EXPERIMENTATION AND MODELING OF CHEMICAL INTERACTION OF PCBN AND INCONEL 718

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Abstract: The paper investigates the mechanisms governing the wear of pcBN tool materials when high speed machining superalloy Inconel 718. The approach includes application of diffusion couples that were exposed to high temperature (1250 ºC) and high pressure (2.5 GPa). Two grades of pcBN tool material were selected for the analysis: binderless materials and grade with low cBN content and TiC-based binder. Results indicate that the interaction proceeds with intensive formation of Nb_2N, Mo_2B and NbB_2 for binderless grade and less intensive reaction also including formation of Nb_2C, TiB, and TiN for the grade with TiC binder.

Keywords: pcBN; Inconel 718; chemical wear; diffusion couple

1. INTRODUCTION

Tools from polycrystalline cubic boron nitride (pcBN), which possess high hardness, wear resistance, and thermal conductivity, are widely used in machining hardened steels and superalloys. These positive properties are slightly lower than those for polycrystalline diamond, however chemical inertness to ferrous alloys is substantially higher. Nevertheless the wear mechanism changes from abrasive to chemical for pcBN tooling when applying high cutting speeds which is accompanied by increased cutting temperatures (Huang, *et al.*, 2007).

At the moment no single view exists on the nature of chemical wear of pcBN tool when machining ferrous alloys. For example some studies register the absence of chemical interaction of pcBN with the iron in the cutting process (Narutaki and Yamane, 1979) and consider the oxidation of cubic boron nitride the cause of chemical wear (Katuku, *et al.*, 2010). This view is experimentally supported by the presence of boron oxide among the wear products. On the other hand, chemical interaction of cBN and nickel powders when heating to 1300 ºC was documented in paper (Bondarenko, *et al.*, 1978), and authors of (Barry and Byrne, 2001) also indicate that the chemical interaction with a workpiece material is the major wear mechanism of pcBN tools. Formation of borides, their subsequent eutectic melting with the being machined material and ejection from the cutting zone has been shown in (Klimenko, *et al.*, 1992). Also, the possibility that the intensive friction in the cutting process can reduce the temperature required for the initiation of chemical interaction cannot be ruled out, and therefore the dominant wear mechanism might be the tribochemical one (Zimmerman, *et al.*, 1997).

The relatively simple procedure used to estimate the possibility of chemical interaction via application of diffusion couples is known. The study of diffusion couple iron-pcBN is carried-out under atmospheric pressure in paper (Gimenez, *et al.*, 2007). It is shown that at temperatures above 1300 ºC an interaction occurs, which the authors relate to the dissolution of carbon present in the binder phase of the pcBN and the subsequent formation of cementite.

High pressure and temperature develops in the zone of tool-workpiece contact in the cutting process, which for example when machining superalloy Inconel 718 can reach 2.5 GPa (Stahl, 2012) and 1250 ºC (Shintani, *et al.*, 1992) at cutting speeds above 4 m/sec. Therefore, an experimental study of chemical interaction is carried-out in the current study via the method of diffusion couples under static pressure of 2.5 GPa and temperature of 1250 ºC, and via the actual machining in the cutting speed range of 2-14 m/sec for superalloy Inconel 718 and several of pcBN materials. Thermodynamic modelling of the chemical interaction was implemented for the same parameters.

2. EXPERIMENTAL SETUP

The bulk Inconel 718 used for diffusion couples and for cutting experiments was supplied in solution annealed and aged state (~ 45 HRC) with composition listed in Table 1.

Table 1. Chemical composition of Inconel 718 in wt.% (Siemens AG Materialdata).

Ni	Cr	Fe	Mo	Nb	Ti	Al	Co	Cu	Mn	Si	C	P	S
bal	18.2	17.8	2.92	5.04	1.01	0.32	0.17	0.04	0.06	0.07	0.03	0.008	0.001

When aged, the microstructure of the superalloy comprises of γ FCC Ni-based solid solution strengthened by precipitates and by NbC and TiC carbides. The precipitates are γ'' BCT Ni_3Nb, γ' FCC $Ni_3(Ti,Al)$ and orthorhombic δ Ni_3Nb plate-like phase precipitating at the grain boundaries (see Figure 1).

