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The Model of Local Fracture on Brittle Material Surface during Machining

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Abstract. Brittle materials such as ceramics, glass or single-crystal silicon are extensively used for industrial applications and recently become an object of actual research due to the development of new products and technologies. In cases, where special attention is paid to the surface layer, mechanical processing with a diamond tool is of interest as one of the most efficient technology to manufacture products from brittle materials. In this paper, simulation method is presented, which allows to estimate an effect of cutting force on the size of defects zone formed in a hard brittle plate during machining. In the proposed model, there is a distinguished surface layer, which can have its own unique properties that differ from the properties of the brittle plate. In this work, the ANSYS finite element program is used to simulate the technological processes and solve the problem of stress distribution in a quasi-static formulation.

Introduction

Slicing single-crystal ingots into thin wafers, dividing semiconductor wafers into crystals, obtaining the required complex geometry, removing a layer from the surface, as well as grinding and polishing [1] are all the main machining technologies for manufacturing electronic and optical components. Usually, cutting tools and modes developed for processing metals and widely used in mechanical engineering are not quite enough viable to perform the listed operations due to the increased brittleness of single-crystal and ceramic or glass materials [2].

The process of machining brittle materials is aimed at local destruction and removal of material from the surface. Information on the fracture of brittle materials is needed to optimize and simulate the process. However, most brittle fracture theories have been developed in detail to ensure structural strength and prevent damage of the structure, so they are not completely meaningful for simulation of machining [3]. Currently, the behavior of brittle materials under the force loading has been intensively studied in connection with hightech applications in the production of high-quality components of optical systems, semiconductor and micromechanical devices [4]. Directional destruction of brittle materials during machining has specific features. In particular, such brittle materials could remain linearly elastic until the last stage of deformation followed by fracture [5].

When modeling the process of machining, a complex of phenomena in the deformation zone of the processed material and on the contact surfaces of the tool should be taken into account [6], for example, it becomes necessary to study the mechanism of local fracture through cracks propagation and formation of chips [7]. To simulate brittle fracture and calculate stresses in the material to be cut, the FE (Finite Element) solver method of CAE (Computer-Aided Engineering) programs can be used [8]. In the general setting, the problem of this simulation includes dynamic, nonlinear and singular effects [9]. The complexity and multiphysical content of the problem being solved often requires the use of supercomputing, which can be easily accessed in a modern infrastructure through cloud services [10]. The purpose of this study is to create a model of brittle materials fracture under force loading, which could be suitable for optimization of cutting parameters and integrating the CAE software tools into the CAM (Computer-Aided Manufacturing) programs.

Brittle fracture model in the case of linear movement of diamond cutter

By means of mathematical and computational modeling, it becomes possible to control the process of brittle fracture during machining through correctly assigned technological parameters, which could be optimized, taking into account some appropriate failure criterion. Figure 1 shows a 3D model of brittle plate in contact with a diamond cutter tip that moves along a straight line at low speed, creating a scratch on the surface of the plate.

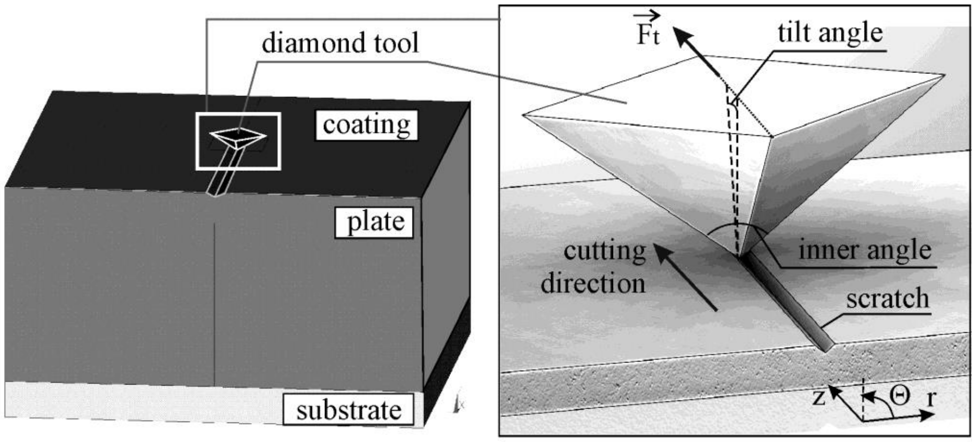


Figure 1. 3D model of a brittle plate in contact with a diamond cutter tip

The failure criterion is used to predict the size of the defects zone, based on the results of stress calculations, and it states that local failure occurs when internal stresses exceed a critical value. When machining, in addition to beneficial fracture required to form a scratch on the surface of the plate, unacceptable cracking can occur. Partial removal of brittle material occurs in a small volume around the cutter tip and goes through three stages. At the first stage, lateral and conical cracks are formed. At the second stage, a favorably located crack grows, which leads to the cleavage of the material fragment and increase of force. In the third stage, the separated fragment leaves the working surface, and the cutting force at the point of contact drops to zero. The location of the cracks along the scratch can be indicated by an isoparametric surface of shear stress τ in a cylindrical coordinate system (r, Θ, z).

