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Effect of Diamond Coatings on Thermal Contact Conductance of Tungsten Carbide Substrates

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Because of its excellent thermal and mechanical properties, diamond appears to be one of the most promising materials for meeting the thermal and mechanical requirements of future advanced engineering design. The thermal contact conductance of diamond coatings on tungsten carbide (WC) was experimentally investigated through the use of diamond coatings prepared by the chemical vapor deposition process. Three different coating thicknesses were used to evaluate the existence of an optimum coating thickness over the pressure range from 1000 to 4000 kPa. Experimental results are presented to illustrate graphically the dimensionless overall thermal contact conductance of diamond coatings on a WC substrate as a function of contact pressure. The surface deformation effect of diamond-coated interfaces on the WC substrate was also investigated.

Nomenclature

H' = effective Vickers microhardness, Pa
h_c = coated thermal contact conductance, W/m^2K
k' = effective thermal conductivity, W/mK
P = contact pressure, Pa
s = asperity slope
σ = surface roughness, μm

Introduction

BECAUSE of the individual surface roughnesses and microscopic asperities, when two surfaces are brought together, only a relatively few discrete points are in real contact. Fletcher[1] reported that the actual contact area is between 2 and 5% of the apparent contact area at the interface. Heat can be transferred across the interface by conduction through the actual contacts, conduction through the substance in the gaps around the contacts, and radiation across the gap, or a combination of all three, called overall thermal contact conductance. Because of this significant area reduction, Yovanovich[2] indicated that the thermal resistance occurs at the interface, resulting in a temperature discontinuity.

To increase the thermal and mechanical characteristics of some specific applications, such as minimizing the thermal resistance between subcomponents and substrates of electric packaging, as well as optimizing the tribological applications of cutting tools, surface treatments shall be considered in the interface of contacting materials. Surface treatments such as coatings and vapor-deposited films are permanent in nature and may be suitable for applications involving device coatings and/or sliding contact between two materials. Several researchers have reported on many metallic and nonmetallic coatings on different substrates to investigate the effect of thermal control management on various applications.[3–6] However, the data of thermal contact conductance of diamond coatings/films are limited, and it is necessary to understand the range of potential applications of diamond coatings/films.

A literature review of the thermal conductivity of synthetic single crystal, polycrystalline, and type 1 and type 2 natural diamond was presented by Blanchard et al.[7] The thermal conductivity of synthetic diamond was found to depend on the crystal size at low temperature, in common with all materials. For natural diamond, the thermal conductivity depends primarily on nitrogen impurity concentrations at high temperatures. Touzelbaev and Goodson[8] developed a model for the thermal resistance near diamond–substract interfaces where the best deposition processes continue to yield high concentrations of amorphous inclusions and nanocrystalline material. The thermal resistance of the diamond boundary varies strongly with microstructural parameters, including the nucleation density and the spatial gradient of the grain dimension. Goodson et al.[9] declare that chemical vapor-deposited diamond layers have the potential to improve thermal conduction in electronic microstructures because of their high thermal conductivities. They developed two independent experimental methods, Joule and laser heating measurement techniques, that measure the total thermal resistance for conduction normal to diamond layers thinner than 5 μm on silicon substrates, yielding an upper bound for the thermal resistance of the diamond–silicon boundary.

Based on these literature reviews, diamond coatings not only increase thermal performance, but also resist wear in sliding contact and galvanic corrosion for engineering applications. Although a wide range of diamond coatings' thermophysical and tribological data exist from which engineering applications can be made, it still appears that there is a lack of interfacial thermal conduct conductance information for diamond coatings. In addition to the limited experimental thermal contact conductance data for diamond coatings, there does not appear to be any surface deformation analysis for diamond coatings that has a strong influence on predicting the thermal conduct conductance of the coating interface. Therefore, an experimental study was conducted for diamond film coated on a tungsten carbide (WC) substrate. It is believed that the using of diamond coatings should be able to decrease the interface thermal resistance and to increase the thermal performance of most thermal systems.

