Computational Materials Science 45 (2009) 358–366

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Graphitization as a precursor to wear of diamond in machining pure iron: A molecular dynamics investigation

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A R T I C L E I N F O

Article history:
Received 1 July 2008
Received in revised form 8 October 2008
Accepted 9 October 2008
Available online 25 November 2008

PACS:
02.70.Ns
81.65.Ps
87.85.Va

Keywords:
Diamond
Graphite
Grinding
Machining
MD simulations

A B S T R A C T

It is well known that although diamond is the hardest known material, it cannot be used effectively for machining pure iron or low carbon ferrous alloys due to extremely rapid tool wear. Several research groups have postulated that the mechanism for the observed wear of diamond tools involves the initial transformation of tetrahedral diamond into hcp graphite, the thermodynamically more stable form of carbon under the usual conditions of machining/grinding. The next step in the postulated mechanism involves the diffusion of graphitic carbon into the iron workpiece. In spite of the wealth of publications reporting experimental investigations of this phenomenon, this proposed mechanism still remains no more than a hypothesis, albeit, a reasonable one. The problem is that the time scales (a few seconds to a minute or more) over which the experiments are conducted are too long to permit direct observation of the diamond → graphite transformation, which occurs on a nanosecond to picosecond time scale, if it occurs at all. In this paper, we utilize molecular dynamics (MD) and realistic interaction potentials to provide the first direct evidence that the diamond → graphite transformation does occur and, therefore, could be the principal mechanism of wear of single-point diamond tools in the machining of ferrous materials. MD simulations of nanometric cutting of pure iron oriented in (100) and cut along ⟨100⟩ direction have been conducted in different orientations of the clearance face, namely, (110), (111), and (100) with a diamond tool at a cutting speed of 100 m s^{-1} to investigate the micromechanisms of diamond tool wear. A modified embedded atom (MEAM) potential was used for the Fe–Fe and Fe–C interactions, and a Tersoff potential for the C–C interactions. The computations employed the large-scale atomic/molecular massively parallel simulator (LAMMPS) software developed at the Sandia National Laboratory. The results provide the first direct evidence that as cutting commences, the structure of diamond at the cutting edge begins to transform from diamond cubic into hexagonal graphite in the presence of iron. Subsequent to this transformation, the graphitic carbon diffuses into the iron. The diamond (100) plane was found to be the most resistant and the (011) plane the least resistant to graphitization with the (111) plane showing intermediate propensity for transformation to a graphite structure. These results are in accord with reported experimental observations. Thus, the MD observations provide direct evidence supporting the wear mechanisms that have been proposed in the literature.

1. Introduction

Diamond, as a cutting tool material, is used extensively in ultraprecision machining and grinding on a wide range of workmaterials, including, semiconductors, soft metals, such as aluminum and copper and their alloys, and numerous polymers. The ubiquitous use of diamond is a result of its unique features, namely, highest hardness, its availability in single-crystal form (no grain boundaries), its ability to form an extremely sharp cutting edge, very high thermal conductivity, low friction, non-adhesion to most workmaterials, and high wear resistance [1]. It is amazing but a fact that diamond, the hardest known material, is not suitable for machining pure iron or ferrous alloys, such as low carbon steels, due to rapid tool wear. This is because carbon has a strong affinity for iron to form iron carbide, especially at temperatures above and pressures below the diamond stable region [2,3]. Ikawa and Tanaka [4] proposed a mechanism of wear involving initial phase transformation of diamond into graphite and subsequent diffusion of carbon into the iron workpiece.

Komanduri and Shaw [2,3] postulated that diamond at room temperature is in a metastable state (sp^3 bonding) and will transform into graphite (sp^2 bonding) under the appropriate conditions of pressure and temperature. An increase in temperature in cut-

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0927-0256/$ - see front matter © 2008 Published by Elsevier B.V.
doi:10.1016/j.commatsci.2008.10.007

ting/grinding of ferrous materials without a concomitant increase in pressure (relative to diamond-graphite equilibrium) can promote graphitization [5]. This can be accelerated under the influence of properly directed shear stress [6]. The presence of a catalyst/solvent material, e.g. iron, that rapidly displaces graphite from the surface of diamond at high temperature can aid in this transformation [7]. It may be noted that iron is used as a catalyst/solvent in the synthesis of diamond under high pressure-high temperature conditions [8]. It can play a similar role in reverse, namely, the transformation of diamond into graphite in the graphite stable region. During machining, the freshly generated surfaces between the chip and the tool face, as well as under the machined surface and the clearance face can further assist the graphitization process [9]. All of the above mentioned conditions, namely, high temperatures, pressures below the diamond stable region, presence of hot iron, and newly generated machined nascent surface exist at the tool–workpiece interface. In this investigation, we report the results of direct investigations of the micromechanisms underlying the wear of diamond in the machining of iron, using molecular dynamics (MD) simulations.