The field of elastic stresses τ in a brittle isotropic plate under loading by force Ft co-directed with the cutting speed is determined within the framework of Cherutti problem [2], the solution of which in spherical (ρ, Θ, φ) and cylindrical (r, Θ, z) coordinate systems can be represented as:

$$\tau_{rr} = \frac{F_t}{2\pi\rho^2}\, cos\theta \left(\frac{(1-2\mu)\, sin\varphi}{1+cos\varphi} - 3\, sin^3\varphi\right) = \frac{F_t}{2\pi}\, cos\theta\, \frac{r}{r^2+z^2}\left(\frac{1-2\mu}{z+\sqrt{r^2+z^2}} - \frac{3\, r^2}{(r^2+z^2)^{3/2}}\right),$$

$$\tau_{\theta\theta} = \frac{(1-2\mu)\, F_t}{2\pi\,\rho^2}\, cos\theta\, sin\varphi \left(1 - \frac{1}{(1+cos\varphi)^2}\right) = (1-2\mu)\frac{F_t}{2\pi}\, cos\theta\, \frac{r}{r^2+z^2}\left(\frac{1}{\sqrt{r^2+z^2}} - \frac{\sqrt{r^2+z^2}}{\left(z+\sqrt{r^2+z^2}\right)^2}\right),$$

$$\tau_{zz} = \frac{F_t}{2\pi\rho^2}\, cos\theta\, (-3\, sin\varphi\, cos^2\varphi) = -3\frac{F_t}{2\pi}\, cos\theta\, \frac{r}{r^2+z^2}\, \frac{z^2}{(r^2+z^2)^{3/2}}, \qquad (1)$$

$$\tau_{rz} = \frac{F_t}{2\pi\rho^2}\, cos\theta\, (-3\, sin^2\varphi\, cos\varphi) = -3\frac{F_t}{2\pi}\, cos\theta\, \frac{r}{r^2+z^2}\, \frac{zr}{(r^2+z^2)^{3/2}},$$

$$\tau_{r\theta} = \frac{F_t}{2\pi\rho^2}\, sin\theta\, \frac{(1-2\mu)\, sin\varphi}{(1+cos\varphi)^2} = (1-2\mu)\frac{F_t}{2\pi}\, sin\theta\, \frac{r}{r^2+z^2}\, \frac{\sqrt{r^2+z^2}}{\left(z+\sqrt{r^2+z^2}\right)^2},$$

$$\tau_{r\theta} = 0\,,$$

where μ is Poisson's ratio; the polar coordinates ρ and φ are related to the cylindrical coordinates r and z by the relations: r = ρsin φ, z = ρ cos φ; and when ρ → 0, τ → ∞, which leads to the appearance of singularity.

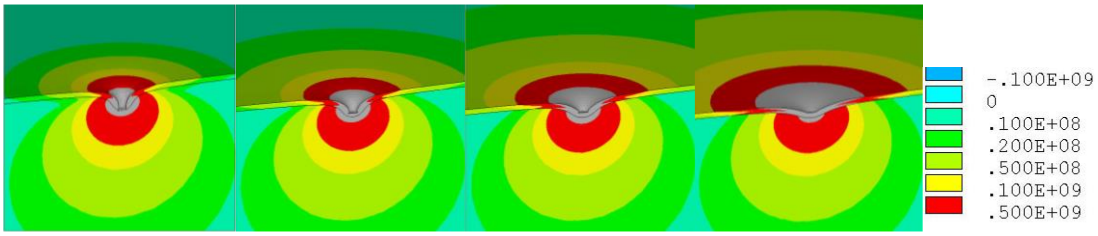
Due to the low speed of the cutter movement, the problem of stresses in the plate can be solved on a FE mesh in a simplified quasi-static formulation. The model was described by a set of parameters, including dimensions of the tool and plate itself, substrate and surface layer, as well as the depth of cut and cutting force. An essential geometric parameter of the FE model is the angle of rotation of cutting tool around the normal to the plate surface, which determines orientation of the tool in space and position of the main cutting edge. In accordance with the input parameters, the model was built using preprocessor of CAE ANSYS software. The most important output parameter of finite element modeling for further development of the cutting process is the width of the defect zone along the scratch, which is determined by the r coordinate in the declared cylindrical coordinate system.

