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Energy consumption and material fluxes in hard coating deposition processes



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ABSTRACT

Hard coatings grown by physical vapor deposition (PVD) or chemical vapor deposition (CVD) on cutting tools are applied to considerably increase the tools' performance and lifetime. Besides differences in types, thicknesses, structures and properties of the coatings synthesized by PVD and CVD, the deposition processes differ significantly in their throughput of tools as well as their energy and material consumption. Within this work, a methodology to analyze the energy and material fluxes of typical PVD and CVD processes for the deposition of hard coatings on cutting tools is introduced. Three case studies are considered: (*i*) cathodic arc evaporation of TiCN, (*ii*) magnetron sputter deposition of TiN, and (*iii*) CVD of a TiCN/Al₂O₃ bilayer coating. The material fluxes and energy consumption for each process step of the respective deposition processes were monitored and are illustrated by individual Sankey diagrams. The visualization by Sankey diagrams allows to readily identify the main energy and mass consuming process steps. Finally, a normalization procedure enabling the comparison of different hard coating production routes is presented and discussed.

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1. Introduction

Thin hard coatings are commonly used for wear protection to improve the performance of tools, dies and molds [1,2]. Overall, about 75% of all cutting tools and in particular more than 90% of all cutting inserts made of cemented carbide are coated by chemical vapor deposition (CVD) or physical vapor deposition (PVD) techniques, with CVD being used in more than half and PVD in slightly less than a quarter of the cases, while the remaining fraction is uncoated [1,3,4]. Table 1 summarizes the main characteristics of the two PVD techniques, i.e. cathodic arc evaporation (CAE) and magnetron sputter deposition (MSD), and the thermally activated CVD process which were analyzed in the current study. In addition to the different deposition temperatures, which determine possible substrate materials, also the typical coating thicknesses and sample loads vary among PVD and CVD, where significantly higher sample loads and coating thicknesses are common for the latter method. Further, CVD and PVD processes differ with respect to typical coating materials, structure and properties, but also in their energy and material consumption. However, a systematic evaluation of the efficiency of these coating processes is not available in literature.

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The aim of the present work is to develop a methodology to analyze the energy and material fluxes for typical PVD and CVD processes used for the deposition of hard coatings on cutting tools. The material and energy fluxes for each deposition step have been recorded and Sankey diagrams were generated, where the main energy and material consuming process steps are readily identifiable. In 1898, Sankey suggested a diagram to illustrate the efficiency of steam engines, describing the energy flow graphically by the arrangement of arrows illustrating different contributions [5,6]. The advantage is that the quantity of all flows can be summarized and so the summed up respective arrow width corresponds to the total flow within a defined system. Later on, Sankey diagrams were also used to compare different processes, like the efficiency of diesel and gas engines [7]. Today, they are used in very different fields like for monitoring biomass streams [8], the global water flow per annum [9] or the efficiency limits of energy converting devices [10]. Sankey diagrams are an important tool in identifying inefficiencies and potential for savings when dealing with resources. They are typically used to visualize energy, material or cost transfers between processes.

Within this work, the Sankey diagrams are applied to visualize the mass throughput and the respective energy contributions of the process steps for three case studies based on exemplary lab deposition processes, i.e. arc evaporation of TiCN, magnetron sputter deposition of TiN and CVD of TiCN/ α -Al₂O₃. Thereby, the energy contributions are quantified

50 Table 1

Overview of typical features of the different deposition techniques considered in the case studies [17,25–28]. Values for the typical loads are given considering cemented carbide half-inch cutting inserts of 12.7 mm.

Process parameter CAE MSD CVD	
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as electrical power per process time interval. These case studies have been chosen as typical processes for the deposition of hard coatings. The demonstrated quantification and visualization by Sankey diagrams allow to determine the fraction of the total material that is incorporated in the coating. To generalize the methodology, the determined mass and energy fluxes are normalized per micrometer coating thickness.

2. Deposition techniques

In PVD methods, solid precursor materials, so-called cathodes or targets, are used. Depending on how the solid material is transferred into the (ionized) vapor phase, evaporation and sputtering can be distinguished [11]. Evaporation is based on the transfer of the solid target material into the vapor phase by applying heat. Using a cathodic arc, evaporation of the target material is realized using a high current, low voltage electrical discharge, the so-called arc. It is ignited between the anode, typically the grounded chamber wall, and the cathode to be evaporated [12]. Within the first case study, TiCN coatings were grown by arc evaporation. The TiCN coating was deposited at a substrate temperature of ~450 °C under a constant flow of Ar (700 sccm) and C_2H_2 (100 sccm) (see Ref. [13] for more details on the deposition process), whereas the N₂ flow was adjusted in order to maintain a total pressure of 3 Pa. The arc current was set to 180 A for each of the four arc sources equipped with Ti targets. A bias voltage of -100 V was applied to the substrates.

