

Effects and possible role of atmospheric molecules in ultra-micro-cutting of monocrystalline silicon

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Abstract

The effect of atmospheric gas during cutting of silicon monocrystals has been investigated experimentally. Two problems investigated in this study are the change of the critical depth of cut from ductile-to-brittle mode cutting with the existence of air and the change of the cutting force when the atmospheric molecules are sandwiched between the rake face of a tool and chips. The result obtained for the critical depth of cut shows that the value is smaller in air than in a vacuum. On the other hand, it is found that atmospheric molecules can serve as lubricant so that they reduce cutting force if they are sandwiched between the rake face of a tool and chips. This may be one of the reasons why applying ultrasonic vibration in the direction of cutting can reduce cutting force.

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1. Introduction

The cutting mechanism has long been studied mainly from mechanical and thermal points of view, even though the chemical effect in cutting has also attracted some interest [1–3]. This is because the quantities considered as mechanical and thermal effects are related to the volume of the cutting area and thus dominate conventional cutting compared with the chemical effect that arises only through boundaries to the area. In micro-cutting, however, the ratio of the boundary area to volume increases so that the chemical effects play an important role. Based on this point of view, the authors carried out a study on the effect of surface oxidation in ultra-micro-cutting of silicon monocrystals, as a first step in investigating various aspects of chemical effects in cutting. The results, which were reported in CIRP, indicated that the micromachinability of silicon monocrystals decreases considerably when their surface is oxidized before cutting [4]. It is considered, however, that the chemical effects are not factors to be considered only before cutting but also during cutting. The possibility that the chemical effect plays some role in cutting

has been pointed out in phenomena such as the brittle-to-ductile transition that occurs when cutting brittle materials [5] and the increase of machinability of difficult-to-cut materials upon applying ultrasonic vibration to a tool in the direction of cutting [6,7]. In this study, the effect of atmospheric gas during cutting of silicon monocrystals has been investigated experimentally, as the continuation of a series of studies concerning chemical effects in cutting. Two problems investigated in this study are (1) the change of the critical depth of cut from ductile-to-brittle mode cutting with the existence of air, and (2) the change of cutting force when the atmospheric molecules are sandwiched between the rake face of a tool and chips. Simulation studies reported so far will be introduced first for each of these problems to show why these problems should be investigated experimentally. Then the experimental procedure and the results obtained from the experiments will be described, together with the discussion on what has been found and what must be clarified further.

2. Change of brittleness with and without air

2.1. Results of simulation study

The authors have been studying the simulation of micro- and ultra-micro-cutting using molecular dynamics. Specifically, the

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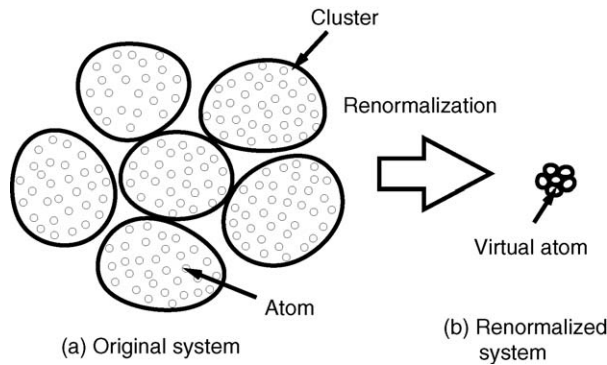


Fig. 1. Concept of renormalized molecular dynamics.

