First-Principles Evaluations of Machinability Dependency on Powder Material in Elastic Emission Machining

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Machining mechanism of EEM (Elastic Emission Machining) is investigated at the atomic level by employing first-principles molecular-dynamics simulations. Based on experimental results it has been suggested that the removal of surface atom occurs through a surface chemical reaction between the work surface and the powder surface. This reaction has been so explained that powder particle chemisorbs on the work surface, and is subsequently separated, removing a work-surface atom. In this paper, we investigate the machining mechanism by the analyses of the reaction process and the binding energy between work and powder surface based on the molecular-dynamics method. First, dependency of machinability on the powder materials is evaluated. It is recognized that the bond between the machined surface atom and the work surface is weakened, and the dependency on powder material is consistent with experimental results. Second, the molecular-dynamics analysis shows that the removal actually occurs in the unit of atom without any potential barrier and without introducing any defect around the machined atom.

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1. Introduction

Elastic Emission Machining (EEM) is an ultra-precision machining, which has performances to create atomically flat surface without introducing any defects on the work surface.¹⁴ In the EEM process, ultra-fine powders dispersed in the water are transported by water flow and come into soft contact with a work surface. This water flow leads them to immediate separation, and work-surface atoms can be readily removed in this process. The following experimental results suggest us that chemical effects should be dominant in this removal: Firstly, the removal is realized in the unit of atom, since the roughness of finished surface is at atomic level. Secondly, the dependence of the machining rate on powder and work materials disagrees with that of mechanical strength. Finally, no defects are induced on work surfaces. These properties indicate a possibility of EEM as an ultimate ultra-precision machining.

On the other hand, there is a disadvantage that removal rate is very low in spite of the above favorable properties. Therefore, selections of suitable powder materials are required to achieve the enhancement of removal rate for work materials. Experimental approach for this selection, however, needs too much effort such as troublesome experiments, production of various kinds of powders, etc. On the contrary, theoretical methods are comprehensive and beneficial to select powder materials.

Machining process should occur breaking back-bonds of a work surface on which a powder particle chemically absorbs, when the powder separate again from the surface. Therefore, evaluation of binding energies of the bonds is very important to discuss machinability dependence on powder materials.

In this paper, we evaluate the machinability dependency on powder materials and analyze the processes and the mechanisms of surface atom removal as a step of powder-material designing for EEM. The first-principles molecular-dynamics methods are employed to analyze this chemical reaction.


An atomic removal mechanism in EEM has been proposed¹⁶ as follows: In water, surface atoms of both ultra-fine powders and the work surface are believed to be terminated by hydroxide species, as shown in Fig. 1(a). When they approach and contact each other, the binding structure shown in Fig. 1(c) might be constructed through intermediate hydrogen bonding state and by dehydration reaction. The interfacial structure is unclear yet, but it is natural to assume the existence of this structure, because this kind of interfacial structure is same as usual metal oxide, e.g., SiZrO₂. Subsequently, water flow lifts up the powder, with breaking the back bonds between the work-surface atom at the interface and second-layer atoms. Monoatomic-removal process is considered to occur in this way.

3. Calculation Method

The applied simulation method is based on the density-functional theory and the local-density approximation.⁷⁻⁹ The norm-conserving pseudopotential¹⁰ is adopted. The plane wave expansion method and repeated slab model are applied with the cut-off energy 24Ry. Although this energy is not fully adequate for precise calculation of the total energies of models including oxygen atoms or zirconium atoms, the value is just enough to calculate binding energies,
4. Binding Energy Analysis

When the binding structure of powder and work is separated to each other, the weakest bond will break. In order to search which bond is the weakest, we evaluate the binding energies at separating planes 1, 2 and 3 indicated in Fig. 3 as follows: Firstly, the most stable adsorption structure of powders on the work surface is obtained through calculations of the total energies in several heights of the powder with optimization of the interfacial structure. The optimized region in the molecular dynamics is indicated in Fig. 3. Next, this optimized structure is divided into two parts at three different separating planes. Then, the binding energies are evaluated by subtracting the total energy of binding model from the sum of the total energies of divided models. The convergencies of binding energies are depicted in Fig. 4. Since the binding energies are almost converged at 24Ry, all calculations are performed at this point to save computational cost. Calculated binding energies are summarized in Table 1. It is clear that the binding energy at separating plane 3 is the smallest in both cases of powder materials, which reveals that the back bond of the surface Si atom is the weakest and that the removal of surface atom is feasible. Moreover, since the binding energy in the case of ZrO2 powder is smaller than that of SiO2, the removal of atom is easier in the case of ZrO2. Thus, the EEM machinability is higher in the case of ZrO2. This result is consistent with experimental results of the machinability dependency of Si(001) on powder materials.