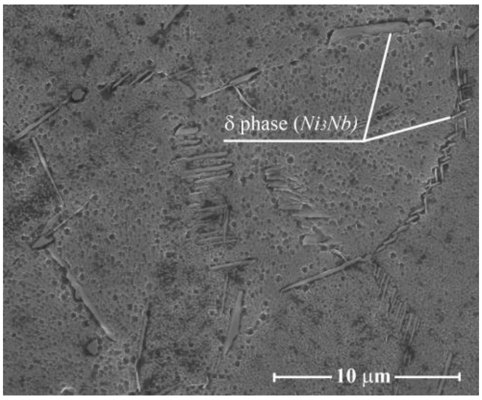

Fig. 1. Microstructure of Inconel 718.

Two grades of PCBN were selected for the diffusion and machining tests. Binderless (bcBN) grade was sintered at the Institute for Superhard Materials (Ukraine) under the pressure of 7.7 GPa and the temperature 2250 ºC. bcBN grade has the cBN grain size of 5-7 µm and 3% stress-inducing inclusions of beta silicon nitride (β-Si_3N_4) (see Figure2.a). Grade with low content of cBN (pcBN-L) was a commercially available product supplied by SECO Tools AB. pcBN-L has the cBN grain size of 0.5-2 µm with ceramic TiC-based binder containing other secondary phases (see Figure 2.b) altogether approx. 50% vol.

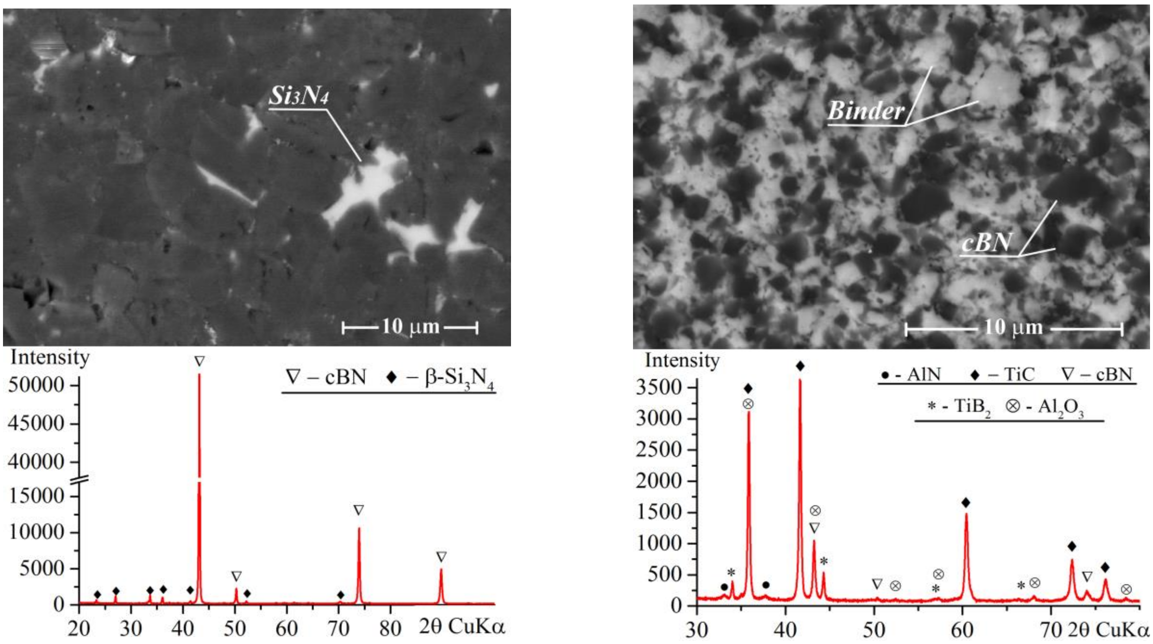

Fig. 2. Microstructure and XRD analysis of (a) binderless pcBN grade and (b) grade with low cBN content.