authors have been trying to extend the molecular dynamics so that phenomena on a micrometer scale can be handled. The extended method is named ‘Renormalized Molecular Dynamics’ (RMD) which consists of two steps: renormalization and MD simulation. In renormalization, an original system which contains huge number of atoms is, first, regarded as a collection of atom clusters as shown in Fig. 1(a). These atomic clusters containing arbitrarily specified number of atoms are regarded as particles and each cluster is reduced to atomic size as shown in Fig. 1(b). The MD simulation is then carried out on these virtual atoms. This method had been expected to be able to simulate brittle-to-ductile transition phenomena in cutting silicon monocrystals. The result obtained, however, did not show any such phenomena for any depth of cut, though the results showed the possibility that spaces were created in the size of several tens angstroms dynamically for a very short time, but repeatedly, in the workpiece during cutting. Because the existence of atmospheric molecules was not taken into account in the simulation, the result raised the issue that in real cutting, atmospheric molecules might fly into the crevices found in the above spaces and might change the material property there so that cracks could develop. Indeed, the result of simulation carried out with weakened interparticle potentials for those areas resulted in brittle-mode cutting [5], as shown in Fig. 2. This possibility is also consistent with the experimental result that glasses exhibited more brittleness in air than in a vacuum when being ground [8]. On the other hand, however, it was also found that the interaction between particles in the aforementioned areas in RMD should be changed not only because of the possibility mentioned above but also from a theoretical point of view. The reason for the latter arises from the demand for energy conservation which states that the interparticle potentials for a particle must be constructed so that the particle has the total potential energy of atoms included in that particle. In RMD, the interatomic potentials were used between particles based on the result that the interatomic potentials could be used for a particle if similarity existed between the particle arrangement around the particle and the atomic arrangement in that particle. This assumption is valid under pure elastic deformation of a monocrystal but it may not be valid for those areas in which the material is subjected to plastic deformation. Thus a more general form of the interparticle potentials that can be used for both elastic and plastic

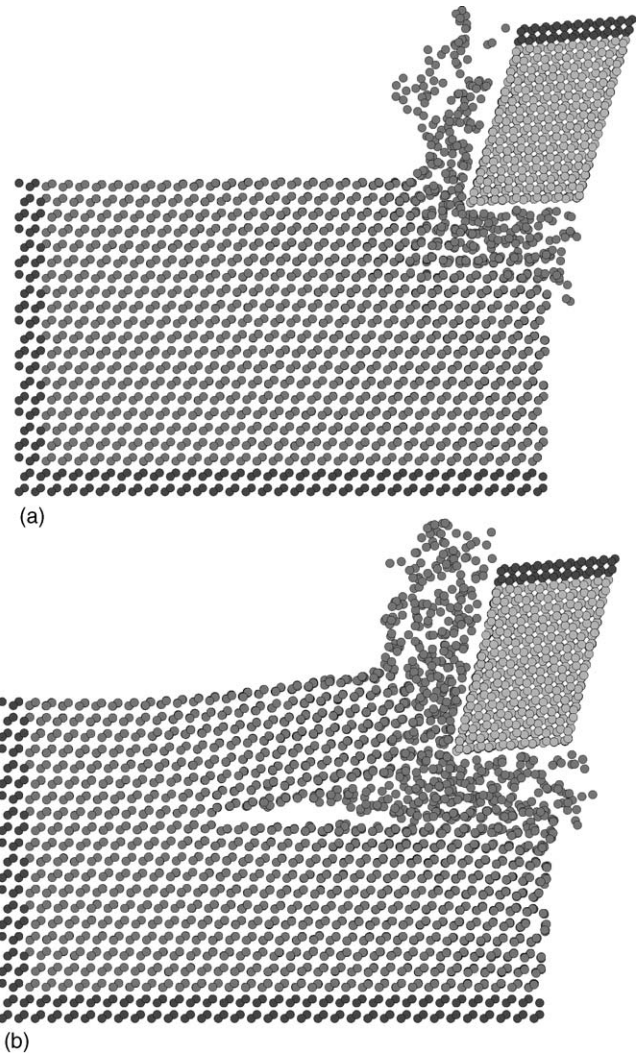


Fig. 2. Results of simulation obtained by taking into account the effect of atmospheric gas. (a) Undeformed chip thickness 0.5 μm, ductile-mode cutting (no crack appeared). (b) Undeformed chip thickness 1.0 μm, brittle-mode cutting (crack appeared in front of a tool).

deformation of a monocrystal has been derived [9]. The derived form can express the fact that both the material strength (which is proportional to the depth of the bottom of the potential curve) and the tangent stiffness (which can be related to the curvature at the bottom of the potential curve) decrease when the material is subjected to plastic deformation. Because this kind of change of the potential function is similar to that in the above simulation and thus the similar results to those obtained above could be derived without taking into account the effect of atmospheric molecules, the above results raise a new question as to what degree atmospheric molecules really affect the brittleness of a silicon monocrystal.

2.2. Experimental verification

The schematic view of the experimental setup is shown in Fig. 3. The setup consists of a machining unit, as shown in the upper part of this figure, in a vacuum chamber in which 2.0×10^{-6} Pa

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