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Mitigation of chemical wear by graphene platelets during diamond cutting of steel

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ABSTRACT

The diamond cutting of transition metal alloys, particularly steel, is severely hindered by accelerated chemical wear of the tool. Recent experimental findings show that the presence of graphene platelets mitigates this problem. However, the specific mechanisms responsible for this wear mitigation are currently unknown. In this paper, molecular dynamics techniques are successfully used to identify these diamond tool wear mitigation mechanisms. A modified embedded atom method force field is first evaluated for its ability to accurately simulate the catalyzed graphitization of diamond in the presence of steel. This force field is then used to simulate nanometric diamond cutting of steel in the presence of a 1 or 3 layered graphene platelet. Coordination analysis of these simulations shows that the presence of the graphene platelet results in 34%–96% reduction in tool wear, when compared to the graphene-free cutting condition. This is attributed to the graphene platelet serving as a physical barrier protecting the tool cutting edge, and also as a sacrificial source for carbon transfer into the workpiece. Other mechanisms, such as platelet cleaving and interlayer sliding, are also observed. The reduction in tool wear reported by the simulations is comparable to the trends observed in prior experiments.

1. Introduction

The hardness of diamond makes it an attractive tool material for various manufacturing operations [1]. Diamond is particularly well-suited for ultra-precision machining operations involving materials such as glass [2], ceramics [3], and aluminum [4]. However, it is common knowledge that diamond tools are ill-suited for cutting transition metals and their alloys (e.g. steel) that are commonly used in engineering applications. The reason for this is two-fold. First, the high temperatures encountered in the cutting zone cause spontaneous graphitization of the diamond tool [5]. This is exacerbated by formation of metal-carbon or metal-carbon-oxygen complexes that increase the rate of graphitization [6]. Since the graphitic phase of carbon is significantly softer than diamond [7], this results in the tool rapidly losing its hardness. The second mechanism is the transfer of carbon atoms into the workpiece by the formation of metal carbides [8]. Both these mechanisms are known to cause rapid wear of the diamond tool, ultimately leading to tool breakage and deterioration of part quality.

There is a wealth of literature related to the mitigation of diamond tool wear while cutting steel. The use of ultrasonic tool vibrations [9], cryogenics [10], inert cutting atmospheres [11] and carbon-rich cutting atmospheres [12] have shown varying levels of success. However, all these methods require expensive modifications to the process. Recently, the work of Smith et al. [13] has shown that the use of cutting fluids laden with graphene platelets provides a more economical solution to the problem. Their experimental results showed that the introduction of graphene platelets into the cutting zone resulted in a ~30% reduction in diamond tool wear during the machining of low-carbon steels. While these results are promising, the specific mechanisms responsible for this wear mitigation are currently unknown.

Cutting processes involve high pressure surface contact and high strain rates. This coupled with the chemical nature of the diamond tool wear and the nanoscale thickness of the graphene platelets, makes it difficult to design experiments that can shed light on the graphene-induced wear mitigation mechanisms. Alternately, molecular dynamics (MD) techniques provide one feasible route for this investigation [14–17]. MD simulations have been used to provide atomic-scale insight into key cutting process phenomena, including chip formation [14] and tool wear [15]. In

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addition, MD simulations have also been used widely to study carbon materials in its various allotropes [16,17].

The objective of this research is to use MD simulations to investigate the wear mitigation mechanisms active during the diamond cutting of steel in the presence of graphene platelets. A modified embedded atom method (MEAM) force field is first evaluated for its ability to accurately satisfy three qualifying criteria, viz., 1) the structural parameters of iron, diamond and graphite; 2) temperature-driven graphitization of diamond; and 3) catalyzed graphitization of diamond in the presence of iron. This force field is then used to simulate nanometric diamond cutting of steel in the presence of graphene platelets. The tool wear trends predicted by the simulations are comparable to the findings of Smith et al. [13]. The graphene platelets are seen to serve as a physical barrier, protecting the tool cutting edge, and also as a sacrificial source for carbon transfer into the workpiece. Other mechanisms, such as platelet cleaving and interlayer sliding, are also observed.

The remainder of this paper is organized as follows: Section 2 provides a summary of the Smith et al. [13] experimental results that demonstrated the efficacy of using graphene platelets to mitigate tool wear during diamond cutting of steel. Section 3 provides the rationale behind the choice of the interatomic force field and discusses the results from the calibration tests for the same. It also describes the frame work for the cutting simulations. Section 4 presents the results from the cutting simulations. Section 5 compares the simulation findings to the experimental results of Smith et al. [13] and also presents a discussion on the wear mitigation mechanisms. Finally, Section 6 summarizes the specific findings of this paper.

2. Review of experimental findings

This section briefly reviews the key findings from the experimental study of Smith et al. [13], where graphene platelets were introduced into the workzone during the diamond cutting of low-carbon steel. Table 1 provides a summary of the micro-scale cutting conditions and tool geometry used for their experiments. In this study, the platelets were delivered in the form of a colloidal dispersion in Castrol Clearedge 6519 semisynthetic cutting fluid.