When preparing the diffusion couples, the round inserts of bcBN and pcBN-L with the diameter of 6.35 mm were placed into the cylindrical capsules machined from the aged Inconel 718, which were then heated to 1250 ºC under the pressure of 2.5 GPa for the duration of 5 minutes. An hBN sleeve was used between the graphite heated and the Inconel 718 capsule. The high pressure apparatus of the toroid type (Khvostantsev, et al., 1977) HPAT-30 was used for the p,T-treatment. The samples were cut in the axial direction with the diamond cut-off wheels upon the release of temperature and pressure and were then polished with diamond and SiO_2 suspensions to a mirror surface finish.

Cutting experiments employed finishing conditions with feed rate and depth of cut being constant: f= 0.1 mm/rev and a_p= 0.2 mm. Cutting speed was selected as a variable. The speeds were changed from conventional to high speed range: v_c=2, 3.5, 5, 6.5, 8, 9.5, 11, 12.5 and 14 m/sec. Round RNGN120300E25 inserts were used in the experiments. All machining was done with use of 8% semi-synthetic coolant supplied at 5 bar and 40 l/min. Electron microscopy was done on *LEO SEM 1560*. Energy dispersive X-Ray (EDX) analysis was performed with *Oxford INCA* at 15 kV. XRD measurements were performed on a STOE Darmstadt diffractometer operated at 40 kV and 40 mA with Cu Kα source.

3. RESULTS

Figure 3 shows the backscatter electron images of the cross sections of the diffusion couples of bcBN-Inconel 718 (Fig. 4.a) and pcBN-L – Inconel 718 (Fig. 4.b) after p,T – treatment at 1250 ºC and 2,5 GPa. In both cases the interface between the two materials has the layer of interaction products with thickness up to 10-15 µm. The grain size of Inconel 718 in this interaction zone is 2-5 µm and is significantly smaller than the grain size of the bulk material (15-20 µm), which provides an evidence to the severe plastic deformation generated when machining the capsules. Precipitation of new phases on the grain boundaries is clearly visible.

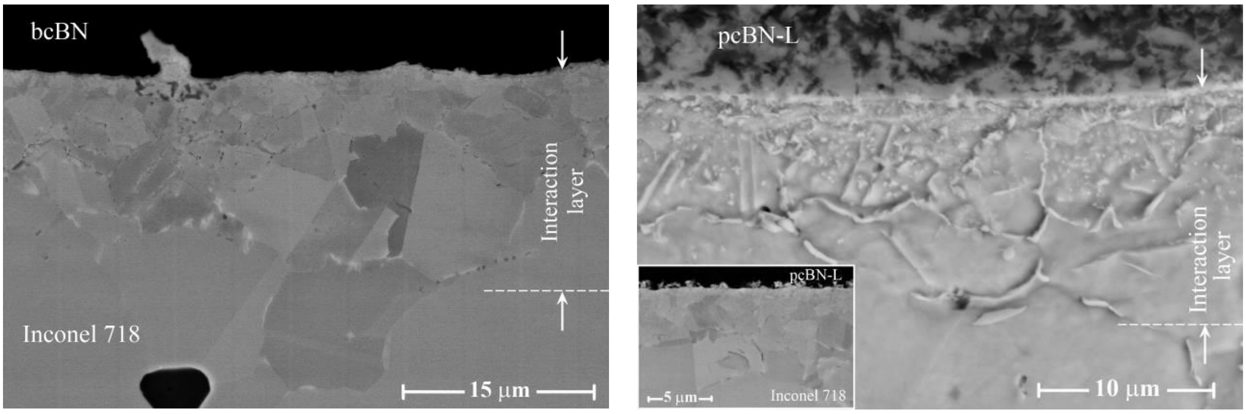

Fig. 3. Backscatter electron images of diffusion couples (a) bcBN – Inconel 718 and (b) pcBN-L – Inconel 718.

