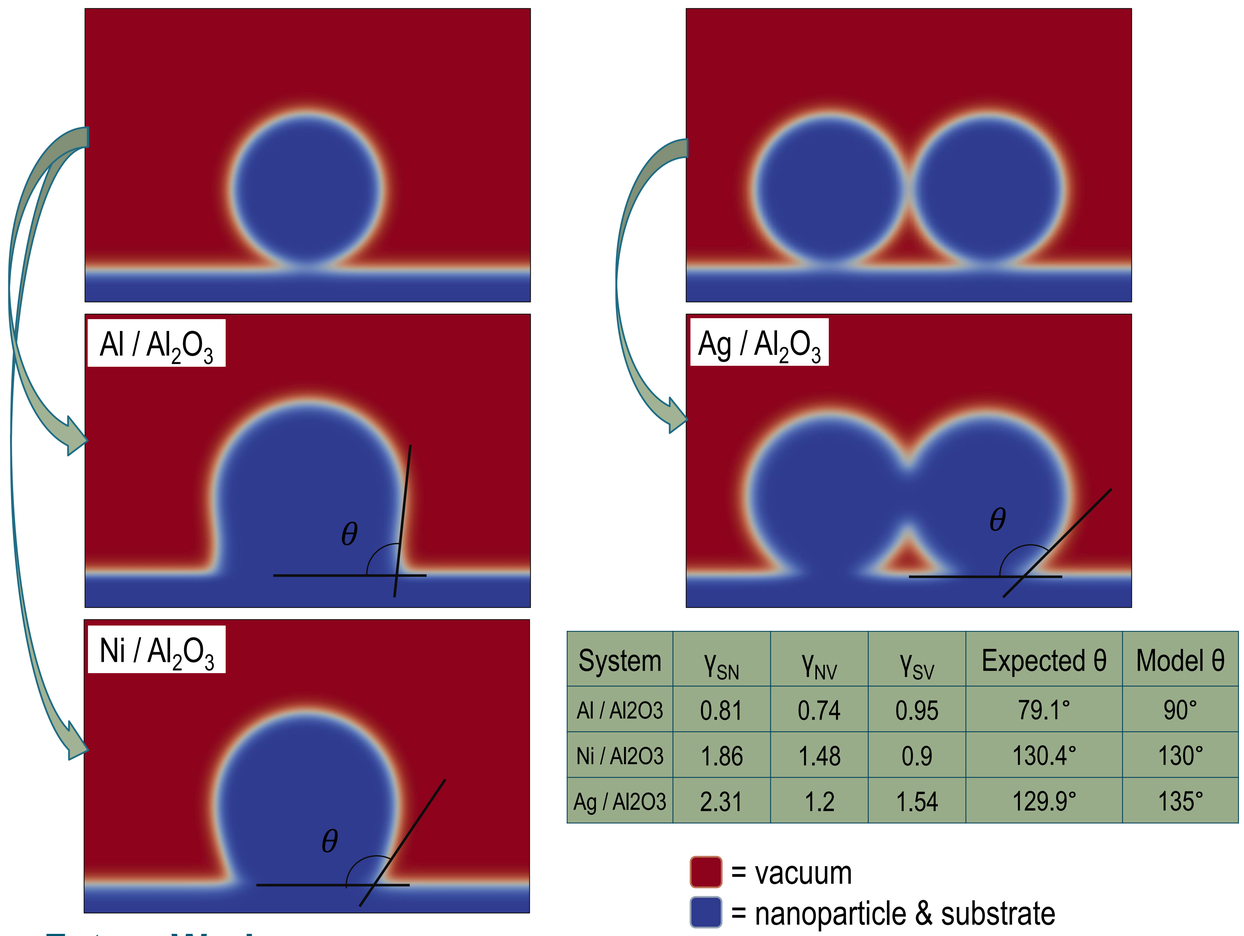
The contact angle, a way to quantify adhesion of wetted nanoparticles on a substrate, was calculated from surface energies using the equation:

$$\theta = \cos^{-1}\left(\frac{\gamma_{SV} - \gamma_{SN}}{\gamma_{NV}}\right)$$

S = substrate
N = nanoparticle
V = vacuum

Results

Results shown for sintering of one and two nanoparticles on a substrate. Nanoparticles are 20 nm in diameter. Surface energies taken from theoretical studies.



System	γ_{SN}	γ_{NV}	γ_{SV}	Expected θ	Model θ
Al / Al2O3	0.81	0.74	0.95	79.1°	90°
Ni / Al2O3	1.86	1.48	0.9	130.4°	130°
Ag / Al2O3	2.31	1.2	1.54	129.9°	135°

Future Work

- Continue to refine current phase field model via parameterization
- Include multiple nanoparticle materials
- Validate with experimental results