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Applicability of random sequential adsorption algorithm for simulation of surface plasma polishing kinetics

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ABSTRACT

Applicability of random sequential adsorption (RSA) model for the material removal during a surface plasma polishing is discussed. The mechanical nature of plasma polishing process is taken into consideration in modified version of RSA model. During the plasma polishing the surface layer is aligned such that molecules of material are removed from the surface mechanically as a consequence of the surface deformation induced by plasma particles impact. We propose modification of RSA technique to describe the reduction of material on the surface provided that sequential character of molecules release from the surface is maintained throughout the polishing process. This empirical model is able to estimate depth profile of material density on the surface during the plasma polishing. We have shown that preliminary results obtained from this model are in good agreement with experimental results.

We believe that molecular dynamics simulation of the polishing process, possibly also other types of surface treatment, can be based on this model. However influence of material parameters and processing conditions (including plasma characteristics) must be taken into account using appropriate model variables.

1. Introduction

Standard random sequential adsorption (RSA) is a process in which objects are placed at random on a surface such that they do not overlap with any that have already been successfully placed. Once the object is placed on the surface, the position of this object remains permanently fixed. This fact ensures the irreversible character of the adsorption process. Initially, the probability of placing a new object is high and objects fill surface rapidly. As the surface coverage increases, the adsorption probability decreases. It is due to exclusion effects from pre-adsorbed objects. Process continues until it is impossible to place another object without overlap. This condition, associated with a zero probability of adsorption, is commonly known as the "jamming limit". For a RSA on a continuous uniform surface, the approach to the jamming limit is characterized by specific time dependence.

In the past much interest has been devoted to the study of the adsorption of colloidal particles in solid surfaces [1,2]. In general, RSA process becomes complex because one should take into account the different forces which influence the rate of the arrival of each particle at the surface, as well as its relative position with respect to the pre-adsorbed ones [3,4]. In order to study the adsorption kinetics, attention has been focused mainly on the effect of surface exclusion. It is necessary to consider the fact that once a particle is adsorbed it reduces the available surface for further adsorbing ones. Two models have been proposed to take these effects into account. First of them is RSA model [5,6]. In this model if the center of the incoming particle, whose position has been randomly chosen on the surface, overlaps with a previously adsorbed one, it is rejected and a new random position is selected. Otherwise, the particle is located irreversibly at that position. Despite its simplicity, experimental results on the adsorption of diffusing latex spheres and polymers seem to agree with its predictions [7,8]. Further the ballistic model (BM) [9,10] was proposed. In this model if the center of the incoming particle overlaps with a previously adsorbed one, it is allowed to roll over it, approaching the surface along the steepest descent path. The particle is rejected only when it cannot reach the surface. Otherwise, it is irreversibly located at that position as well [11].

It is no problem to understand why the RSA model has received so much attention [12–22]. Although the defining algorithm for this irreversible process is simple, obtained results are complex. Simulation studies, particularly of non-spherical particles, require considerable computational resources. Such resources were not available when the model was first proposed [23,24]. Currently the RSA is thought to be applicable to a wide variety of physical,

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chemical and biological processes. A number of related models have also been studied using RSA algorithm [25–28] including surface development [29,30].

A lot of models to describe the kinetics of polishing process have been proposed up to now [31–34]. In this article we introduce a new possibility to use RSA technique for the modeling of plasma polishing kinetics. We suggest to apply this algorithm in the case when particles are not adsorbed on the surface according to standard RSA rules, but conversely they gradually escape from the surface. This is a particular type of desorption which can be regarded as an inverse process to adsorption. The particles may evaporate from the surface only in such a case when they do not overlap with any that have been placed above them. We assume that sequential character of this process is dominant. Our goal is to describe kinetics of the particles vaporization from the surface through a statistical probability analysis.