Figure 4 shows the results of EDX-mapping of the interaction layer and the adjacent regions. An increased concentration of niobium, molybdenum, boron and nitrogen in the interaction layer is detected on the bcBN – Inconel 718 diffusion couple. In case of pcBN-L – Inconel 718, primarily a sharp increase in the concentration of carbon, and then later niobium, titanium, molybdenum, boron and nitrogen was identified (Fig. 4.b).

Comparison (see Fig. 5) of the phase composition of the bulk Inconel 718 prior and post HP-HT treatment indicates that a dissolution of both Ni_3Nb intermetallic γ’ and γ’’ precipitates in the FCC solid solution takes place. Such dissolution allows interpreting the high concentration of niobium only as the formation of nitrides and borides of Nb, Mo, and Ti in both diffusion couples.

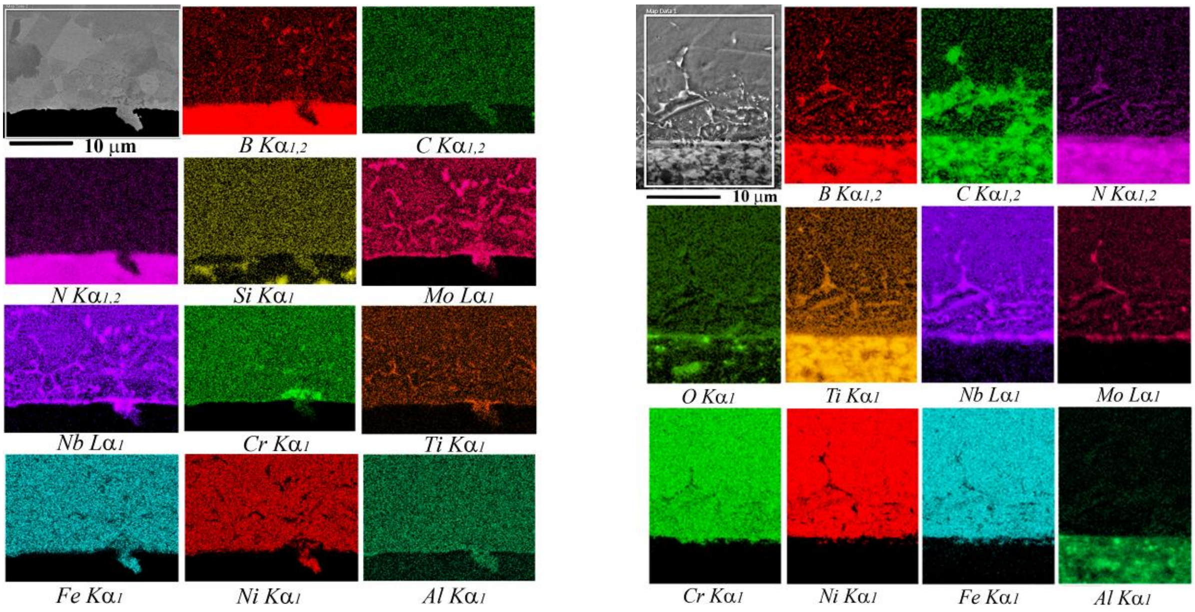

Fig. 4. EDX-mapping of the interaction layer for (a) bcBN – Inconel 718 and (b) pcBN-L – Inconel 718.

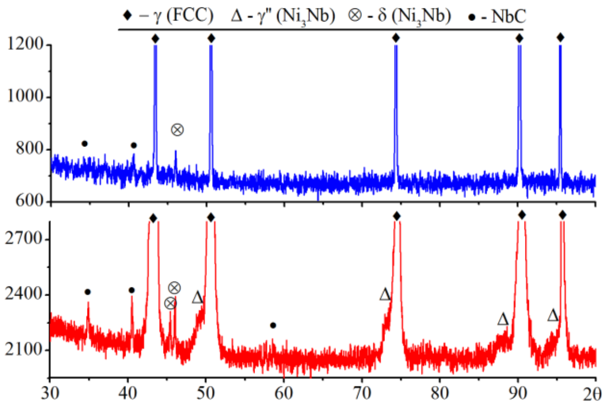

Figure 5. XRD analysis of (a) as received Inconel 718 and (b) of superalloy from the diffusion couple.