Test Specimen Preparation

The uses of diamond as an abrasive and cutting tool material, exploiting its extreme hardness and wear resistance, have been long recognized and constitute the basis of a relatively mature industry. Recent progress in chemical vapor deposition (CVD) synthesis technology has made it possible to manufacture very high-quality polycrystalline diamond components of large dimensions, either as flat plates or three-dimensional shapes such as domes. The ability to manufacture CVD diamond as a reliable and robust engineering material at a viable price is opening the way to the use of this material for numerous technically demanding applications. Diamond offers excellent thermophysical properties that have always made it attractive as coatings. In addition to the high thermal conductivity, Coll

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Table 1 Detailed surface characteristics of test specimens

Specimen	t,[a] μm	R_a,[b] μm	R_q,[c] μm	R_s,[d]	W_t,[e] μm
1	Bare	0.53	0.67	0.158	6.06
2	6	1.32	1.61	0.098	10.12
3	14	1.16	1.95	0.016	16.5
4	31	1.01	1.45	0.037	12.3

[a]Diamond coating thickness.
[b]Arithmetic average roughness.
[c]RMS roughness.
[d]Average asperity slope.
[e]Maximum waviness height.

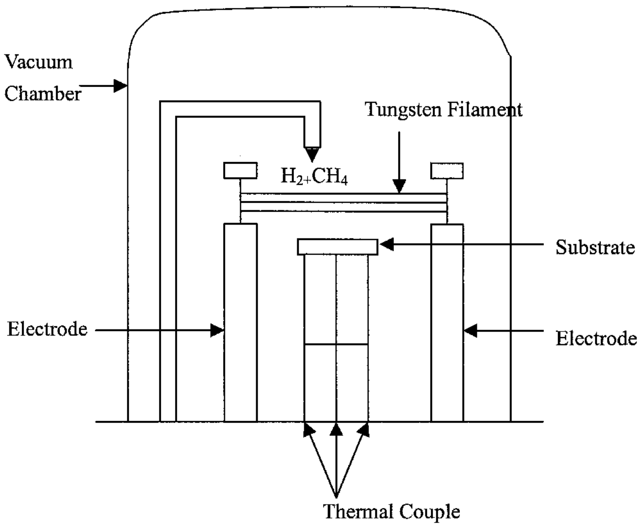

Fig. 1 Chemical vapor deposition chamber for diamond coatings.

et al.[10] reported that diamond is the hardest material and possesses a low friction coefficient. Consequently, it is a good candidate material for tribological applications. Many research efforts have focused on developing diamond films as a hard coating on tool materials.[11,12]

The application of CVD diamond technology to cutting tools is an obvious choice, given the established and growing market for diamond cutting tools in the aerospace, woodworking, and automotive markets. In this paper, a WC substrate was chosen for investigating the effect of diamond coating on thermal contact conductance because tungsten carbide is the most widely used material in cutting tool inserts for machine operations. The WC samples were both cut from standard bar stock and turned to the appropriate diameter, 2.54-cm diam and 0.2-cm thickness. Three different coating thicknesses are adopted for WC test specimens. The detailed surface characteristics and coating thicknesses for all test specimens are listed in Table 1.

A CVD system was used to coat the diamond on the WC substrates, as shown in Fig. 1. A mixture of H_2 and CH_4 was employed as the reactant to synthesize diamond film by a hot filament made of tungsten wire with a diameter of 0.127 mm (0.005 in.). The power input for the filament is 250 to 350 W, and the filament temperature is about 2200°C. The substrate temperature is 750–850°C as measured by three K-type thermocouples. The pressure of the reactor chamber was maintained at approximately 20 torr, and the flow rate of mixture gas is 100 cm^3/min. All of the diamond coating test specimens are fabricated using the same CVD system.

Experimental Program

An experimental investigation was conducted to determine the degree to which the thermal contact conductance at the interface of a contacting WC surface could be enhanced through the use of diamond coatings. Potential optimum diamond coating thickness was evaluated under four different contact pressures. Also, the hysteresis effect of diamond coatings on the WC substrate was examined using the experimental data.

