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Microstructure replication using high frequency vibroactive pad

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1. Introduction

Micro level relief formation on the surface of polymer is demanded technique in various application fields like: optics, electronics, microfluidic devices [1]. In the case of this paper, created microstructure will be employed as a diffractive optical element, thus diffraction efficiency is considered as significant quality parameter.

Typically microstructures of high aspect ratio are produced by the method of injection molding, hot embossing and ultrasonic hot embossing [2]. Because of advantages, like: high aspect ratio and low cost equipment, hot embossing is chosen to replicate microstructures in this paper [3].

Hot embossing [2] is a microstructure formation technique, used for imprinting microstructures on a substrate, using preheated master mold. It consists from following steps. First of all polymer is being preheated until polymer glass transition temperature (T_g), this allows minimize the force, required to deform the polymer. Then, the polymer is being imprinted with the desired imprint with particular imprint force, at the temperature, under which it behaves fluid-like. Finally, the mold is being withdrawn from the surface of polymer [4].

Besides process advantages, it is necessary to take into account possible risks of potential defects of the microstructure that can occur as a result of the melting the material and withdrawal of mold from the surface of polymer. Most common defects include material shrinkage, bubbles of residual gas, which remain within the polymer after the process, insufficient filling ratio of the master mold shape, high surface roughness, non-uniform mold imprint, cracks (mainly because of adhesion between mold and polymer) etc. [5-10]. Insufficient filling ratio of microstructure, i.e. master mold is not being replicated precisely according to its shape, causes lower diffraction efficiency.

Major factors, which influence the quality of created microstructure are: temperature, pressure and time of process[11-13]. High frequency excitation is another contributor, which, when properly exploited can significantly enhance outcomes of the process. Ultrasonic excitation can be exploited for different purposes. It is widely applied in welding, replicating and joining of thermoplastic materials with low softening temperature [14-17]. In these processes ultrasonic energy is converted into heat through the phenomena of intermolecular friction within the thermoplastics [18]. The generated heat melts thermoplastics and causes the melt to flow and fill the interface between master mold and polymer surfaces.

When working with already preheated polymer, high frequency is used with a purpose to force preheated polymer to flow towards the mold and to move to the central part of pattern area in a mold, thus better filling empty cavities of the mold. It allows diminish bubble of residual gas effect in the pattern. Furthermore, during demolding step vibration excitation allows avoid surface distortions, which are possible due to adhesion between master mold and polymer.

Most of the authors apply excitation from the upper side to polymer by using sonotrode. Earlier was revealed, that ultrasonic excitation from the bottom side of the polymer using vibroactive pad, which is based on single layer piezoceramic as an actuator is able to enhance the quality of microstructure [19-20].

Problematic of the paper is related with previously created vibroactive pad. This vibroactive pad generates first vibration mode at 5.2 kHz and second vibration mode is obtained at 8.8 kHz [21]. Vibroactive pad has several disadvantages, which are necessary to solve, in order to go further towards hot imprint process, with usage of high frequency excitation, optimization. These imperfections include:

- Single layer vibroactive pad (Fig. 1) is not able to generate large displacements, what in turn diminishes the effect of high frequency excitation, because lower force forces polymer to flow.
- Indentation of vibroactive pad (Fig. 2) (especially it's center), under the action of mechanical load. This causes lower filling of the mold in the center of microstructure, thus remaining empty cavities.

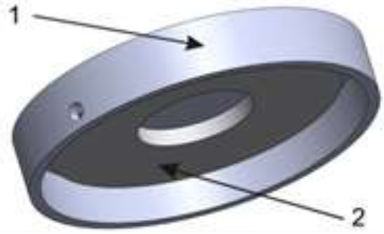


Fig. 1 Vibroactive pad: frame *1* and piezoelectric element *2* [21]

Moreover previously microstructures were created by using second vibration mode at frequency of 8.8 kHz. This causes uneven contact between surfaces of vibrating vibroactive pad and polymer, thus diminishing the effect of high frequency excitation during the process (Fig. 2).