As seen on the Figure 6, during the contact interaction of pcBN-L and Inconel 718, a diffusional dissolution of cBN grains takes place and the space between the TiC grains is occupied by the saturated FCC solid solution. The SEM image indicates the relative stability and invariable position of the titanium carbide grains. At the same time, the EDX analysis shows a raise of the carbon content in the interaction layer. It is clear that the source of this carbon, which diffuses into FCC solid solution, is the TiC phase. At the temperature of 1250 ºC, an increase of the amount of vacancies in the carbon sublattice of titanium carbide can reach the composition of $TiC_{0.7}$ (Frisk, 2003).

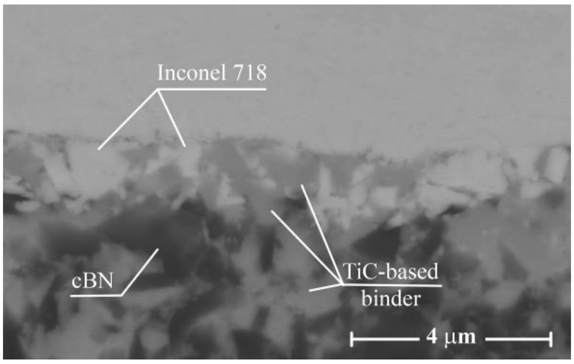

Fig. 6. Dissolution of cBN in the FCC solid solution of Inconel 718.

Tool life was estimated in terms of maximum wear land (VB_{max}) on the tool flank upon the end of tool engagement which was kept on a constant level of L=440 m for all the tests. Analysis of the tool wear is summarized in Figure 7. It can be seen that pcBN-L tools with low cBN content and TiC binder have a significantly lower level of tool wear than bcBN especially in the range of low to moderate cutting speeds. pcBN-L outperforms bcBN grade by more than 4-5 times under cutting speeds below 5 m/sec. Further increase in speed gradually equalizes such stark difference and the wear for both tool grades becomes almost equal above cutting speed 11 m/sec. Typical morphologies of the worn tools are shown on Figure 8. It is seen that bcBN attains significant wear not only on the flank wear land, but also both the crater wear and contact length on the rake face of the tool is bigger than for pcBN-L counterpart.

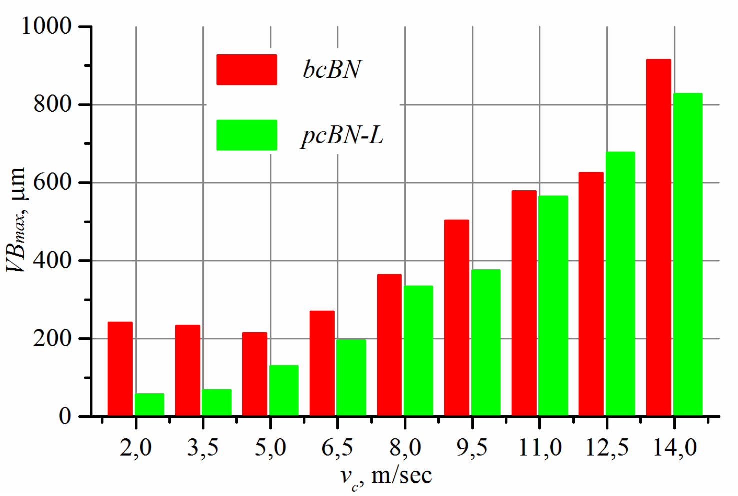

Fig. 7. Tool wear of bcBN and pcBN-L tools when turning Inconel 718.