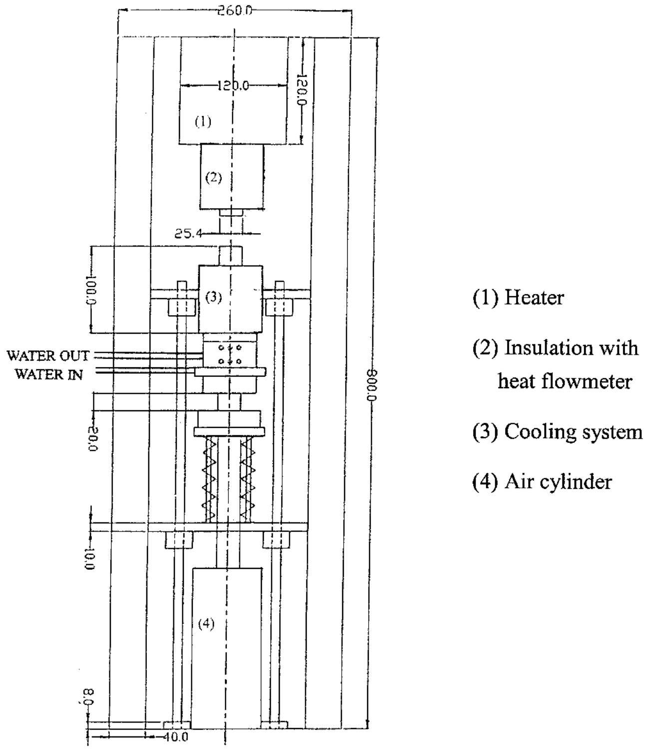

Fig. 2 Experimental test apparatus.

Test Apparatus

An experimental apparatus was built to measure the thermal contact conductance of the WC substrate coated by diamond. The experimental apparatus consists of an electrical heater, two heat flowmeters, a test specimen, a cooling unit, a load cell, a load bellow, and a pneumatic pressure cylinder. A schematic diagram of the complete test apparatus is shown in Fig. 2. The heat flowmeters were made of 304 stainless steel and were approximately 10.16 cm long and 2.54 cm in diameter. Each heat flowmeter had four holes that were radially drilled to accommodate the thermocouples. The diameter of each hole was 1.6 mm, and the hole was 1.27 cm deep, drilled perpendicular to the axes of the heat flowmeters. J-type thermocouples were installed in each hole, located at 1.5-cm intervals, for measuring the temperatures along the heat flowmeters' centerline. To ensure good contact between the thermocouples and the test specimens, thermal grease was inserted in the thermocouple holes. A 32-point data logger and a personal computer were applied to acquire the thermoelectric voltages and convert the signals to temperatures. The electrical resistance heater and water cooling systems were employed to create a one-dimensional, steady-state heat flow across the test interface. Fiberglass insulation was wrapped around both of the heat flowmeters, and the heat loss due to convection and radiation were assumed to be negligible for the experimental temperature range. The measured interface temperatures ranged from 35 to 55°C, so that the radiative effect is quite small when compared with the conduction effect. Temperatures at the contact interface were determined by extrapolating the temperatures along the heat flowmeter centerlines. The heat flux was calculated using these temperatures, the distance of the thermocouples, and the known thermal conductivity of the WC substrate. The thermal conductivity of the WC specimens is 120 W/mK (Ref. 13).

The influence of contact pressure on the diamond coating interface was also investigated in this paper. The contact pressure was applied by pumping high-pressure air into the pneumatic pressure control system, which consisted of a load cell, pressure transducer, air cylinder, and the base plate. By the use of a compression load cell and pressure transducer located under the heat flowmeter, the contact pressures were monitored at the interface.

Experimental Procedure

Tests were conducted to determine the overall thermal contact conductance for the WC substrate with diamond coatings. Uncoated interfaces for the WC substrate were tested first to establish a baseline overall thermal contact conductance value for each coating specimen. Three different coating thicknesses of WC test samples were employed to investigate the effect of coating thickness on the overall thermal contact conductance.

The same experimental procedure was followed for all of the tests. All of the sample pairs were stored in a vacuum environment before testing. Each test pair was removed from the vacuum container when needed. The test specimen was installed in the test facility and the vertical heat flowmeters were aligned to ensure that the contacting surfaces remained parallel during the tests. It is important to ensure that the test column be in perfect alignment. If it were not, then there would be uneven pressure across the interfaces in the stacked column, and this would skew thermal resistance measurements. These resistances could produce nonuniform temperature distribution on local cross sections of the test column near the interfaces, and, hence, the temperature measurements of the heat flowmeter would not represent the appropriate value.

The temperature and pressure test conditions were set by adjusting the heater current and pressurizing the load bellows, respectively. Tests were conducted at an average contact interface temperature of $45 \pm 2^\circ$C by adjusting the power to the heater. The average heat flux for a test was calculated by using a linear regression difference approximation for the temperature gradient. The thermal contact conductance was then calculated using the average heat flux of the heated and cooled specimens divided by the temperature drop across the test interface.

