Journal of Engineering Physics and Thermophysics, Vol. 76, No. 2, 2003

MODELING OF THE SURFACE STRUCTURE IN GASDYNAMIC PROBLEMS WITH THE USE OF THE DATA OF ATOMIC-FORCE MICROSCOPY

O. E. Gerasimova,[a] **S. F. Borisov,**[a]
C. Boragno,[b] **and U. Valbusa**[b]

UDC 533.722:541.183

The morphology of the surface of single-crystalline silicon as a function of the degree of oxidation has been investigated by the method of atomic-force microscopy. The roughness of the surface at different stages of treatment has been evaluated with the use of topographic images. It has been found that the standard deviation characterizing the distribution of microroughnesses by height, or the roughness, increases with oxidation of the sample. A histogram of the distribution of structural surface elements has been presented. The data obtained can be employed in specifying boundary conditions to gasdynamic problems.

Investigations aimed at studying the surface structure and the kinetics of interphase interactions have been activated significantly in recent years. This is dictated by the needs of various fields of science, engineering, and technology. Thus, for example, the development of new semiconductor devices and the element base of microelectronics necessitates fundamental research of the surface properties of semiconductor materials. A study of the surface microstructure is topical for such fields as cryosorption engineering, techniques of production of materials with specified properties (in particular, CVD-techniques), and the aerodynamics and heat exchange of aircraft.

It is well known that the microstructure of the surface exerts a substantial influence on the parameters determining the interaction between it and gases. Such parameters include, for example, the momentum and energy accommodation coefficients, the probability of scattering of molecules by the surface, and the condensation coefficient. The microstructure of the surface is of considerable importance in the formation of a rarefied-gas flow in the case of external and internal flow past it [1–6]. It has been shown experimentally in [7] that the method of treatment of the surface exerts a significant influence on the gasdynamic conductivity of a cylindrical channel, especially for light gases.

Until recently, the shortage of information on the surface microstructure was compensated for with construction of different models, each of which reproduced the structure of specific surfaces by prescribing the shape of the hypothetical elements of the microstructure and angles of orientation of crystal faces. Following this path, Sazhin et al. [8] attempted to construct a microstructure model on the basis of the method of direct statistical modeling of Monte Carlo — the probe-particle method — and to apply this model to description of the results of an investigation of rarefied-gas flow in a rectangular channel. The surface microstructure was modeled in the shape of triangles with specified average heights of microroughness and base angles. Another (statistical) model given in [9] is based on the assumption that individual elements of the surface microstructure represent cones with equal heights and base angles. The cones are in contact, as is shown in Fig. 1. In our opinion, this model approaches an actual situation and it is promising. The next step on the road to modifying it could be to account for the distribution function of the cones by height and slope. It becomes possible to obtain such a distribution function from experiment at present owing to the development of the methods of probe scanning microscopy and, in particular, of atomic-force microscopy.

By the atomic-force-microscopy method we have investigated the microstructure of the surface of single-crystalline silicon subjected to chemical cleaning and subsequent oxidation. We determined the parameters of the surface microstructure, in particular, the standard deviation characterizing the distribution of microroughnesses by height (or the roughness), and the average height of the microroughnesses and evaluated the fractal dimension.

Measurement Procedure and Technique of Processing of the Initial Data. To investigate the evolution of the microstructure of the sample's surface we employed an AutoProbe CP atomic-force microscope (Park Scientific In-

[a]Ural State University, Ekaterinburg, Russia; email: Sergei.Borisov@usu.ru; [b]Genoa University, Genoa, Italy.
Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 76, No. 2, pp. 151–154, March–April, 2003. Original article submitted October 11, 2002.

1062-0125/03/7602-0413$25.00

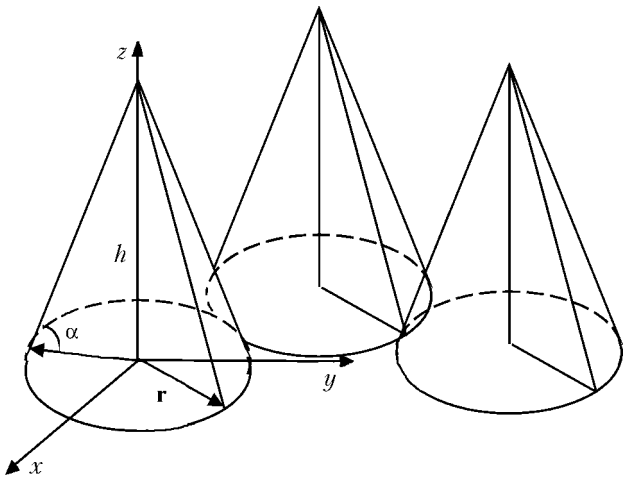

Fig. 1. Statistical model of roughness [9].

