

# Contribution of the Interface Energies to the Growth Process of Cemented Carbides WC-Co

Sabine Lay<sup>1,a</sup>, Jean-Michel Missiaen<sup>2,b</sup>, and Colette H Allibert<sup>3,c</sup>

<sup>1</sup>LTPCM (CNRS/INPG), BP75, 38402 St Martin d'Hères, France <sup>2</sup>LTPCM (CNRS/INPG) BP75, 38402 St Martin d'Hères, France <sup>3</sup>LTPCM (CNRS/INPG), BP75, 38402 St Martin d'Hères, France <sup>a</sup>Sabine.Lay@ltpcm.inpg.fr, <sup>b</sup>Missiaen@ltpcm.inpg.fr, <sup>c</sup>challibert@wanadoo.fr

## Abstract

The driving forces and the probable processes of WC-Co grain growth are reanalysed from recent data of interface energy and microstructure. Grain growth is driven by the disappearing of the high energy WC/WC and WC/Co interfaces with habit planes different from  $\{0001\}$ ,  $\{10\overline{1}0\}$  and  $\{11\overline{2}0\}$  facets and by the area decrease of the WC/WC and WC/Co interfaces with  $\{0001\}$  and  $\{10\overline{1}0\}$  habit planes. Grain growth mainly results of dissolution-precipitation. Abnormal grains are likely formed by defects assisted nucleation.

Keywords : Cemented carbide WC-Co, interface energy anisotropy, abnormal growth

## 1. Introduction

The cemented carbides WC-Co are processed by liquid phase sintering. During the process abnormally large grains develop and the mean WC grain size increases. This growth detrimental for the properties can be limited by inhibitor additions but is difficult to control because the processes of microstructure evolution are complex. Grain growth is driven by the decrease of the total interfacial energy of the WC-Co mixture. It occurs by i) the development of the low energy WC/Co and WC/WC interfaces at the expense of those of high energy ii) the area decrease of the low energy interfaces. The WC hexagonal structure seems simple but the atom positions induce two sets of prismatic  $\{10\overline{1}0\}$ planes (PI, PII) with different distances to the first sublayer. As the basal {0001} B and prismatic planes can be terminated by W or C atoms, six structures are possible for  $\{0001\}$  and  $\{10\overline{1}0\}$  habit planes forming the most frequent WC/Co and WC/WC interfaces [1].  $\{0001\}$ ,  $\{10\overline{1}0\}$  and  $\{11\,\overline{2}\,0\}$  habits can generate grain boundaries with high density of coincidence atom sites due to the close values of the lattice parameters (a=0.2906, c=0.2837nm) [2].



Fig. 1. Atom positions in the WC crystal structure.

Therefore the driving force for grain growth depends on the respective stability of the various types of WC/WC and WC/Co interfaces. The microstructure evolution processes are defined by the relative mobility of the different interfaces. This presentation analyses the probable grain growth processes from recent interfacial and microstructure data.

# 2. Driving forces

The good wetting of WC by Co was well known but the energy range of the main WC/WC and WC/Co interfaces was evaluated only recently by atomistic calculation [3]. Upper and lower bounds were obtained from probable atom configurations of the interfaces. They were calculated for the W or C terminated planes and for the W rich and C rich limits of the field {WC+Co}. The more stable facets are W terminated. The interface energy decreases from PII (2.14-3.02 Jm<sup>-2</sup>) to PI (1.43-1.89 J.m<sup>-2</sup>) and to B (1.07-1.34 Jm<sup>-2</sup>). The stability that increases as PII<PI<B, with differences slightly higher on the C limit, is confirmed by crystal shape measurements [4].

The WC/WC interface energy was evaluated for the grain boundaries the most frequent in the microstructure [3]. The high coincidence  $\Sigma 2 90^{\circ}$  twist  $\{10\bar{1}0\}//\{10\bar{1}0\}$  has the highest stability (0.02 J.m<sup>-2</sup>). Configurations derived from  $\Sigma 2 90^{\circ}$  twist or  $\Sigma 2 90^{\circ}$  tilt  $\{0001\}//\{11\bar{2}0\}$ , representative of general boundaries lead to energies in the range 2.1-2.6 Jm<sup>-2</sup> and 3.8-4.4 Jm<sup>-2</sup> for the lower and upper bounds respectively. Fig. 2 shows that the boundaries derived from  $\Sigma 2$  twist with energy lower than that of the two relevant WC/Co interfaces cannot be infiltrated by Co.  $\Sigma 2$  tilt grain boundaries the energy of which is higher than that of the two related WC/Co interfaces could be infiltrated by Co. Grain boundaries with other habits, are less stable but can be retained in the microstructure by geometry constraints.