Experimental data were only recorded when steady-state conditions were achieved after approximately 1 h following each increased loading step. The recorded data included the temperatures of the heat flowmeters, specimen thickness, and applied contact pressure. From these data, the overall thermal contact conductance and uncertainty in thermal conductance measurements were computed. The uncertainty in the temperature drop across the coating interface is the result of the uncertainties associated with the thermocouple readings and the extrapolated temperature. An estimate of the total uncertainty was approximately $\pm 8\%$ for all test samples. The uncertainty associated with any single thermal conductance measurement was a function of the uncertainty of the temperature measurements, the heat flux calculations, pressure measurements, and the thermal conductivity of the coatings. When these uncertainties were combined, the overall uncertainty of all experimental data was estimated to be $\pm 8.5\%$.

Results and Discussion

Because of its excellent thermal and electrical properties, diamond appears to be the most promising material for meeting the thermal and electrical requirements for future advanced industrial applications. Besides being the hardest known material, diamond also has other unique properties that makes it ideal for many engineering applications. The most widely used material in cutting tool inserts for machining operations is WC. Thus, the effect of diamond coatings on thermal contact conductance at the interface of a WC substrate using a CVD technique were studied experimentally. The entire idea of this experimental setup was to provide a means to determine the influence of coating thickness on joint thermal conductance and investigate the optimum coating thickness of diamond coatings. The data obtained from the thermocouples were used to calculate the temperature jump across the test interface. The temperature drop across the test specimen was determined by subtracting the upper interface temperature from the lower interface temperature. The overall thermal conductance across the interface was calculated by dividing the average heat flux by the temperature drop across the interface.

The uncoated WC substrate sample is tested first. Based on these baseline thermal performance characteristics, it is possible to determine potential improvements in the thermal performance with coated surfaces experimentally. To evaluate the diamond coating effect on the thermal conductance of the WC substrate at the interface, the calculated overall thermal conductance data for a bare surface sample is compared with those of coated surface pairs under the same pressures.

The results of the bare specimen and three different thicknesses of WC substrate with diamond coatings samples are presented in Fig. 3. Under the constant interface temperature, contact pressures were varied from 1.37 to 3.73 MPa. The three diamond coating thicknesses are 6, 14, and 31 μm, respectively. Basically, the overall thermal conductance increased with increasing interfacial load. As expected the measured results for each sample are different due to minor variations in the surface characteristics of the contacting surfaces. The greatest enhancement of the overall thermal conductance was obtained for 14-μm diamond coatings, as shown in Fig. 3. The thicker coating sample (31 μm) presented a lower overall thermal conductance at the interface. To investigate the optimum thicknesses of the layer for different interface pressures, the dimensionless overall thermal contact conductance, defined as the ratio of overall thermal contact conductance for the coated joint and the overall thermal contact conductance for the uncoated joint at the same pressure, were curve fitted using a linear regression technique.

The dimensionless overall thermal conductance data for diamond coatings are presented in Fig. 4. The ratios of the coated overall thermal contact conductance to the overall uncoated thermal contact conductance at four different pressures are plotted as a function

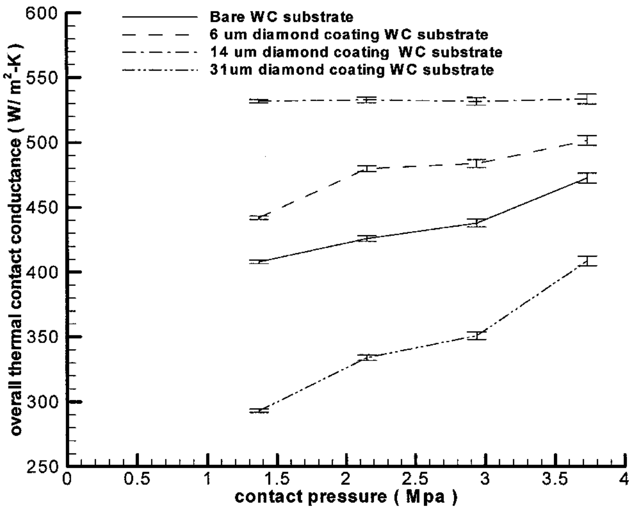

Fig. 3 Overall thermal contact conductance of WC substrate with different diamond coating thicknesses as a function of pressure.

