66a Thermal Decomposition Mechanism of Nickel Oxalate in an Aerosol Flow Reactor

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The morphological changes accompanying the thermal decomposition of nickel oxalate dihydrate and nickel oxalate (dried) within an aerosol flow reactor are investigated. Feed precursor particles can be thought of as microcontainers. Reaction takes place within each microcontainer. As the decomposition process begins, nickel primary particles, or grains, are nucleated within the microcontainer and continue to grow. Coalescence of adjacent grains occurs at elevated temperatures. Image analysis of the particle interior confirms that reaction occurs everywhere within the microcontainer, no preferred reaction zones or geometrical advance patterns are observed. Specific surface area increases as the reaction initiates occurs due to grain breakup resulting from increased lattice strains imposed by the vacating gaseous carbon dioxide gas. As the reaction rate slows, grain coalescence results in specific surface area reduction. A model describing the internal morphological changes that occur within the microcontainer during the thermal decomposition process is developed. Surface or grain boundary self-diffusion of nickel are the likely sintering mechanisms. Nickel self-diffusion coefficients can be estimated from the best fit parameters. The self-diffusion coefficient has an Arrhenius relationship with temperature. For surface self-diffusion, the pre-exponential self-diffusion coefficient is $2.3 \times 10^{-16} \pm 2.1 \times 10^{-16}$ m^2/s and the self-diffusion activation energy is $1.1 \times 10^5 \pm 3.9 \times 10^4$ J/mol. For grain boundary self-diffusion, the pre-exponential self-diffusion coefficient is $1.3 \times 10^{-9} \pm 1.2 \times 10^{-9}$ and the self-diffusion activation energy is $1.2 \times 10^5 \pm 6.9 \times 10^4$ J/mol. The reported uncertainties are the 95% joint confidence intervals. Similar values are found when nickel oxalate (dried) is used as the solid precursor.