# Fig. 2. Energies of the most frequent grain boundaries and of the two corresponding WC/Co interfaces. $\Sigma 2$ twist should not be disintegrated by Co.

Finally the driving forces for grain growth are the energy decrease leading to i) the disappearing of the highest energy WC/WC and WC/Co interfaces and ii) the decrease of the area of the grain boundaries and interfaces with  $\{0001\}$  and  $\{10\overline{1}0\}$  habits that have energies of the same order.

## 3. Possible processes and mechanisms

The abnormal growth of WC-Co, consistent with the interface anisotropy, is well known. However the growth mechanism is not proved by the published models [5] and numerical simulations (for example [6]). In fact two processes are required to produce the area decrease of the interfaces and of the boundaries with {0001} and { $10^{\overline{1}}0$ } habits, for which the driving forces are of the same order.



Fig. 3. TEM micrograph showing the typical features of WC abnormal grain in C rich WC-Co (8 wt%) treated at 1450°C, 2h.

The most probable processes are dissolution-precipitation for the grain coarsening by interface motion and grain boundary migration and for the coalescence of contiguous grains. Two mechanisms of precipitation on faceted crystals are possible: 2D-nucleation or nucleation assisted by defects [5, 7]. Information on the major process and on its most likely mechanism is given by the typical features of the large grains microstructure observed by Transmission Electron Microscopy (TEM) (Fig. 3):

- 1) Dissolution-precipitation is likely the major process: the large grains are bounded by Co interfaces more developed than the boundaries with the small grains in contact.
- 2) Abnormal grains are in contact with small grains and sometimes contain tiny grains. Marks of migration are detected neither for the high energy boundaries with the small grains in contact nor for the low energy  $\Sigma 2$  twist boundaries with the trapped tiny grains.
- 3) Nucleation assisted by defect is the probable mechanism starting abnormal growth. All the large grains contain local defects zones and the dislocation /interface junctions create atom size steps that are preferred nucleation sites.

As the different structures of the WC facets that generate energy anisotropy can also induce mobility anisotropy, the area quantification of the interfaces with the preferred habits should determine if the interface mobility anisotropy contributes to the abnormal WC growth.

## 4. Summary

The WC-Co growth is reanalyzed from published data of interface energy accounting of the interface anisotropy and from recent microstructure results. Driving forces of the same order are found for the development of the WC/WC and WC/Co interfaces with {0001} and { $10\overline{1}0$ } habits. The features of the large grains microstructure lead to propose that growth mainly proceeds by dissolution - precipitation. Nucleation assisted by defects is the probable precipitation mechanism. No mark of migration could be detected for either the high energy or the low energy boundaries.

# 4. References

1. C. S. Kim, G. Rohrer. Interface Sci. special issue on metal/ceramic interfaces, **12**[1] 19(2004).

2. J. Vicens, E. Laurent - Pinson, J. L. Chermant and G. Nouet, J. Physique **49** C5-271(1988).

3. M. Christensen and G. Wahnström, Acta Mater., **52** 2199 (2004).

4. M. Christensen, G. Wahnström, C.H. Allibert and S. Lay, Phys. Rev. Letters, **94** 066105 (2005).

5. Y.J. Park, N.M. Hwang, D.Y. Yoon, Met. Mat. Trans A 27A 2809(1996)

6. J. <u>Kishino</u>, H. <u>Nomura</u>, S.-G. <u>Shin</u>, H. <u>Matsubara</u>, T. <u>Tanase</u>, Int. J. Refractory Met. Hard Mater. **20**[1] 31(2002).

7. S.D. Peteves, R. Abashian Met. Trans 22A 1259(1991).