To solve previously mentioned problems vibroactive pad, based on the multilayer actuator is proposed. This type of actuator is located in the centre of vibroactive pad, this precludes indentations, which emerge under the action of mechanical load.

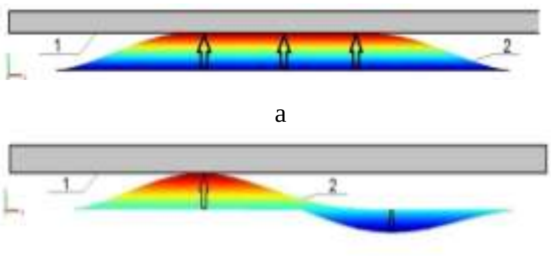


Fig. 2 Contact patterns between vibroactive pad and polymer: a - first vibration mode; b - second vibration mode

According to theory multilayer, because of several layers of piezoceramic added one to another is able to generate bigger displacements and forces, than single layer is able to do [22-23]. In this way it forces preheated polymer to flow more rapidly and better fill empty cavities of master mold.

As well first vibration mode will be applied in the process of mechanical hot imprint. This mode acts to the surface of polymer symmetrically, thus causing better and more symmetric flow of polymer.

The goal of the work is to improve the quality of periodic microstructures, by employing vibroactive pad, based on multilayer actuator. In this paper analysis of vibroactive pad, which is based on multilayer actuator, together with its application in the process of mechanical hot imprint are presented. Finally analysis of results is presented and outcomes are discussed.

2. Design of vibroactive pad

Literature review shows, that higher displacements and force cause polymer to flow more rapidly, in this way better replicating mold. Stack type actuator, which is composed from multiple layers of piezoceramic is able to generate higher displacements, than single layer is capable to do [22]. Larger number of piezo layers stacked on top of one another increases the energy that may be delivered to a load.

Total mechanical energy E of piezoceramic is equal to:

$$E = \Delta F \, \Delta l \, , \tag{1}$$

where Δl is displacement; ΔF is force generation.

Creating multilayer construction from several layers of piezoceramic, in order to get thickness mode (d_{33} effect) increases total stroke (due to superposition of single layers) In ideal conditions multilayer actuator can reach up to 0.2% of total actuator length and higher force [26].

Another important thing is that this type of vibroactive pad is located in the centre of the pad, thus obstructing indentation of the centre during the process.

The piezoelectric low voltage stack type piezoactuator (PSt 150/4/20 VS9) was chosen as a source of high frequency vibrations – it is a 9 mm diameter cylinder of 31 mm height.

Vibroactive pad (Fig. 3) is based on the actuator in the center of construction and aluminum frame, whose purpose is to increase operating area, secure the pad from mechanical load and possible damage of actuator. Both elements of the frame were produced with turning lathe. The piezoelectric actuator is mounted to aluminum frame with M3 (according to ISO 261 standard) bolts. Material and geometrical parameters of the vibroactive pad were selected according to application– the pad should sustain the pressure of 506625 N/m^2. At the same time it should be flexible enough to transmit vibrations to the polymer, in order to do this more efficiently the upper side of wall was turned more than the lower side. This decreases the stiffness of the upper side of the frame, thus allowing get bigger displacements and lower resonant frequencies, than it would be with thicker walls. In the same time thicker lower side of the frame gives more stability for the vibroactive pad.