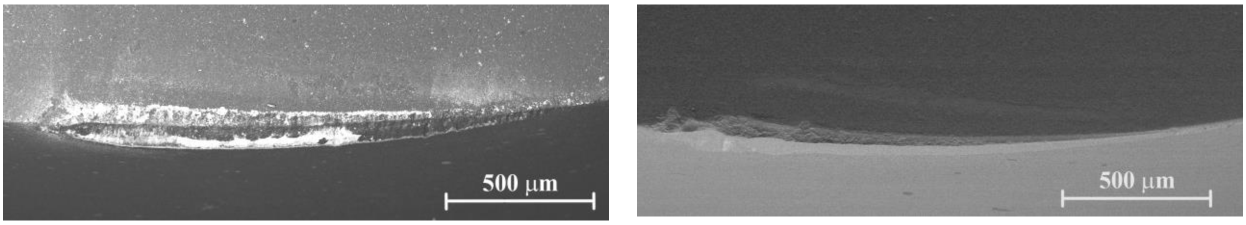

Fig. 8. SEM image of the wear morphology for (a) bcBN and (b) pcBN-L tools (v_c=5 m/sec).

4. THERMODYNAMIC CALCULATIONS

Inconel 718 is a Ni-based alloy with FCC lattice containing 50.0-55.0 wt.% Ni, 17.0-21.0 wt.% Cr, 15-17 wt.% Fe, 4.8-5.5 wt.% Nb, 2.8-3.3 wt.% Mo and Ti, Al, Co, C, Mn, Si, P, S, B, Cu in total not exceeding 3 wt.% (see Table 1). Therefore, in the current study, in the thermodynamic calculations the alloy was considered as the FCC solid solution with the following content 55.0 at.% Ni, 17.4 at.% Fe, 22.4 at.% Cr, 3.2 at% Nb and 2.0 at.% Mo. Earlier publications on Cr-Fe (Andersson and Sundman, 1987), Cr-Ni (Kajihara and Hillert, 1990), Fe-Ni (Servant, *et al.*, 2001), Cr-Fe-Ni (Hillert and Qiu, 1990), Mo-Ni (Frisk, 1990), Nb-Ni (Kajikawa, *et al.*, 2010) were used for description of thermodynamics of these systems. No other literature data for the system Ni-Cr-Fe-Nb-Mo were found available. Therefore the Gibbs free energy of Inconel 718 was described as follows:

$$\begin{aligned} G_{Inco} &= x_{Cr}{}^{o}G_{Cr} + x_{Fe}{}^{o}G_{Fe} + x_{Ni}{}^{o}G_{Ni} + x_{Nb}{}^{o}G_{Nb} + x_{Cr}{}^{o}G_{Mo} + \\ &+ RT\left[x_{Cr}\ln(x_{Cr}) + x_{Fe}\ln(x_{Fe}) + x_{Ni}\ln(x_{Ni}) + x_{Nb}\ln(x_{Nb}) + x_{Mo}\ln(x_{Mo})\right] + \\ &+ x_{Cr}x_{Fe}L_{Cr,Fe} + x_{Cr}x_{Ni}L_{Cr,Ni} + x_{Fe}x_{Ni}L_{Fe,Ni} + x_{Fe}x_{Ni}x_{Cr}L_{Fe,Ni,Cr} + x_{Mo}x_{Ni}L_{Mo,Ni} + x_{Nb}x_{Ni}L_{Nb,Ni} \end{aligned} \quad , \tag{1}$$

The interaction parameters, included in the equation (1) are consolidated in Table 2.