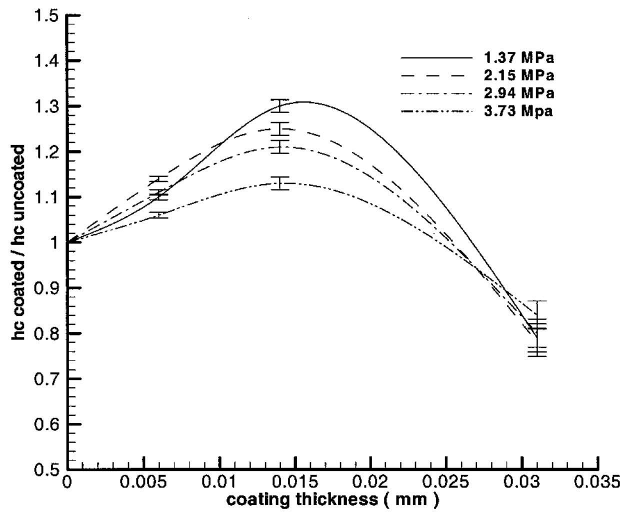

Fig. 4 Improvement in the overall thermal contact conductance of WC substrate as a function of diamond coating thickness.

of the coating thickness t. As illustrated in Fig. 4, three different coating thicknesses were tested and the ratio of the coated thermal contact conductance to the uncoated thermal contact conductance at four different pressures was plotted as a function of the coating thickness. The results indicate that the dimensionless overall thermal contact conductance increases as the coating thickness increases, up to thickness of 14 μm. At this point, the dimensionless overall thermal contact conductance decreases with increasing coating thickness. The reason might be because, when the coating thickness is increased at constant pressure, the enhancement of the thermal contact conductance results from the increase of contact area. If the coating thickness is increased further, the enhancement due to the increase in area is overshadowed by the increase of the bulk thermal resistance of the coating material. An optimum thickness is reached when the combination of these two effects results in the minimum resistance. It is believed that an optimum coating thickness exists in diamond-coated junctions. Basically, moderate coating thickness can enhance thermal conductance due to the coating material displacing the interstitial gas and increasing the contact area. However, an excessive coating thickness will increase the bulk thermal resistance of the coating material and decrease the thermal conductance at the interface.

It is also apparent from Fig. 4 that the enhancement of the overall thermal contact conductance decreases as the pressure increases at a constant coating thickness. When the pressure initially increases, the contact area of the coated joint increases much faster than for the uncoated joints. As the pressure continues to increase, the rapid increase in contact area is decreased by the surface asperities that have penetrated the coatings and are in contact with the WC substrate. However, for the 6-μm coating thickness sample, a deviation was found at 1.37-MPa pressure. This is probably in large part due to differences in the surface profile of the specimens. The surface of this specimen exhibited significant crowning. This would prohibit contact over the annulus surrounding the raised portion of the surface, causing decreased thermal conductance.

The nature of the deformations of surface asperities had a strong influence on the thermal contact conductance. Based on classical theories of contact mechanics, the surface deformations could be either elastic or plastic. How the different coating materials, coating thicknesses, and surface roughness influence the surface deformation is still not clear. To determine whether elastic or plastic deformation was dominant at the diamond-coated interface, the contact pressure was increased from approximately 1.4 to 3.8 MPa and back to 1.4 MPa. When the pressure reached 3.8 MPa, the pressure remained steady for 1 h. After all of the temperatures from the thermocouples were recorded, the contact pressure was decreased from 3.8 back to 1.4 MPa. If plastic deformation of the diamond coating interface occurred, one would expect to observe an increase in the conductance during unloading over that during initial loading. However, if the surface deformation is predominantly elastic, the increase and decrease of real contact area during loading and unloading, respectively, are reversible. Hence, there would not be any difference in the measured conductance. After a maximum load was reached, similar measurements were taken for decreasing load.

The overall thermal conductance results of diamond coatings during the first loading–unloading cycle are shown in Fig. 5. The thermal contact conductance of all experimental data is observed to increase with pressure. It is clear that the overall thermal conductance during the first unloading was greater than that for the initial loading at the same applied contact pressures. This seems to indicate that the diamond-coated interface deformation is predominantly plastic during the initial loading. Comparing the results of a constant coating thickness specimen shows that higher contact pressure data present less hysteresis than lower contact pressure data. This is because the contact area has been increased gradually during the loading process and still retained some part of real contact area at the coating interface when the contact pressure returned to the original level.

