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Modeling a material from packing, through sintering and to the final microstructural properties

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We present a combination of numerical models that can together simulate the initial packing of particles, followed by sintering and finally the resulting microstructural properties. For the latter we here focus on the magnetism of a sintered sample, and the associated coupling between heat and magnetism known as the magnetocaloric effect. We present a 3-dimensional time-dependent numerical model that spatially resolves samples down to the grain size, and includes the demagnetizing field, chemical inhomogeneity realized as a spatial variation of Curie temperature across the sample, local hysteresis and heat transfer. We can thus model how particle size, packing, sintering and chemical inhomogeneity affect the observed properties of magnetocaloric samples. For example, we show that even a modest distribution in Curie temperature (T_C) across the sample results in a significant broadening and lowering of the total entropy change of the sample around T_C. We discuss how clustering of grains with similar values of T_C across the sample influences the results.