Table 2. Inconel 718 FCC solid solution parameters used in the present work, J/mole.

$$L_{Cr,Fe} = 10833 - 7.477T + 1410(x_{Cr} - x_{Fe})$$

$$L_{Cr,Ni} = 8347 - 12.1038T + (29.895 - 16.3838T)(x_{Cr} - x_{Ni})$$

$$L_{Fe,Ni} = -12054 + 3.274T + (11082 - 4.45T)(x_{Fe} - x_{Ni}) - 725.8(x_{Fe} - x_{Ni})^2$$

$$L_{Fe,Ni,Cr} = 16580 - 9.7835T$$

$$L_{Mo,Ni} = 4803.7 - 5.96T + 10880(x_{Mo} - x_{Ni})$$

$$L_{Nb,Ni} = -128814 - 63.1T + 41652(x_{Nb} - x_{Ni})$$

The rest of the calculations used the information about Gibbs free energy of the substances and their compounds, as the phases of constant content, that are published in the FactSage 6.3 package database (CRCT, 2014). Data on the pressure-temperature potential of cBN were taken from (Solozhenko, *et al.*, 1999). Reactions for the formation of borides and nitrides that are listed below:

BN + 2 Cr = Cr_2N + B (ΔG = 98.5 kJ, T = 1520 K)
BN + 4 Fe = Fe_4N + B (ΔG = 190.1 kJ, T = 1520 K)
BN + 2 Mo = Mo_2N + B (ΔG = 132.6 kJ, T = 1520 K)
BN + Cr = CrB + 0.5 $N_2\uparrow$ (ΔG = 36.5 kJ, T = 1520 K)
BN + 2 Fe = Fe_2B + 0.5 $N_2\uparrow$ (ΔG = 61.2 kJ, T = 1520 K)
BN + 1.333 Ni = 0.333 Ni_4B_3 + 0.5 $N_2\uparrow$ (ΔG = 90.0 kJ, T = 1520 K)

are thermodynamically unfavorable, on the contrary to the following reactions:

BN + 2 Nb = Nb_2N + B (ΔG = -6.5 kJ, T = 1520 K)
BN + 2 Mo = Mo_2B + 0.5 $N_2\uparrow$ (ΔG = -0.1 kJ, T = 1520 K)
BN + 0.5 Nb = 0.5 NbB_2 + 0.5 $N_2\uparrow$ (ΔG = -1.4 kJ, T = 1520 K)

Therefore, nitrides Cr_2N, Fe_4N, Mo_2N and borides CrB, Fe_2B, Ni_4B_3 were not considered as the competitive phases in all subsequent calculations. Formation of Nb_2N, Mo_2B and NbB_2 in the course of interaction between cBN and Inconel 718 leads to the removal of niobium and molybdenum from the FCC solid solution with the corresponding change to its free energy. Free energy of the reaction of binderless cBN with Inconel 718 is calculated as follows:

0.0148 BN + 1 Inconel718 (0.55Ni, 0.174Fe, 0.224Cr, 0.02Mo, 0.032Nb) =
= 0.948 (0.58Ni, 0.184Fe, 0.236Cr) + 0.01 Mo_2B + 0.0024 NbB_2 + 0.0148 Nb_2N (2)

and equals: ΔG = +2.21 kJ/mole.

High pressure increases the free energy of a phase m on $\int_0^p V^m dp$ value. The first approximation of this input can be estimated when excluding the dependence of the volume from the temperature because, for a wide class of substances, compressibility is compensated by the thermal expansion and the volume of a phase at 2.5 GPa and 1520 ºK (1250 ºC) is close to equal to its value under normal conditions. It should be noted that gaseous N_2 is under atmospheric pressure because neither the high pressure cell no the tool/workpiece contact zone are gastight. Values of the molar volume, calculated according to (ICDD, 2014), are used in the current study. Free energy for the reaction (2) at 1520 K and 2.5 GPa equals ΔG = +2.55 kJ/mole, i.e. the energy of niobium and molybdenum losing the bonding with the atoms of nickel, iron, and chromium in the FCC solid solution of Inconel 718 is higher than the energy of formation of the mentioned borides and nitrides. Therefore the chemical interaction between cBN and Inconel 718 is thermodynamically unfavorable.

pcBN-L contains up to 40 vol.% of TiC which will not react with the elements contained in Inconel 718:

TiC + 3 Fe = Fe_3C + Ti (ΔG = 157.3 kJ, T = 1520 K)