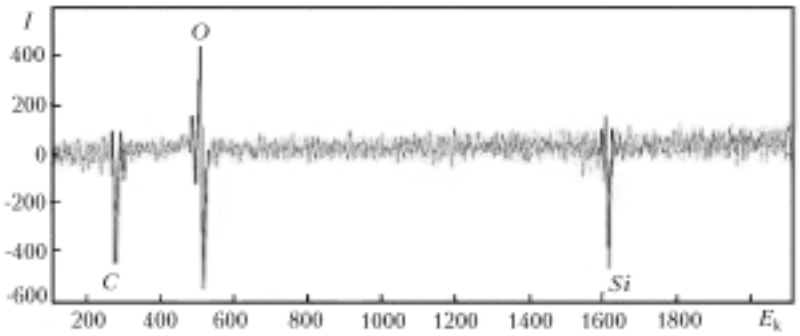

Fig. 2. Auger spectrum of the silicon surface, which has been obtained after the storage of the samples in air for several hours.

struments). The measurements were performed in air in the contact regime. We employed a V-shaped cantilever with a conic probe of silicon nitride with a radius of curvature at the base of ~10 nm. The size of the scanning region varied from 5 to 20 μm.

We cut (1 × 1)-cm samples with surface Si(100)–(2 × 1) from a single-crystalline-silicone plate. The surface of the samples was initially covered with a layer of natural oxide. To remove it we held the samples for 10 min in a 1% solution of hydrofluoric acid. To clean organic contaminants from the surface we treated it with acetone. As is well known, such a treatment does not lead to a change in the surface structure of silicon at the atomic level. At the same time, chemical etching with hydrofluoric acid can cause a significant change in the surface roughness.

A chemical analysis of the surface was made by the method of Auger-electron spectroscopy with the use of a PHI Model 5600 Multi-Technique system. As the analysis showed, the silicon peak was the main signal in the Auger spectrum after the chemical etching of the sample's surface. Storage of the samples for several hours in air led to the appearance of a signal corresponding to oxygen. An example of the Auger spectrum obtained is shown in Fig. 2.

The procedure of measurement of the degree of microroughness of the samples in the process of natural oxidation of the surface involved recording of the microstructure image using the atomic-force microscope.

In describing the evolution of the surface microstructure, we calculated the parameters characterizing the microroughness of the surface at different stages of the experiment.

The microroughness of the surface was determined by the value of the standard deviation of the microroughness or by the fluctuations in height [10]:

$$w = \frac{1}{N}\sqrt{\sum_{i}^{N} (h_i - \bar{h}_i)^2} \quad . \tag{1}$$

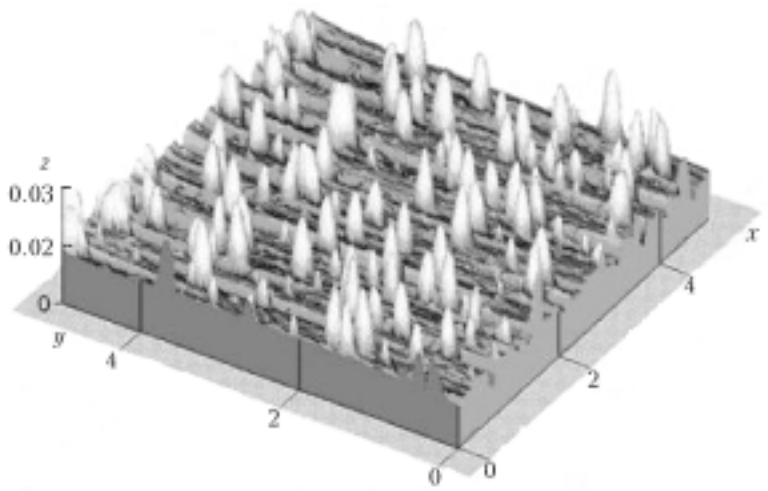

Fig. 3. Topogram of the silicon surface totally covered with silicon dioxide. The size of the scanning region is $(5 \times 5) \cdot 10^{-6}$ m.

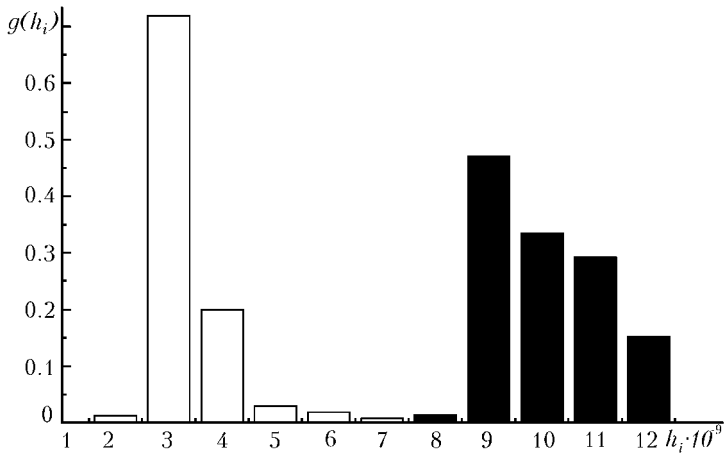

Fig. 4. Histogram of the size distribution of the elements of the surface microstructure. Light columns, sample's surface totally covered with the layer of natural oxide; dark columns, cleaned surface of the sample.

