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Design of metal-cutting tool coatings at the atomic level

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Abstract. The research aims to lower tooling costs by reducing the time allotted to designing coatings on domestic cemented carbide metal-cutting tools by using the atomic force approach. The object of the study is coatings on cemented carbides of the tungsten carbide group such as titanium carbide (TiC), titanium nitride (TiN), and titanium (Ti) coatings or a nitride-based titanium, chromium and aluminum (Ti,Cr,Al)N composite coating. To select the most rational coatings, the article employed the method of calculating the functionals of interatomic systems using the density functional description of single atoms. The simplest measure to reduce the cost of designing metal-cutting instruments for manufacturing parts made of difficult-to-machine materials is to develop coatings for this tool type. The article considers various atomic arrangements in the coating material in relation to the WCo8 cemented carbide (VK8, tungsten carbide-cobalt alloy containing 8% cobalt). The calculated values of the interaction energy of the coating material atoms with one another and with the cemented carbide material ranged from 3.04 to 3.5 J/m². Moreover, the research has established a correlation between the calculation results and the performance parameter of metal-cutting tools considering fracture toughness K_{1c} (MPa · √m). The main result of the study is that the employed computational method made it possible to determine the adhesion value for the atoms of the above-mentioned coating materials with tungsten carbide and cobalt atoms packed in different scale configurations. This enables the classification of coatings from the perspective of ensuring maximum performance properties of the tooling material. The present article assumes that the higher the adhesion value, the better the performance properties. The hypothesis has been confirmed experimentally as well as by the values of fracture toughness K_{1c}. Thus, the most rational coating options have been selected for specified operating conditions of a metal-cutting tool, which permits reduction of tool design costs and makes it possible to predict the performance properties of tools at the design stage.

Keywords: atomic force approach to coating design, cemented carbide coatings, tooling cost reduction

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МАШИНОСТРОЕНИЕ

Научная статья

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Проектирование покрытий металлорежущего инструмента на атомарном уровне

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Резюме. Цель работы – снизить инструментальные затраты за счет сокращения времени на проектирование покрытий на твердосплавном отечественном металлорежущем инструменте путем применения атомарно-силового подхода. Объектом исследования являются покрытия на твердом сплаве группы карбидов вольфрама, например: покрытия карбидом титана TiC, нитридом титана TiN, титаном Ti или нитридом сложносоставного покрытия смеси титана, хрома и алюминия (Ti,Cr,Al)N. Для выбора наиболее рациональных покрытий применен метод расчета функционалов межатомных систем с использованием функциональной плотности одиночных атомов. Наиболее простой мерой, позволяющей снизить расходы на проектирование металлорежущего инструмента для изготовления деталей, выполненных из труднообрабатываемых материалов, является разработка покрытий для данного вида инструментов. Рассмотрены различные схемы расположения атомов в материале покрытия по отношению к твердосплавному

материалу ВК8. Рассчитанные величины энергии взаимодействия атомов материала покрытия между собой и с материалом твердого сплава составили от 3,04 до 3,5 Дж/м². Установлена взаимосвязь результатов расчета с эксплуатационным параметром металлорежущего инструмента по коэффициенту трещиностойкости K_{1c} (МПа·√м). Главным результатом проведенных исследований является то, что расчетным методом определена величина адгезии для атомов материала покрытий, указанных выше, с атомами карбида вольфрама и кобальта, уложенных в разные масштабные конфигурации. Это позволяет классифицировать покрытия с позиций обеспечения максимальных эксплуатационных свойств инструментального материала. Предполагается, что чем выше величина адгезии, тем лучше эксплуатационные свойства. Это подтверждено экспериментально и по значениям коэффициента трещиностойкости K_{1c} . Таким образом, выбраны наиболее рациональные варианты покрытий под заданные условия эксплуатации металлорежущего инструмента, что позволяет сократить затраты на проектирование инструмента и обеспечивает возможность прогнозирования эксплуатационных свойств инструмента на этапе его проектирования.

Ключевые слова: атомарно силовой подход к проектированию покрытий, покрытия на твердом сплаве, сокращение инструментальных затрат

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INTRODUCTION

Designing coatings for metal-cutting tools for specified operating conditions is a labor-intensive process. The study [1] presents the results of designing coatings based on the atomic force approach. In it, the adhesion between the atomic layers of the coating material is used as a criterion for coating selection. As for foreign scientific literature, this approach is outlined in specialized sources [2–4]. In the Russian Federation, the founder of this approach is Professor V.G. Zavodinsky [5, 6].

In works [1, 5, 6], the adhesion energy value E_{ad} is determined by the formula:

$$E_{ad} = \frac{E_{system} - E_1 - E_2}{S},$$

where E_{system} is the total energy of the system. The system is conventionally divided into parts 1 and 2 (top and bottom), J/m². E_1 and E_2 are the energies of the system parts calculated separately, without interaction with each other, J/m². Part 1 can be a substrate or a WC substrate with a layer on it. Part 2 can be all other layers (one or two). The symbol S denotes the interface area.