Using MSD, the solid target material is transferred into the vapor phase by energy and momentum transfer from impinging ions. These ions, usually Ar^+ , are provided by igniting a glow discharge between the target (cathode) and the chamber wall (anode) [14,15]. The TiN coatings considered within the second case study were grown using unbalanced pulsed direct current magnetron sputter deposition. The TiN coating was synthesized under a constant Ar flow (200 sccm) and the chamber was backfilled with N₂ to a total pressure of 0.58 Pa. The four magnetrons equipped with Ti targets were operated in constant power mode set to 7 kW for each magnetron, applying bipolar pulses at a frequency of 50 kHz and a duty cycle of 50%. The bias voltage was set to - 50 V with a pulse frequency of 350 kHz (bipolarily pulsed) and a reversal time of 1000 ns (for more details on the deposition process see Ref. [16]).

In contrast to PVD, in thermally activated CVD gaseous precursors are introduced into the deposition reactor and form the desired chemical compound of the coating at elevated temperatures [17]. In the third case study considered here, TiCN/ α -Al₂O₃ bilayer coatings were deposited. The α -Al₂O₃ layer was synthesized from AlCl₃-CO₂-H₂-H₂S precursors at a temperature of ~1000 °C [18] and a pressure of 7.5 kPa (for more details on the deposition process see Ref. [19]). As base layer, TiCN was deposited via medium-temperature CVD at 900 °C using a gas mixture of TiCl₄-CH₃CN-H₂-N₂ at a pressure of 10 kPa (for more details on the deposition process see Refs. [18,20–22]). The use of CH₃CN instead of CH₄ enables deposition of TiCN at lower temperatures, which prevents formation of the brittle η phase in cemented carbide substrates [20].

3. Methodology

For all deposition processes, the mass and energy fluxes were recorded and divided into steps. Fig. 1 gives an overview of the different deposition steps. The energy consumption was calculated from the nominal capacity and the effective utilization during the respective process steps for each component involved in the deposition plant (bias generator, heaters, pumps, cathodes, filament and coils, ventilators). For MSD and CVD, the calculation was based on the effective utilization during the process steps. For CAE all pumps are considered to run at full power during the deposition cycle, accepting the fact that this would lead to an overestimation in energy consumption. For the mass flux diagrams, the streamed-in gas fluxes were considered for each process step and the mass flux was determined by the read-out of the mass flow controllers and the respective gas density. In the two PVD processes, prior to mounting on the cathode holders or magnetrons, all targets were weighed to determine the initial mass. After deposition, the mass of the targets was measured again and the mass loss per coating deposition time was calculated. The amount of water for cooling was not considered in any case study, because all deposition systems are working with a closed cooling water circuit, with several coating units which makes a separation impossible. To provide a reference point for a rough estimation, a typical chiller system for the two PVD processes considered here will consume an approximate energy of 6 kWh, contributing to about 6% of the overall energy consumed. For the CVD process, the liquid components for neutralization of the reactions products were considered according to manufacturer's instructions.

For all processes, prior to mounting in the chamber, the substrates were cleaned in ethanol in an ultrasonic bath. They were weighed before and after the deposition process to determine the mass gain of the coated substrates. The mass loss according to the ion etching step prior to coating deposition in the two PVD processes could not be considered, because it was close or even below the resolution limit of high-precision mass balances. The coating thickness was determined by a spherical abrasion test, averaged for at least three substrates mounted on representative positons at the substrate holders. It should be noted that the remaining positions were filled by dummy substrates. Using the chemical composition of the synthesized coating, which was determined for the CVD and MSD processes by energy dispersive Xray spectroscopy and for the CAE process by elastic recoil detection analysis, the mass fraction of each element in the deposited substrates was calculated. All other masses, which were not incorporated in the coating on the substrates, were assumed to be deposited on the carousel and/or substrate holder and the chamber walls or, in the case of gaseous components, left the process as outgoing gas.

For MSD, cemented carbide substrates in three different geometries were used. Three disks (\emptyset 30 mm × 4 mm) and three SNUN 120412 inserts (according to ISO 1832) were mounted on a substrate holder operating in twofold rotation. In addition, nine CNMG 120408 inserts (according to ISO 1832) were mounted to undergo threefold rotation. The material flux during CAE was recorded using three high-speed



Fig. 1. Sequential steps of deposition processes. In the case of the PVD processes, the steps Pumping, Purging and Venting have been included into the steps Heating and Cooling, respectively. In the case of the CVD process, the step Pumping/Purging was included into the step Heating; the steps Plasma etching and Venting are absent.

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