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Mesoscale Thermodynamically motivated Statistical Mechanics based Kinetic Model for Sintering monoliths[1] NISHA MOHAN, Los Alamos National Laboratory — Modeling the evolution of microstructure during sintering is a persistent challenge in ceramics science, although needed as the microstructure impacts properties of an engineered material. Bridging the gap between microscopic and continuum models, kinetic Monte Carlo (kMC) methods provide a stochastic approach towards sintering and microstructure evolution. These kMC models work at the mesoscale, with length and time-scales between thoseof atomistic and continuum approaches. We develop a sintering/compacting model for the two-phase sintering of boron nitride ceramics and allotropes alike. Our formulation includes mechanisms for phase transformation between h-BN and c-BN and takes into account thermodynamics of pressure and temperature on interaction energies and mechanism rates. In addition to replicating the micro-structure evolution observed in experiments, it also captures the phase diagram of Boron Nitride materials. Results have been analyzed in terms of phase diagrams and crystal growth. It also serves with insights to guide the choice of additives and conditions for the sintering process.While detailed time and spatial resolutions are lost in any MC, the progression of stochastic events still captures plausible local energy minima and long-time temporal developments.

[1]DARPA

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