Fig. 1 provides an example of the arrangement of one row (monorow) of the coating material atoms in the conventional XYZ coordinate system.

From a geometric perspective, this is an ideal atomic arrangement (packing). It assumes:

- 1) in each row the atoms are in contact with one another;
- 2) each atomic row in the following similar rows

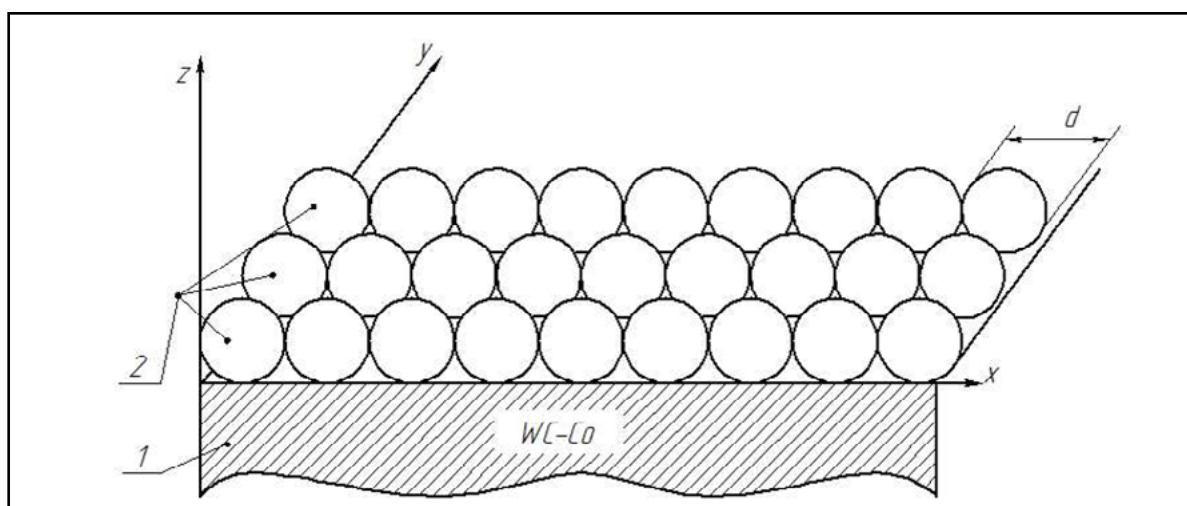


Fig. 1. A conventional arrangement picture of a coating material atom layer (monolayer) on the WC group hard alloy (1 – hard-alloy material, 2 – atoms of the coating material, d – atom diameter, WC – tungsten carbide atoms of hard alloy, Co – cobalt atoms)

Рис. 1. Условная картина расположения ряда (монослоя) атомов материала покрытия на твердом сплаве группы ВК (1 – твердосплавной материал, 2 – атомы материала покрытия, d – диаметр атомов, WC – атомы карбида вольфрама твердого сплава, Co – атомы кобальта)

