

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Sintering Behavior of Metallic Nanoparticles¹

MARTIN FENDRICH, RALF MEYER, RUSLAN ZINETULLIN, DIETRICH E. WOLF, PETER ENTEL, Theoretical Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — Novel technological applications call increasingly for the controlled production of nanoparticles with well-defined physical properties. An important subject in this field is the sintering of agglomerated particles. We employ two different computer-simulation techniques to simulate the sintering of metallic nanoparticles. Molecular-dynamics simulations are used to study the early stage ($t < \approx 100$ ns) of the sintering of two Ni nanoparticles with a size of about 4 nm. These simulations make it possible to observe important metallurgical details, like the role of (partial) dislocations in the process of the alignment of the crystal lattices. The data of the molecular-dynamics simulations are then used to calibrate the time-scale of kinetic Monte-Carlo simulations which can follow the sintering process over a much longer time-scale. A special technique is used in these simulations which makes it possible to take the misaligned crystal lattices into account.

¹Supported by the Deutsche Forschungsgemeinschaft (SFB 445)

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Date submitted: 27 Nov 2007

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