

Elimination of an isolated pore: Effect of grain size

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The effect of grain size on the elimination of an isolated pore was investigated both by the Monte Carlo simulations and by a scaling analysis. The Monte Carlo statistical mechanics model for sintering was constructed by mapping microstructures onto domains of vectors of different orientations as grains and domains of vacancies as pores. The most distinctive feature of the simulations is that we allow the vacancies to move. By incorporating the outer surfaces of the sample in the simulations, sintering takes place via vacancy diffusion from the pores to the outer sample surfaces. The simulations were performed in two dimensions. The results showed that the model is capable of displaying various sintering phenomena such as evaporation and condensation, rounding of a sharp corner, pore coalescence, thermal etching, neck formation, grain growth, and growth of large pores. For the elimination of an isolated pore, the most salient result is that the scaling law of the pore elimination time t_p with respect to the pore diameter d_p changes as pore size changes from larger than the grains to smaller than the grains. For example, in sample-size-fixed simulations, $t_p \sim d_p^3$ for $d_p < G$ and $t_p \sim d_p^2$ for $d_p > G$ with the crossover pore diameter d_c increasing linearly with G where G is the average grain diameter. For sample-size-scaled simulations, $t_p \sim d_p^4$ for $d_p < G$ and $t_p \sim d_p^3$ for $d_p > G$. That t_p has different scaling laws in different grain-size regimes is a result of grain boundaries serving as diffusion channels in a fine-grain microstructure such as those considered in the simulations. A scaling analysis is provided to explain the scaling relationships among t_p , d_p , and G obtained in the simulations. The scaling analysis also shows that these scaling relationships are independent of the dimensionality. Thus, the results of the two-dimensional simulations should also apply in three dimensions.

Keywords: Computer simulation; Diffusion; Sintering

Materials:

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