To further analyze the relationship between the hysteresis effect and diamond coating thickness, a relative conductance ratio of loading and unloading was applied in this study. The relative conductance ratio is defined as the overall thermal conductance of unloading divided by that of loading. The hysteresis effect was investigated using the relative conductance ratio, as shown in Fig. 6. The higher hysteresis effect can be observed at the contact pressure returned to the lower level during the first loading–unloading process. Note that the higher coating thickness can result in larger hysteresis effect. For example, the 31-μm diamond coating test results present, on average, 25, 32, and 38% larger hysteresis effects than that of the of 14-μm, 6-μm, and bare specimen, respectively. However, further experimental data of different coating materials and substrates are recommended to substantiate this result.

The preceding experimental results clearly show that the diamond coating interfaces were predominantly plastic deformation for the first loading of a fresh surface. Hence, some appropriate theoretical or empirical models can be applied for comparison with the test results, but existing theoretical models for nonmetallic coatings and overall thermal contact conductance are limited. However, some metallic coating thermal contact conductance models are applied to evaluate the test data. Lambert and Fletcher[14] reviewed the published thermal contact conductance data for metallic coated metals. Using 654 data chosen from 99 separate contact conductance experiments, they presented a regression analysis that utilized expressions for dimensionless thermal contact conductance and relative

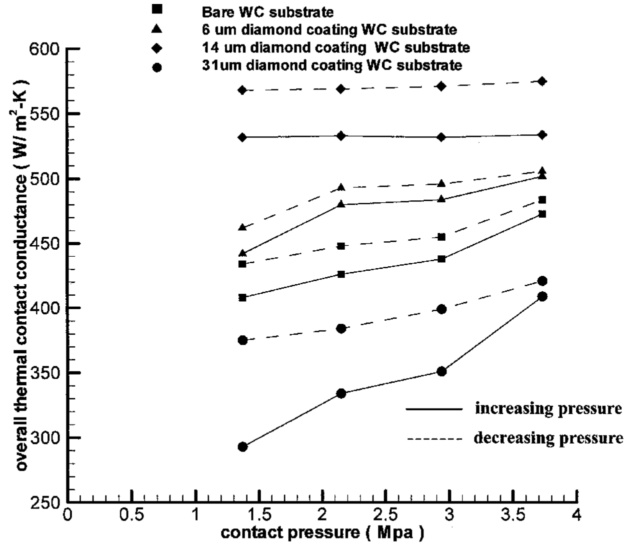

Fig. 5 Overall thermal contact conductance as a function of contact pressure for diamond coatings on WC substrate during first loading–unloading process.

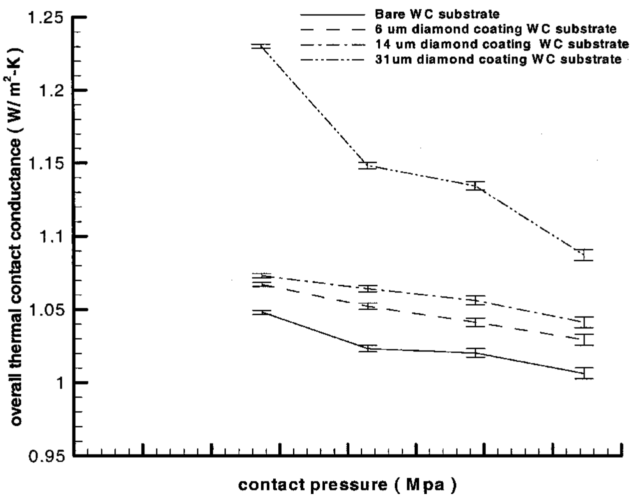

Fig. 6 Relative conductance ratio of WC substrate with diamond coatings during first loading–unloading process.