Although there exist plausible arguments that support a wear mechanism comprising the initial transformation of cubic diamond into a hexagonal graphitic structure followed by diffusion of the graphitic carbon into the iron workpiece, the fact remains that there have been no direct observations of such a transformation actually occurring in the machining of iron with a diamond tool. The problem is one of time scales. Machining experiments are conducted of necessity over a time scale of a few seconds to a minute or more whereas MD simulations are conducted over a pico-to-nanosecond time scale. A potential problem that may arise is the possibility that the cubic diamond to graphite transformation, if it occurs, might occur over an intermediate time scale, such as a microsecond. In such a case, it will be unobservable in both the experiments and in the MD calculations as well. Fortunately, this transformation was found in this investigation to be observable at the pico-to-nanosecond time scale.

Thus, although the MD methods cannot be used to simulate the actual cutting experiment, they can be employed to study atomic level processes occurring over the pico-to-nanosecond time domain. The objective of this research is to use MD methods with realistic interaction potentials to investigate the question of whether or not cubic diamond can be transformed to a graphitic structure over the first few nanoseconds of a cutting experiment.

2. Simulation setup and test conditions

In machining, almost all of the plastic deformation energy is converted into heat. It has been shown experimentally that of

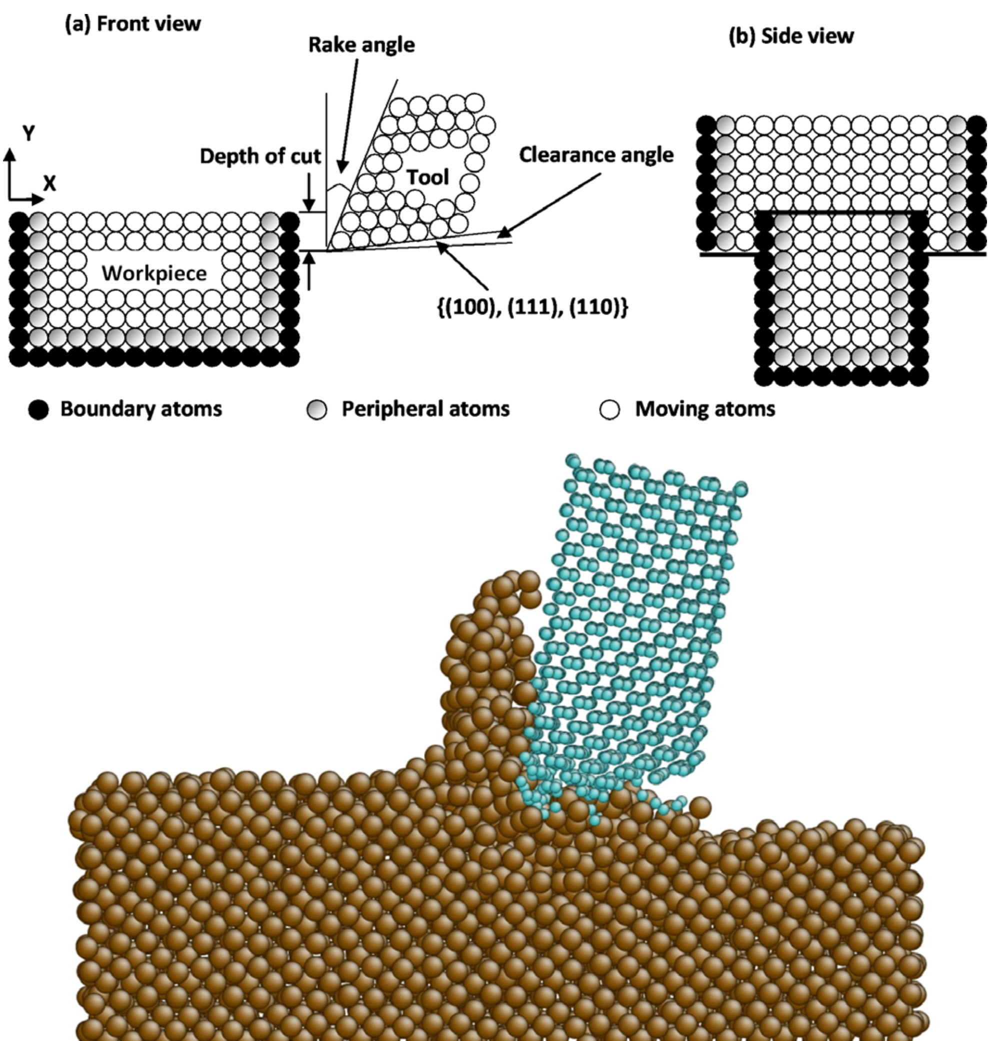

Fig. 1. (a) Schematic of MD simulation of orthogonal (or 2D) machining with a deformable tool. (b) Snapshot of MD simulation of orthogonal machining (carbon atoms are shown in cyan color and iron atoms are shown in ochre color). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)