Simulation of stresses in brittle material under force loading

Machining of brittle materials is a special class of technological processes in mechanical engineering, which is the most difficult object for simulation by the FE method. In the simulation, it is necessary to take into account a large number of nonlinear parameters that determine the local destruction of brittle material, local heating, cutting speed and force, tool geometry, its friction and wear, formation and removal of chips, behavior of the surface layer, contact of the cutting tool with the material. In this work, FE simulation was performed using interface of the ANSYS Mechanical program and ANSYS parametric programming language (APDL).

The parametric simulation model considers static effect of cutting tool on a brittle plate with coating layer and set by parameters the materials properties, geometry, boundary conditions, type and size of FE elements, contact and solver settings. It is assumed that increased strength, optical, semiconductor and other advantageous properties in the surface layer of the brittle plate can be obtained by coating with a material, which differ from the brittle material due to chemical composition or special treatment, for example, doping or heat treatment. In this case, the advantage of cutting with diamond tool is the ability to maintain a low temperature in the cutting zone, which is important for doped and organic coatings.

The parametric simulation model can be used for studying a wide range of brittle materials, coatings and machining conditions. As an example, Figure 2 graphically presents the results of such study for silicon wafer covered with film of 2 µm thick. The wafer is loaded by a diamond cone, the same force loading is applied to the cone, while the hardness of the coating varies in computational experiments. The pictures show the influence of Young modulus on the distribution of stress intensity over the film and in the cross section of the silicon wafer. The stress intensity is defined as the maximum difference in principal stresses $S_I = \max(|S_1 - S_2|, |S_2 - S_3|, |S_3 - S_1|)$.



a b c d

Figure 2. Distribution of stress intensity (Pa) in the cross section of a silicon wafer for Young modulus of the coating material equal to (a) 25, (b) 70, (c) 200 and (d) 800 GPa

Stresses in coatings and especially at the interface with the base plate must be taken into account when manufacturing and using components of electronic and optical devices. The functional coating on the plate can be thin or thick depending on its thickness. Films on the surface of a silicon wafer less than 1 µm thick are considered thin. Thick films have a thickness of 1 to 100 microns or more, such films have their own structural rigidity.

To provide special properties on the surface of components, thin metal and dielectric films are created, flat or spatial structures are formed by various methods, in particular, on single-crystal silicon wafers. Thin-film coatings are created by vacuum thermal evaporation, ion sputtering and thermal ion evaporation. To create the most perfect structures, epitaxy is used, which consists in the deposition of single-crystal semiconductor films on single-crystal wafers. Epitaxy forms a thin layer of deposited semiconductor material that closely follows the surface structure of the base plate. Epitaxial heterostructures, such as quantum wells and superlattices, have unique optical and electrical properties, so that bulk materials similar in composition do not show such properties.

A significant advantage of parametric modeling is that the model is represented by a short program code and can be used to work in the cloud. In the case when the simulation is performed in the cloud, the model is transferred as a text file and launched into the command line of the ANSYS program installed on the remote workstation. The calculated stresses are also saved to the text file and transferred back to the user's computer. A distinctive feature of the developed model is the ability to set input parameters that determine the conditions of force loading, and after the completion of simulation, the user can process the output parameters that determine the mode of cutting technology. Due to the parameters, it becomes possible to create an information link between CAE and CAM programs. The CAE/CAM integration meets the latest requirement in CAM software development to physically justify the assignment of cutting parameters.

Observation of cracks in silicon wafer along the scratch

To compare the calculated width of defect zone with the experimental one, a full-scale experiment was carried out. Scratches were made with a diamond tool on the surface of silicon wafer and then observed with optical microscope. Figure 3 (a) shows a dark-field image of the scratch made by the edge of the tool in the crystallographic direction <112> on the surface {111} of the wafer. Dark field imaging reveals subsurface cracks along the scratch, the estimated width of the defects zone is about 30 μkm. Figure 3 (b) shows an optical image of the scratch applied with conical tool. The experimentally observed width of the defect zone corresponds to the calculated data. The stresses calculated using the program within 4% coincide with the theoretical ones. The analysis of the observed defects along the scratch line confirms the theoretical approaches to modeling the fracture on brittle material surface during machining.