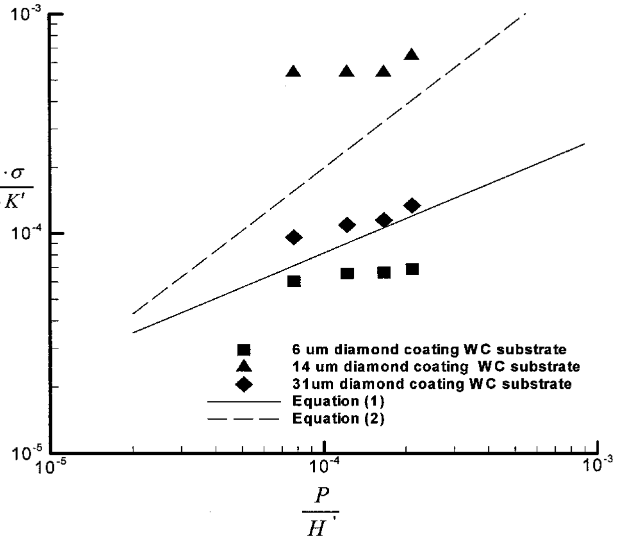

Fig. 7 Comparison between existing models and test results for diamond coatings.

pressure developed for optically flat surfaces. The dimensionless contact conductance relationship is

$$h_c\sigma/sk' = 0.00977(P/H')^{0.52} \tag{1}$$

Antonetti and Yovanovich[15] employed only roughness and asperity slope in their expression for dimensionless conductance because they dealt with optically flat surfaces that were bead blasted to achieve various roughness values. They also utilized an effective thermal conductivity k', which takes into account the generally different conductivities of the substrate and coating and their effect on the geometrical constriction resistance at the idealized microcontact spots. The dimensionless contact conductance vs relative pressure relationship developed by Antonetti and Yovanovich is

$$h_c\sigma/sk' = 1.25(P/H')^{0.95} \tag{2}$$

The overall thermal contact conductance and apparent contact pressure values are reduced to dimensionless terms to facilitate comparison of data from different coating surfaces involving various surface profiles and contact pressures. A comparison of the dimensionless thermal contact conductance values obtained from present study with earlier models is shown in Fig. 7. Some surface parameters in linear regression models, such as asperity slope, waviness, and flatness deviation, may influence the predicted results from approximately two orders of magnitude to more than three orders of magnitude. Nevertheless, the linear regression model might offer reasonable predicting agreement for test data ranging from 1.4 to 3.8 MPa. The theoretical model of Eq. (2) underpredicted the very thick coating samples, as shown in Fig. 7. It seems that deformation of contact spots at the interface may exhibit some unknown contact mechanism for very thick coatings. When the contact pressure is increasing or contact microhardness is decreasing, the predicted values may approach closer to test data. This may be attributed to high contact pressure extruding the void/gap spaces at joints, which may cause some extra hysteresis effect at the interface. It may dramatically increase the heat flow through contact areas at the interface, but an upper limitation may exist. However, further investigations are needed to study this phenomenon from an experimental as well as an analytical point of view.

Conclusions

The theoretical models of the heat transfer at the junctions can provide excellent opportunities for parametric investigations. Such studies are extremely useful in analyzing new machine tools designs. However, a comprehensive theoretical model that can predict optimal coating thickness, resulting in higher thermal enhancement effects, is not available. The geometry of real design systems is sufficiently complex that analytical techniques are difficult to use in most instances. Therefore, experimental investigations have been conducted and reported in this paper to provide useful data for diamond coating applications.

To study the effects of coating thickness, a steady-state conductive heat transfer experiment was performed. The phenomena of optimum coating thickness were observed in this investigation. Basically, moderate coating thickness can enhance thermal conductance due to the coating material displacing the interstitial gas and increasing the contact area. However, excessive coating thickness will increase the bulk thermal resistance of the coating material and decrease the thermal conductance at the interface. When the coating thickness is too thick, exceeding the optimum coating thickness that produces the high thermal contact conductance, a negative effect on the enhancement thermal contact conductance can result. The experimental results show a common tendency for the enhancement of the dimensionless thermal contact conductance to increase as the contact pressure decreases. The discrepancy of some measured data is probably in large part due to differences in the surface profiles of the specimens caused by the manufacturing process. The overall thermal contact conductance can be enhanced by the use of coatings of 6 and 14 μm of diamond, but the opposite effect can be observed in 31-μm diamond coatings.

The experimental results do also present a trend for increasing hysteresis as the diamond coating thickness increases. Note that experimental results from this study may only be valid for contacting surfaces that have surface characteristic values similar to those tested in the experimental investigation.

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