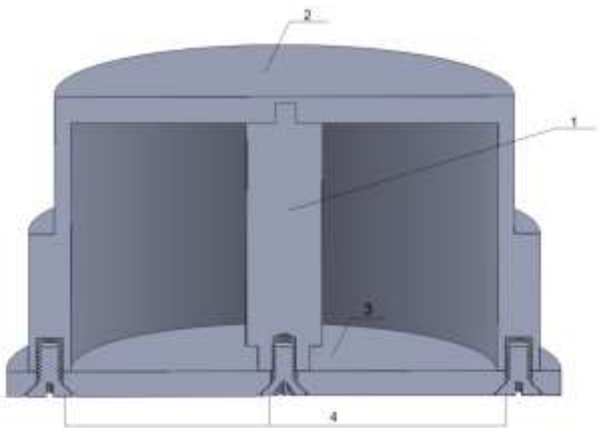


Fig. 3 Cross section of vibroactive pad: *1* - multilayer piezoactuator PSt 150/4/20 VS9; *2* - upper side of the frame; *3* - bottom side of the frame; *4* - M3 bolts

In order to use the multilayer as the high frequency generator during the process of mechanical hot embossing it is necessary to analyze its characteristics (Table 1) and verify its suitability for this process.

Table 1

Characteristics of PSt 150/4/20 VS9 actuator

Type	PSt 150/4/20 VS9
Max. stroke, µm	27/20
Length of actuator, mm	28
El. Capacitance, nF	340
Stiffness, N/µm	12
Resonance frequency, kHz	30
Prestress force, N	approx. 40
Max. load force, N	300
Max. force generation, N	300

Multilayer is able to operate, when load force is no more than 300 N, thus it is necessary to confirm, that impressing force would satisfy these conditions. Press is able to attain the pressure of 5 Atmospheres. Converting to SI system units 506625 N/m^2 or 50662.5 kg/m^2 are obtained. Thus mechanical load, which acts on the area of multilayer actuator (0,000063 m^2) is equal to 31.92 N, this satisfies boundary conditions of the actuator.

3. Simulation and experimental research of vibroactive pad

To exploit all potential of vibroactive pad it is necessary to get highest displacements and forces, what is only possible, when vibroactive pad works under first resonant frequency.

In order to precisely find resonant modes, numerical simulation and further experimental verification must be performed.

Primarily Comsol Multiphysics 3.5a., is used in order to find eigenfrequencies of the system and thus simplify further experimental analysis.

Before the modelling, it is necessary to determine boundary conditions of the construction. Like in real conditions, bottom surface vibroactive is fixed (Fig. 4). During the modelling bolts were neglected, but in order to maintain the same boundary conditions, frame was considered as solid single body. Diameter of Stack type actuator's frame is considered as 9 mm. Diameter of PZT-4 multilayer ring was considered as 3 mm, other dimensions are represented in Fig. 4.

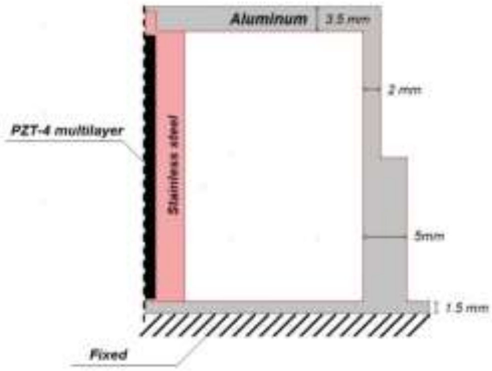


Fig. 4 Computational scheme of vibroactive pad

The material properties, included in modelling (Table 2) were taken from Comsol Multiphysics materials library.

Table 2

Material properties

Material properties	Aluminum	Stainless steel	PZT-4
Young modulus E, Pa	$6.9\cdot10^9$	$200\cdot10^9$	$7.5\cdot10^9$
Poisson's ratio ν	0.334	0.33	0.35
Density ρ, Kg/m^3	2700	7850	7500

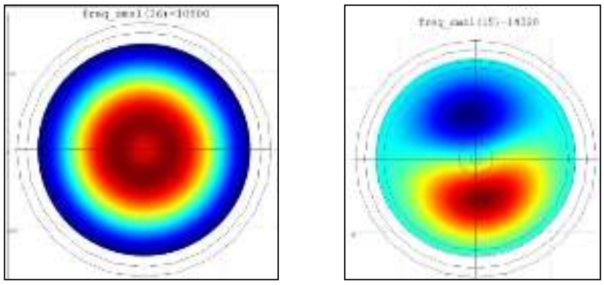
The element of tetrahedral form, defined by ten nodes (three degrees of freedom at every node: displacement in the x, y and z directions.), was chosen as mesh element.