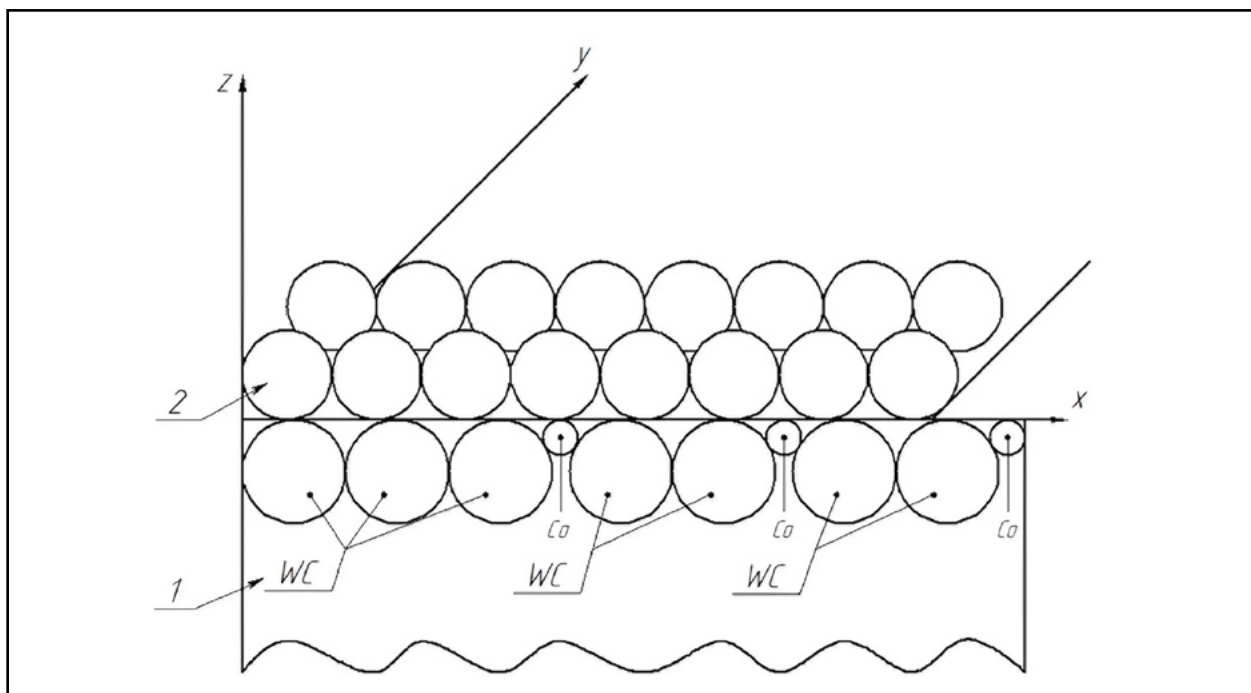


Fig. 2. An example of the coating material mono layer arrangement on a hard-alloy material WC – Co (1 – carbide material, 2 – coating material atoms)

Рис. 2. Пример расположения монослоя материала покрытия на твердосплавном материале WC – Co (1 – твердосплавный материал, 2 – атомы материала покрытия)

is located so that the atoms in the XY plane are in contact only with a similar atom in the preceding row.

In a real situation, this ideal packing scheme changes. Fig. 2 shows one example of the change.

Fig. 2 conventionally shows an example when (from left to right) 3 coating material atoms are in contact with the tungsten carbide (WC) atoms, then a gap occurs between the atoms due to the presence of cobalt (Co) atoms and again two

atoms are in contact with atoms 2 of the coating material, and so on.

Fig. 3 shows an example of close packing of the coating material atoms. Undoubtedly, other combinations of atomic arrangements are possible, including the formation of discontinuities (absence of one or more atoms in a row).

As applied to titanium atoms, the calculation results obtained by the adhesion energy formula (see above) are given in Table 1.

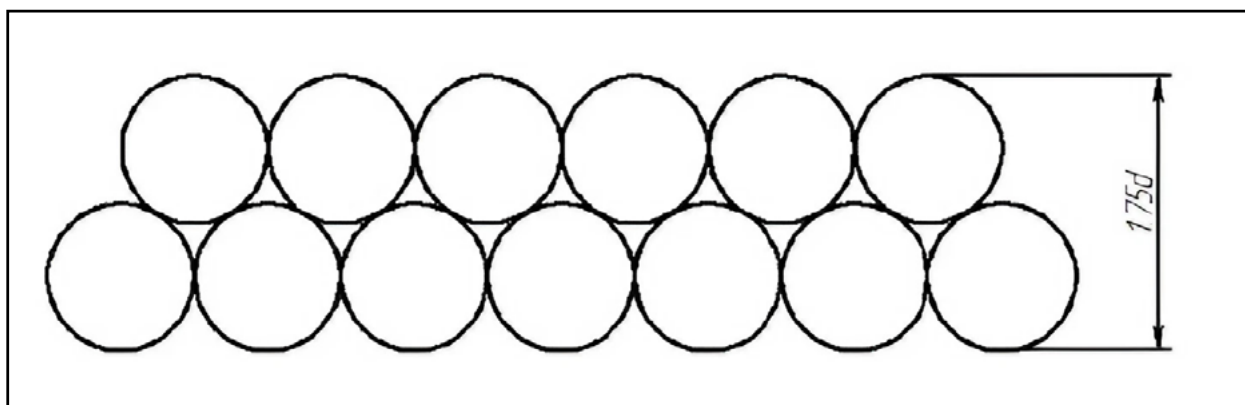
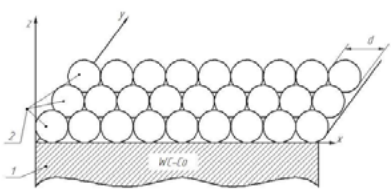
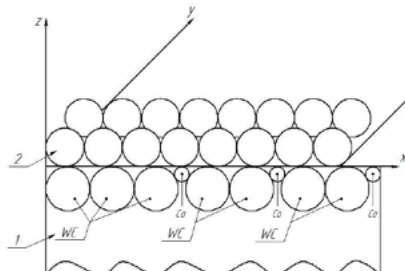
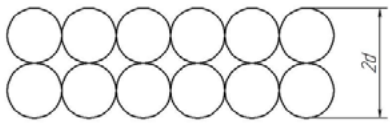
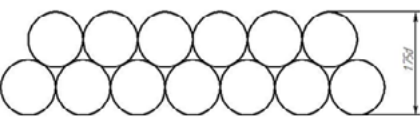
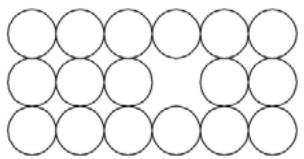
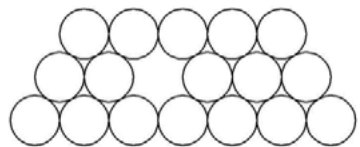