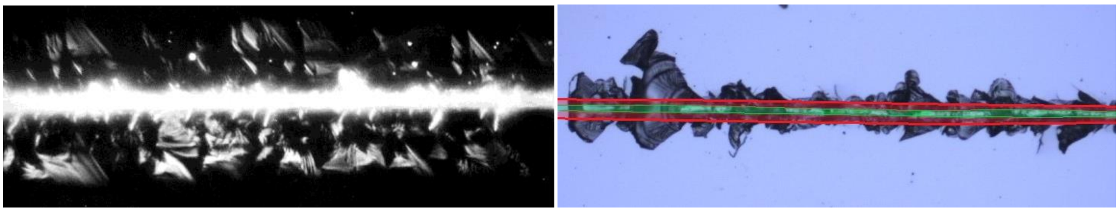

a b

Figure 3. Defects zone along the scratch, including subsurface cracks (a) and chips (b) on the surface of silicon wafer

The observed strip of subsurface defects along the scratch consists of cracks that have grown in the brittle material from the points of contact with the cutting edge of the tool. Having initiated cracks propagate in the area of increased stresses and stop, reaching the area in which the maximum shear stresses are less than the destructive stresses. Some cracks reach the plate surface and form visible chips, which violate the flatness of the processed surface.

The formation of defects along the scratch can be explained similarly to the theory of turning with a lathe tool. The position of the front surfaces and cutting edges of the cutting tool, when scratching silicon wafer, corresponds to the theoretical model of oblique non-free cutting. The most unfavorable option is cutting with large and negative rake angles for the edges forming the sides of the scratch and large positive values of the tool main cutting edges inclination angles. The type of chips and the mechanism of their formation at the contact with the front surface of the tool also appears to be similar. In the case of processing brittle materials with large cutting depth and large front angles, tearing stresses appear in the cut layer, and large particles of irregularly shaped material are torn out or chipped off, so, breakage chips are formed. Elemental chips are generated, if the cutting speed is increased.

When scribing silicon wafers with a diamond tool, defects and local fracture depend on the normal force applied to the cutting tool. Under normal tool load 0.001 ... 0.1 N and a depth of cut of 0.1 ... 0.5 µm, elastic-plastic deformation is observed. At a load of 0.5 ... 1 N and a depth of cut of 0.7 ... 5 µm, brittle fracture occurs, respectively, cracks and chips cover micron volumes of silicon along the scribing line. At loads 3 ... 12 N the processes of microplastic deformation of the surface layers are insignificant, and the stage of plastic deformation in the cut volume of the brittle material is not observed. Force loading at values over 12.. .15 N leads to unacceptably large chips and destroys the plate.

To obtain a high-quality processed surface, it is required to achieve local brittle fracture by setting the depth of cut, which exceeds the thickness of the surface layer with high ductility. On the one hand, a too shallow scratch depth corresponds to plastic deformation and ductile fracture in the surface layer. On the other hand, an excessive increase in the scratch depth provides a transition to elastic behavior and uncontrolled brittle cleavage. The nature of local fractures on the surface of a brittle plate can be controlled by a reasonable choice of the normal force load on the cutter and its edge radius. Large cutting edge radius and low loading forces plastically deform the surface and can be the physical basis for single-point turning technology. Small cutting edge radius, which is less than the depth of cut, and medium loading forces provide a sharp scratch tip and reliable separation of the silicon wafer along the scribing line.

Various types and modes of processing a brittle material with a diamond tool can be simulated using the created computational model.

Summary

In conclusion, the model of machining brittle material is proposed, which is suitable to estimate stresses in FE simulation and predict formation of large defect zone along the scratch. The model emphasizes the relationship between essential process parameters and surface quality. The essential technological parameters for cutting brittle materials are cutting force, cutting depth and angles of tool geometry. Since the cutting speed is low and therefore does not significantly affect the formation of defects, the process of cutting brittle materials is simulated under conditions of quasi-static loading. The surface quality of a brittle material after cutting is determined not only by the appearance of visible chips on the surface, but also by the presence of subsurface cracks.

A criterion is formulated for evaluating the zone of subsurface defects along a scratch based on the results of stress calculations. The criterion takes into account the initiation and propagation of subsurface cracks in the stress field. Under force loading, cracks appear in the zone of destructive normal compressive stresses, propagate along the trajectory of maximum shear stresses, and stop growing on the iso-parametric surface of the critical stress. In the case where the cutting tool forms a scratch on the surface, for example, during scribing or engraving, the calculated stress field can be analyzed in a cylindrical coordinate system.

The use of the parametric model and a solver of the CAE program in the cloud makes it possible to effectively optimize parameters of cutting mode for brittle material that provide a minimum defect zone on the surface.

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