# Unified Molding and Simulation for Nano-structured Tungsten Carbide

Seong Jin Park[1,a], John L. Johnson[2,b], and Randall M. German[1,c]

[1]Mississippi State University, P.O. Box 5405, Mississippi State, MS 39762, USA
[2]Kennametal Inc., 1600 Technology Way, Latrobe, PA 15650, USA
[a]sjpark@cavs.msstate.edu, [b]JohnL.Johnson@kennametal.com, [c]german@cavs.msstate.edu

**Abstract**

*Nano-structured tungsten carbide compacts with cobalt matrices (WC-Co) offer new opportunities for achieving superior hardness and toughness combinations. A unified modeling and simulation tool has been developed to produce maps of sintering pathways from nanocrystalline WC powder to sintered nano-structured WC-Co compacts. This tool includes (1) die compaction, (2) grain growth, (3) densification, (4) sensitivity analysis, and (5) optimization. All material parameters were obtained by curve fitting based on results with two WC-Co powders. Critical processing parameters are determined based on sensitivity analysis and are optimized to minimize grain size with high density.*

**Keywords : tungsten carbide (WC), densification, grain growth, modeling, and optimization**

## 1. Introduction

Nanoscaled WC grains in a cobalt matrix may enable simultaneous increases in both hardness and toughness [1]; however, appropriate processing techniques to produce such material are generally lacking. In this study, a unified modeling and simulation tool has been developed to produce maps of sintering pathways from nanocrystalline WC powder to sintered nano-structured WC-Co compacts. This tool includes die compaction, grain growth, densification, sensitivity analysis, and optimization.

## 2. Experimental and Results

Die pressing was used as the method of compaction. For developing the die-compaction models, right cylindrical compacts were made from the two powders at compaction pressures ranging from 50 to 600 MPa. One is a standard powder (Powder S, WC-10Co, $D_{50}$ = 480 nm, Kennametal, Inc.), the other one is a nano-crystalline powder (Powder N, WC-12Co-1TiC-3TaC, $D_{50}$ = 188 nm, average crystallite size of 54 nm, Inframet, Inc.) with TiC and TaC as grain growth inhibitors.

All sintering runs were performed using an Anter Laboratories Unitherm[TM] model #1161 vertical tube dilatometer. Three different heating rates were used to obtain master sintering curves (MSCs).

## 3. Modeling, Sensitivity Analysis and Optimization

We elected to use a conventional constitutive model for die compaction proposed by Shima and Oyane based on uniaxial compression tests [2]:

$$F = \left(\frac{q}{\sigma_m}\right)^2 + 6.20(1-\rho)^{1.028}\left(\frac{p}{\sigma_m}\right)^2 - \rho^{\delta} \qquad (1)$$

where $q$ and $p$ are the effective stress and hydrostatic pressure, $\rho$ is the relative density, $\sigma_m$ is the flow stress of the matrix material, and $\delta$ is a material parameter.

The classical model [3] is applied for interface-controlled grain growth:

$$\frac{dG}{dt} = \frac{K_0}{G}\exp\left(-\frac{Q_G}{RT}\right) \qquad (2)$$

where $G$ is the grain size and $K_0$ is the associated preexponential factor.

The master sintering curve (MSC), as defined by Johnson [4], is based on the concept of the work-of-sintering $\Theta_\rho$ [5].

$$\Theta_\rho = \int_0^1 \frac{1}{T}\exp\left(-\frac{Q_\rho}{RT}\right)dt \qquad (3)$$

The activation energy $Q_\rho$ for the sintering system is determined by minimizing the error between the experimental data and the model [5]. It has been shown [6] that a sigmoid function provides a good fit between the relative sintered density and the natural logarithm of $\ln\Theta_\rho$. The sigmoid equation used to define the MSC is

$$\Psi = \frac{\rho - \rho_0}{1 - \rho_0} = \frac{1}{1 + \exp\left[-\dfrac{\ln\Theta_\rho - a}{b}\right]} \qquad (4)$$

where $\Psi$ is the densification parameter, $\rho_o$ is the relative

density at the start of the sintering experiment, and *a* and *b* are constants defining the curve.