Fig. 3. An example of a close-packed arrangement of two rows of atoms of the coating material (1.75d – height of two rows of atoms, d – atom diameters)

Рис. 3. Пример плотного расположения двух рядов атомов материала покрытия (1,75d – высота двух рядов атомов, где d – диаметр атомов)

Table 1. Values of the adhesion energy for the considered arrangement cases of coating titanium atoms
Таблица 1. Величины энергии адгезии для рассмотренных случаев расположения атомов титана покрытия

Example of atom arrangement	Adhesion energy, J/m ²
 a	3.07
 b	3.27
 c	3.34
 d	3.48
 e	3.34 in solid columns (from left to right columns 1, 2, 3, 5 and 6)
	3.11 in column 4
 f	3.50 in the places lacking discontinuity 3.04 in the places close to Discontinuity

The data in Table 1 shows that the adhesion energy is maximum (3.48 J/m²) at the close-packed double-row arrangement of titanium atoms in the coating (case d). It is significant (3.5 J/m²) for the three-row atomic arrangement (case f), but only in

places remote from the discontinuity. The presence of a discontinuity reduces the adhesion energy to 3.11 J/m² for the three-row vertical atomic arrangement (case e) and to 3.04 J/m² for the close-packed three-row atomic arrangement (case f). This per-

mits the conclusion that discontinuities should be classified as defects reducing the metal-cutting tool performance due to the low adhesion energy in the coating layers.

The study has experimentally proved that the more the coating resists the formation and growth of microcracks, including microcrack branching, the higher the cutting tool performance is. In other

words, the higher the adhesion energy between the coating layers, the longer the cutting tool life up to the allowable wear.

Table 2 shows the results of evaluating the fracture toughness of cemented carbide (grade WCo8) used for tool making and several options of its coating according to the K_{Ic} parameter ($\text{MPa} \cdot \sqrt{\text{m}}$).

Table 2. Comparative assessment of crack resistance of the WCo8 grade tool hard alloy and its several coating options
Таблица 2. Сравнительная оценка трещиностойкости инструментального твердого сплава марки ВК8 и нескольких вариантов его покрытий

Materials	VK8	TiC	TiN	Ti	(Ti,Cr,Al)N
K_{Ic} , $\text{MPa} \cdot \sqrt{\text{m}}$	11.4	1.85	1.89	1.94	2.26

Table 2 shows that from the perspective of resistance to microcrack formation and growth, including microcrack branching, in comparison with carbide ($1.85 \text{ MPa} \cdot \sqrt{\text{m}}$) or nitride ($1.89 \text{ MPa} \cdot \sqrt{\text{m}}$) coatings:

- the titanium coating is predicted to be rational ($1.94 \text{ MPa} \cdot \sqrt{\text{m}}$);
- the nitride-based composite coating (Ti,Cr,Al)N is predicted to be the most rational one ($2.26 \text{ MPa} \cdot \sqrt{\text{m}}$).

The obtained results do not contradict the existing ideas [7–20]. Nevertheless, they indicate that it is feasible to use a new approach to tooling materials design for specified operating conditions of metal-cutting tools.

CONCLUSION

Calculating the adhesion energy of atomic interaction, the study has evaluated the adhesion properties which different coating layers display in relation to each other and to the WCo8 hard alloy used for making tools. This approach has been experimentally verified in terms of resistance to microcrack formation and growth, including

microcrack branching. The article has considered various atomic arrangements in the coating material in relation to the WCo8 cemented carbide material. The values of the energy of interaction of the coating material atoms with each other and with the hard alloy material have been calculated. The research has employed the method of calculating functionals of interatomic systems using the density functional description of single atoms. The correlation between the calculation results and the performance parameter of metal-cutting tools according to fracture toughness K_{Ic} ($\text{MPa} \cdot \sqrt{\text{m}}$) has been established. The article proposes to examine tooling materials at the design stage by the adhesion energy value. The novelty of the research consists in determining the adhesion value for atoms arranged in different scale configurations by a computational method. Thus, coatings can be classified from the standpoint of ensuring maximum performance properties of the tooling material. It is assumed that the higher the adhesion value, the higher the performance properties. This has been confirmed experimentally and by fracture toughness K_{Ic} .

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