Table 1
Summary of cutting conditions in Smith et al. [13].

Workpiece	• 3 mm diameter, AISI 12L14 steel rod, turning operation
Tool	• Manufacturer: Sumitomo Inc. • Tool insert#: NF-CCGA21.50.5 • Material: Polycrystalline diamond (PCD) • Right-hand, 7° relief angle, 55° nose angle, 0.0075 inch nose radius.
Cutting velocity	• 3 m/s
Depth-of-cut	• 100 μm (Radial) • 5 μm/revolution (Axial)
Cutting conditions	a. Dry – no cutting fluid b. Baseline cutting fluid – castrol clearedge 6519 semi-synthetic (12.5% dilution) c. Baseline cutting fluid +0.2 wt% graphene platelets.

Two measures were used to determine the extent of the diamond tool wear. The first was optical profilometry of the tool surface after the completion of the cut. This data was used to construct height maps of the worn tools, shown in Fig. 1a–c. These results showed that the presence of graphene platelets led to a ~74% reduction in wear compared to the dry cut and ~32% reduction compared to the cut using the baseline cutting fluid. The second measure involved X-ray photoelectron spectroscopy (XPS) of the workpiece to reveal peaks in the binding energy distribution curve corresponding to the iron-carbon bond involved in carbidization. The percentage contribution of the carbide peak was seen to be 13%, 9% and 6% for the dry machining, baseline cutting fluid and graphene colloidal suspension, respectively. The lower formation of carbides was correlated to the trends seen in the tool wear under the same conditions.

The cutting temperature and cutting force measurements for the baseline cutting fluid were found to be comparable to those for the graphene colloidal suspensions. This meant that the wear reduction in the presence of graphene could not be attributed to lower cutting temperatures or lower cutting forces. Therefore, two alternate mechanisms were hypothesized to explain the tool wear trend. The first was that the graphene platelets potentially serve as a physical barrier around the cutting edge, and the second was that the carbon in the platelet was affecting the chemical reaction rate. However, these specific mechanisms have not yet been confirmed.

3. Interatomic force fields and molecular dynamics simulations

This section will first discuss the selection and evaluation of an appropriate interatomic force field to capture the tool wear mitigation phenomenon during diamond machining of steel, followed by the details of the MD nanometric cutting simulation.

3.1. Selection of interatomic force field

In order to accurately model the dynamics of the cutting zone, the interatomic force field must satisfy three specific criteria. First, it must be able to model metallic elements (iron), non-metallic elements (carbon in graphite and diamond allotropes), as well as compounds/alloys (more specifically steel, which is comprised of interstitial carbon in iron, and iron carbides). Second, the force field must be able to describe the temperature-driven graphitization of diamond and third, the potential must be capable of capturing the catalyzed graphitization of diamond in the presence of iron. With

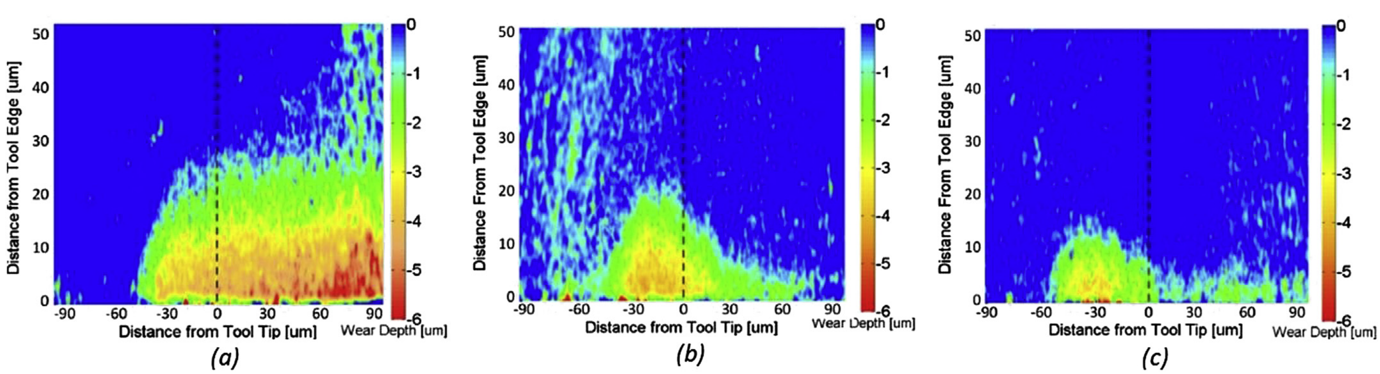

Fig. 1. Volumetric tool wear patterns seen by Smith et al. [13]. (a) Dry machining (b) Baseline cutting fluid (c) Graphene colloidal suspension (Note – The dotted line corresponds to the centerline of the tool). (A colour version of this figure can be viewed online.)