## 4. Results and discussion

Fig. 1 shows the consolidation behavior of WC-Co during die compaction. Powder S is much more difficult to press than powder N. From the simulation results, the final density distribution for Powder S is much wider than that for Powder N.

As shown in Fig. 2, the grain growth for Powder S is more sensitive to compaction pressure than powder N because of greater agglomeration of the smaller particles. The crystallite size data do not work for the grain growth model. It is noted that a role of smaller particle is to reduce sintering temperature and/or to activation energy not to directly reduce final grain size.
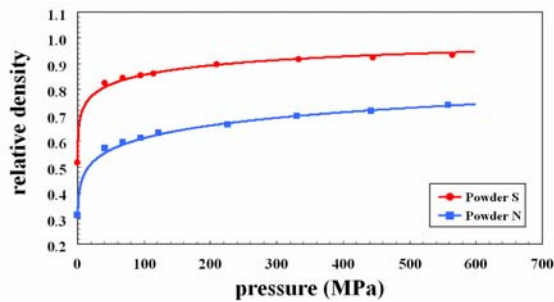


**Fig. 1. Density vs. pressure plot for die compaction. The density is relative to the pycnometer density of the powder/binder mixture.**
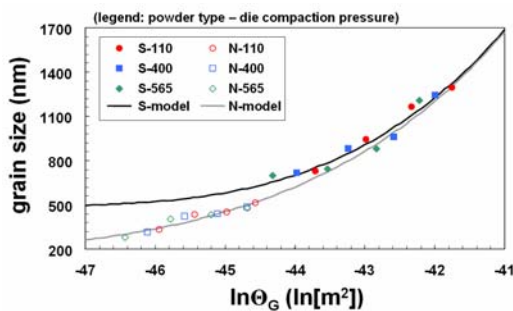


**Fig. 2. Mater sintering curve for grain growth.**

Fig. 3 shows MSC of densification for both powders. Densification in the region of 1100-1310 °C is much more sensitive to temperature than in the region below 1100 °C for Powder N due to the effect of the grain growth inhibitors.

Fig. 4 shows the minimum grain size for a given target density for Powder N. It is noted that Powder S cannot reach a density of > 90 % during solid-state sintering only. From the optimization results, the minimum grain size that

can be achieved at a sintered density of 97 % of theoretical is 332 nm with a compaction pressure of 565 MPa. This value is 1.8 times larger than the initial grain size. Roughly saying, a WC powder with a $D_{50}$ < 50 nm is required in order to obtain nano-structured WC-Co with a sintered grain size of < 100 nm and a density of > 97 % through conventional sintering technology.
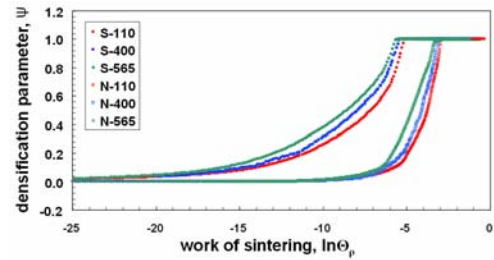

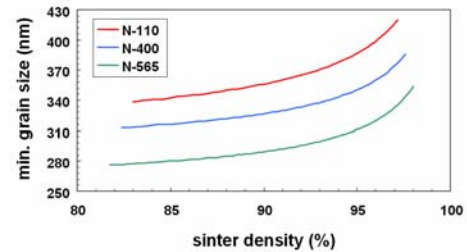
**Fig. 3. Master sintering curve for densification.**



**Fig. 4. Minimum grain size for a given sintered density.**

## 5. Summary

In this study, we developed modeling and simulation tools for assessment and optimization of nano-structured sintered W-Co compacts. A nano-crystalline WC-Co powder with grain growth inhibitors and a crystallite size of 54 nm is unable to maintain a sintered grain size below 200 nm with conventional sintering. The model predicts that a powder with discrete particles < 50 nm is needed.

## 6. References

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