2. Using of random sequential adsorption algorithm in surface plasma polishing regime

A variety of molecules are located at the individual levels in the material surface. We consider that disruption of binding occurs due to the impact of electron from plasma discharge and molecule is vaporized from the surface. Let P is the probability that electron hits the surface in position x. The sequential character of electrons impact and local character of energy transfer between electron and the surface are assumed. Whereas the electrons impact the surface sequentially, it is possible to calculate the probability of removal material from surface at each sequence. We assume that the density of incident plasma electrons is constant and layered structure of surface is considered in the model. Molecule can be released from the surface only in case if this molecule interacts directly with incident plasma electron. If molecule from nth layer on surface has to be released, $n-1$ molecules placed above it must be released before. By means of combinatorial rules it is easy determine probability of release of molecule from nth layer if plasma electrons impact surface sequentially. Therefore the probability of molecule evaporation in position x from the second molecular layer on the surface during individual sequence of plasma electrons impact can be calculated:

in the first sequence: $w_1^{(2)} = 0$, in the second sequence: $w_2^{(2)} = P^2$ in the third sequence: $w_3^{(2)} = \binom{3}{2}(1-P)P^2$, in the fourth sequence: $w_4^{(2)} = \binom{4}{2}(1-P)^2P^2$,

in the fifth sequence: $w_5^{(2)} = \binom{5}{2}(1-P)^3P^2 \ldots$ etc. . .

Similarly, the probability of particle evaporation from second molecular layer on the surface during any kth sequence of electrons impact can be calculated as:

$$w_k^{(2)} = \binom{k}{2}(1-P)^{k-2}P^2 \tag{1}$$

Generally, the probability of particle evaporation from arbitrary ith molecular layer on the surface during any jth sequence is given by formula:

$$w_j^{(i)} = \binom{j}{i}(1-P)^{j-i}P^i \tag{2}$$

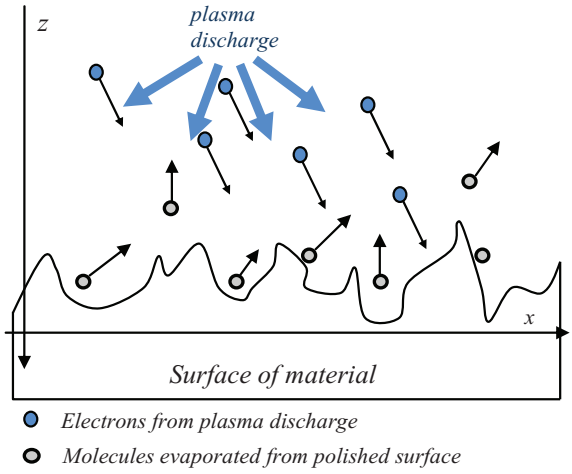

Fig. 1. Scheme of surface plasma polishing.

where binomial coefficients:

$$\binom{j}{i} = \frac{j!}{(j-i)!i!} \tag{3}$$

determine number of distinct subsets with i elements that can be chosen from a set with j elements. We note that $j > i$.

3. Continuum limit

We assume random sequential character of particles evaporation from the material surface during the plasma polishing process. Sequential character is given by the gradual separation of particles from individual layers on the surface toward the volume. Scheme in Fig. 1 intuitive encourages the notion about random and sequential character of removal of material from the surface. Simulation of plasma polishing process requires a definition of algorithm enabling to describe material losses from surface. Fig. 2 explains that the formal concept of this algorithm could be essentially equivalent with RSA technique. We believe that scheme in Fig. 2 is sufficient for gaining deeper understanding of the interpretative key to such algorithm. Limiting case is considered when the material loss occurs point by point and size of vaporized particles is negligibly small (zero). Characteristic parameters of separated particles (their shape, size, binding forces, etc.) and also plasma processing conditions are hidden in the value of probability P in this context. The corresponding correlation functions can be investigated in future. We assume that plasma electrons impact on the

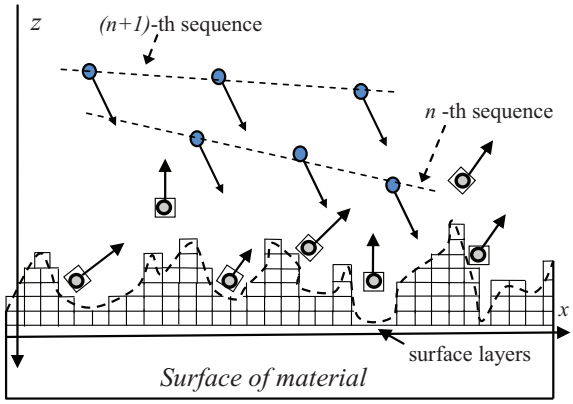

Fig. 2. Concept of modified RSA algorithm application for surface plasma polishing process.