In order to observe simulated resonant frequencies (Fig. 5), it is necessary to solve eigenfrequency equation, where all the variables are chosen according to their real physical characteristics:

$$[M_{UU}]\{\ddot{U}\}+[C_{UU}]\{\dot{U}\}+[K_{UU}]\{U\}=0, \qquad (2)$$

where $[K_{uu}]$ is stiffness matrix; $[C_{uu}]$ is damping matrix; $[M_{UU}]$ is mass matrix; $\{U\}$ is nodal displacement.

Operating frequencies of vibroactive pad are in the order of several kilohertz, and displacements corresponding to these frequencies are in the order micrometers. Therefore system PRISM, produced by company HYTEC (Fig. 6), which works by the principle of electronic speckle pattern interferometry (ESPI) holography, is applied for the visual representation of vibration modes of vibroactive pad.



a b

Fig. 5 Results of numerical analysis: a - first vibration mode frequency 10500 Hz; b - second vibration mode frequency 14320 Hz

Operating principle of ESPI holography: Object beam is being directed to the lens system and further to the object (which is being investigated). Reference beam goes to video camera, where it interferes with registered object beam (this beam is already reflected from the investigated object). Interferential view from camera is transferred to computer, where it is being processed with PRISMA-DAQ software.

The digital holographic interferometry by now is the most effective technique for the analysis of dynamic processes [24]. The results, obtained with PRISM system are images with vibration shapes at desired frequencies.

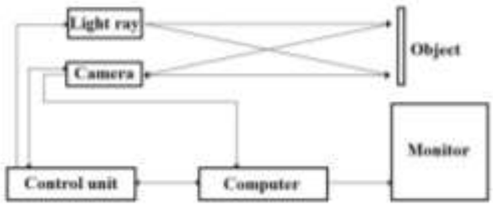
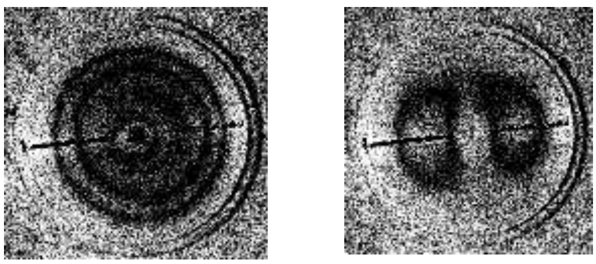


Fig. 6 PRISM systems optical setup

After the analysis with PRISM system, following results of experimental research were obtained: first vibration mode 12.910 kHz; second vibration mode 13.6 kHz (Fig. 7).



a b

Fig. 7 Hologram of vibrating construction: a - obtained at 12.910 kHz; b - at 13.601 kHz

From the Figs. 5 and 7 it is possible to conclude, that simulation results of multilayer pad correspond with experimental. The biggest difference was observed for the first mode of vibroactive pad. The difference between experimental and simulated frequencies is about 22.9%. The difference between simulated second vibration mode and experimentally obtained second vibration mode is 5.28%.

4. Experimental setup for mechanical hot imprint

Experimental setup of mechanical hot imprint, with exploitation of high frequency excitation, is shown in (Fig. 8).