Summation was made over all the points of the data matrix. The global surface roughness was obtained by averaging w over all topograms.

The average height of the microstructure elements was found from the average height within the limits of the selected profile according to the standard definition:

$$R_{\mathrm{a}} = \frac{1}{N} \sum_{i}^{N} h_i \,. \tag{2}$$

To characterize the spatial complexity of the microstructure we made a fractal analysis. The fractal dimension of the surface of the silicon samples was evaluated using the variational method described in [11] in detail.

Discussion of the Results. We obtained images corresponding to the following surface states: a) total coverage with the layer of silicon dioxide, b) cleaned surface immediately after the etching procedure, and c) different stages of oxidation. Figure 3 gives an example of the topogram of the surface totally covered with a layer of natural silicon oxide.

The found values of the silicon-surface microstructure were employed for construction of the model of the microstructure. As such a model we selected the statistical cone model. From a comparison of the topogram of the sur-

TABLE 1. Values of the Parameters Characterizing the Surface Microstructure

Type of the sample surface	Parameters of the surface microstructure			
	$w \cdot 10^{-9}$, m	$R_a \cdot 10^{-9}$, m	D_f	α, deg
Totally covered with silicon dioxide	0.8	5.1±0.1	1.8	80.4
After chemical etching	0.6	16.7±0.3	1.6	60.9
Partially oxidized	0.7	12.5±0.2	1.8	67.2

face (Fig. 3) and the model representation of the structure it is clear (Fig. 1) that the cone model describes the actual situation quite well. In modeling the surface microstructure, we employed the quantity R_a determined experimentally as the parameter of the model h. The radius of the cones was selected to be equivalent to half the distance between the centers of the cones, which was $6 \cdot 10^{-8}$ m in our case. The angle α was easily computed based on the geometry of the problem. The results of the calculation of the above parameters are given in Table 1.

Using the data on the microroughness, we have constructed a histogram of the size distribution of the structural elements of the surface, which is presented in Fig. 4. As is seen in the figure, the peak in the distribution function for the cleaned surface shifts in the direction of increasing values. The reason for this could be the fact that the growth of the natural oxide on the surface is frequently nonuniform.

Thus, in the present work, we have made an attempt to apply the data obtained by the atomic-force-microscopy method on the surface structure to evaluation of the parameters of the microstructure model employed in numerical modeling in gasdynamic problems. At the same time, one can employ these data directly in the boundary conditions in the process of calculation of the heat exchange and gasdynamic resistance of bodies in motion in a rarefied-gas flow.

This work was partially supported by the American Civic Research and Development Foundation for the Independent States of the former Soviet Union (CRDF), No. REC-005. A part of the investigations was carried out within the framework of the INTAS International Program, No. 99-007-49.

NOTATION

h_i, measured values of the height of the surface element at point i, m; w, standard deviation of the roughness; R_a, average height of microroughnesses, m; h, parameter of the microstructure model; N, number of points within the limits of the selected profile; α, slope of the structural elements, deg; D_f, fractal dimension; **r**, radius of the cone in the statistical model, m; $g(h_i)$, distribution function of the structural elements by height; x, y, and z, parameters of the topogram, μm; E_k, kinetic energy, eV; I, intensity, pulse/sec. Subscripts: a, average; f, fractal; k, kinetic.

REFERENCES

1. J. Huggel, *Proc. Roy. Soc.*, **212a**, 123–136 (1952).
2. L. M. Lund and A. S. Berman, *Chem. Phys.*, **28**, 363–364 (1958).
3. B. T. Porodnov, P. E. Suetin, S. F. Borisov, and V. D. Akins, *J. Fluid Mech.*, **64**, No. 3, 417–437 (1974).
4. W. J. Maegle and A. S. Berman, *Phys. Fluids*, **15**, 772–780 (1972).
5. E. Steinheil, W. Scherber, M. Seidl, and H. Rieger, in: *Proc. X Int. Symp. Rarefied Gas Dynamics*, AIAA, New York (1977), pp. 589–602.
6. F. Sharipov and V. Seleznev, *Phys. Chem. Ref. Data*, **27**, No. 3, 657–706 (1998).
7. D. H. Davis, L. L. Levenson, and N. Mileron, *Appl. Phys.*, **35**, 529–532 (1964).
8. O. V. Sazhin, A. N. Kulev, and S. F. Borisov, *Teplofiz. Aéromekh.*, **8**, No. 3, 391–399 (2001).
9. T. Sawada, B. Y. Horie, and W. Sugiyama, *Vacuum*, **47**, No. 6–8, 795–797 (1996).
10. A. L. Barabasi and H. E. Stanley, in: *Fractal Concepts in Surface Growth*, Cambridge (1995), pp. 9–30.
11. L. Spanos and E. A. Irene, *Vacuum Sci. Technol.*, **A12**, No. 5, 2646–2652 (1994).