$TiC + 3\ Ni = Ni_3C + Ti$ ($\Delta G = 176.0$ kJ, T = 1520 K)
$TiC + 3.833\ Cr = 0.167\ Cr_{23}C_6 + Ti$ ($\Delta G = 87.7$ kJ, T = 1520 K)
$TiC + 2\ Mo = Mo_2C + Ti$ ($\Delta G = 109.8$ kJ, T = 1520 K)

except for niobium

$TiC + 2\ Nb = Nb_2C + Ti$ ($\Delta G = -12.2$ kJ, T = 1520 K)

Free energy for the reaction between pcBN-L and Inconel 718 is given as:

$$0.008\ BN + 0.016\ TiC + 1\ \text{Inconel718}\ (0.55Ni, 0.174Fe, 0.224Cr, 0.02Mo, 0.032Nb) =$$
$$= 0.968\ (0.568Ni, 0.18Fe, 0.231Cr, 0.021Mo) + 0.016\ Nb_2C + 0.008\ TiB + 0.008\ TiN \quad (3)$$

and equals $\Delta G = +0.72$ kJ/mole at atmospheric pressure and $\Delta G = +0.98$ kJ/mole at 2.5 GPa and 1520 ºK, which makes reaction (3) thermodynamically unfavorable. The difference between the experimental and calculation results can be explained if considering the input of the excess energy from the deformed subsurface layer of the capsule which was machined from Inconel 718 for the experiments. According to (M'Saoubi, *et al.*, 2012) the maximum residual stresses on a surface of an Inconel 718 workpiece machined with pcBN and cemented carbide tools equals from $0.8 \cdot 10^6$ to $1.2 \cdot 10^6$ kJ/m^3 dependent on the cutting data and tool wear. Hence, the free energy of the subsurface layer of Inconel 718 capsule amounts to $0.8 \cdot 10^6$ kJ/m^3 * $7.27 \cdot 10^{-6}$ m^3/mole = 5.82 kJ/mole, and thus the value of the Gibbs free energies of equations (2) and (3) will be -0.36 kJ/mole and -1.93 kJ/mole correspondingly.

The obtained results make it possible to explain the experimental fact of significantly higher wear resistance (up to 4-5 times) of tool materials of the pcBN-L group over grades with high cBN content and binderless cBN in particular. The temperature (up to 1250 ºC) and pressure (up to 2.5 GPa) that are often reached when machining at speeds 5-6 m/sec enable the chemical reaction between cBN and Inconel 718, where borides of niobium and molybdenum, as well as niobium nitride are formed. The mechanism of the interaction encountered in the diffusion couples includes the steps of diffusion of boron and nitrogen from cBN into Inconel 718; formation of their solid solutions; saturation and precipitation of these new phases on the grain boundaries of Inconel 718. Presence of titanium carbide in the pcBN-L radically changes the picture of the interaction. TiC reacts with niobium resulting in formation of niobium carbide, whereas titanium reacts with cBN and forms titanium nitride and boride. Inconel 718, being depleted of niobium not so intensively reacts by the equation (2). Additionally, the resultant Nb_2C, TiB, and TiN form a layer that infringes the contact of cBN and Inconel 718, and thus reduces the intensity of the chemical interaction.

4. CONCLUSIONS

The paper addresses the issues of mechanisms of chemical wear encountered when high speed machining superalloy Inconel 718 with pcBN tools. The approach of model experiments involving the use of diffusion couples and the real machining tests was taken. A thorough thermodynamic modelling of the anticipated chemical reactions was also carried out. Both, the experimental and theoretical results show that cubic boron nitride is prone to reactions with niobium and molybdenum of the workpiece and these govern the chemical wear. On the other hand, the use of hard and refractory TiC binder, which can serve as the source of carbon during the interaction, can facilitate the formation of carbides when reacting with Nb, Mo, Cr, etc. Because the reaction of these carbides with cBN is thermodynamically unfavorable, they might act as the passivation layer which blocks or retards the interaction of cBN with the workpiece material. This, in turn, was shown to inhibit chemical wear of pcBN tools during high speed machining, which is accompanied by high temperatures in the cutting zone.

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