Next, the weakening of the back-bond strength induced by powder attack is examined. As shown in Table 2, the back-bond binding energy without powder attack is obtained as 6.9 eV, which is smaller in comparison to that with the powder (8.3 eV (7.4 eV) in the case of SiO2 (ZrO2)). Since these
Fig. 3 Region of atoms which is structurally optimized by molecular dynamics.

![Diagram showing separation and optimization process](image)

Fig. 4 Convergence of binding energy on cut-off energy.

(a) SiO₂

(b) ZrO₂

Table 2 Revised binding energies of back-bond.

<table>
<thead>
<tr>
<th></th>
<th>SiO₂</th>
<th>ZrO₂</th>
<th>Without powder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absorption energy in the model without machined surface Si atom</td>
<td>1.7 eV</td>
<td>1.5 eV</td>
<td>—</td>
</tr>
<tr>
<td>Revised back-bond binding energy</td>
<td>6.6 eV</td>
<td>5.9 eV</td>
<td>—</td>
</tr>
<tr>
<td>Back-bond binding energy</td>
<td>—</td>
<td>—</td>
<td>6.9 eV</td>
</tr>
</tbody>
</table>

5. Molecular-Dynamics Analysis of Removal Process of Surface Atom

Though above-mentioned binding-energy analysis reveals a possibility of machining in the unit of an atom, it is still unresolved problem whether this reaction occurs with no energy barrier or not. In order to simulate this process, we perform molecular-dynamics calculations with step-by-step lifting up the powder cluster. The step length is taken to be 0.01 nm. After each lift-up step, topmost 3 layers consisting of 24 Si atoms on the surface and two O atoms (indicated by B in Fig. 2(d)) of the cluster are relaxed (Fig. 3).

Figure 5 depicts some snap shots in the simulation on each powder material. In this figure, grayed spheres represent atoms, and white clouds electron distribution (equivalent valence charge-density surface of 0.65 electrons/a.u.\(^3\)). When powders are lifted up, the Si atom at the interface (indicated by A in Fig. 2(d)) is also lifted up with being captured by the powder. The amount of electronic density at back bond between the Si atom A and the Si atom in the second layer decreases apparently, as shown in Figs. 5(c) and (f). On the contrary, the other surface atoms make no drastic motion. These
results show that the back-bonds are being broken. From the observation of inducing no defect onto the surface even in employing chemically active ideal surface models, we deduce that it is more difficult to induce defects onto real passivated surfaces. Consequently, it is concluded that a removal process in the unit of an atom with introducing no defects on machined surface is theoretically feasible.

Next, we calculate the change of total energy for lifting up the powder, as shown in Fig. 6. The energies in the cases of two powder materials both increase in lifting up them until 0.14 nm (SiO₂) or 0.15 nm (ZrO₂). The maximum values of the energies are smaller than those indicated in Table 1 because of short of lift-up height. Because a powder particle is lifted up by mechanical force generated by water flow in the real machining process, if it conquers the binding energy, the powder can be separated from work surface. It is confirmed that once the separation occurs, the surface Si atom is always removed without any thermal activation.

6. Conclusions

In this paper, we calculated the binding energy and the atomic removal process in EEM and analyzed the dependency of the machinability on powder materials by employing first-principles molecular-dynamics simulations. Obtained results are summarized as follows:

1) The binding-energy analysis reveals the weakening of the Si back-bond strength though chemical interaction originating from powder attack. Moreover, the dependency of machinability on the powder material is consistent with the experimental results.

2) Step-by-step lifting-up processes of the SiO₂ and ZrO₂ powders adsorbed on Si surface shows that the Si atom at the interface is lifted up with being captured by the powder, and the amount of electronic density decreases.

3) Non-induction of defects onto the machined surface is theoretically clarified.

4) From (1) to (3), it is concluded that a monoatomic
removal process with introducing no defects onto the surface is feasible.

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