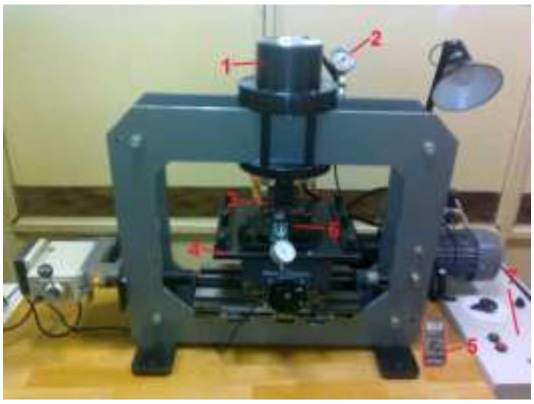


Fig. 8 Experimental setup of mechanical hot imprint: hydraulic hold *1*, measurement of pressure *2*, horn for mold *3*, controlled stage *4*, measurement of temperature *5*, dynamometer *6*, and control block of temperature, time, and pressure *7*

Process mechanical hot imprint consists from three steps:

- Preheating. The initial temperature of the mold and polycarbonate is 20˚C (ambient temperature). In this step, when the mold reaches the surface of polycarbonate, the heating begins up to chosen 148˚C temperature. This temperature corresponds to glass transition temperature of polycarbonate. As the temperature reaches rubbery state of the polymer (Fig. 9), the polymer leaves glassy or brittle state and starts to be reversibly and irreversibly deformated under the action mechanical stress. In other words it becomes viscoelastic.
  In this step heat of the mold is transmitted to the polycarbonate and it starts to deform according to the shape of the master mold.

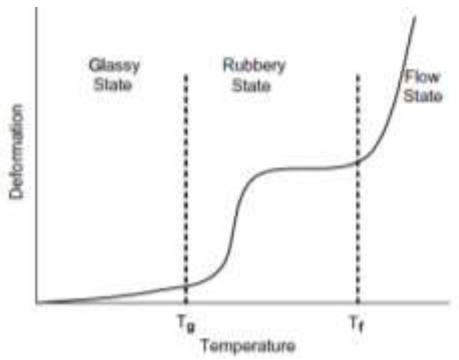


Fig. 9 Deformation behavior of thermoplastic polymer as a function of temperature

Heat transfer conductivity during the process of heating is described by the formula:

$$\rho(T)c_p(T)\frac{\partial T}{\partial t}+\nabla(-k\nabla T)=q\,, \tag{4}$$

where k is thermal conductivity; ρ is density; c_p is heat capacity; T is temperature; q is rate of the heat generation.

- Imprinting. The mold impresses (till reaches nominal pressure (303900 N/m^2) , which is being applied for 10 seconds) polycarbonate- contact force between the mold and polycarbonate increases. Plastic deformation of polycarbonate takes place.
- Demolding. The mold is being withdrawn and polycarbonate is cooled down till ambient temperature. Micro relief of master mold is thus transferred on the surface of polycarbonate.

Structural scheme of mechanical hot imprint process is represented in Fig. 10.

Process parameters (temperature, pressure and imprinting time), except the construction of vibroactive pad, are being held constant (Table 3), thus allowing find out, whether multilayer vibroactive pad allows achieve better quality of microstructure.

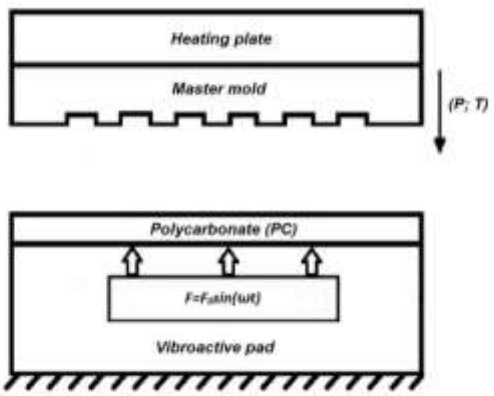


Fig. 10 Structural scheme of hot imprint process with ultrasonic excitation [10; 12]; *P* - pressure; *T*- temperature; *F* - sinusoidal force

Table 3

Experimental matrix of the process of mechanical hot imprint, with usage of high frequency excitation

Vibroactive pad	Multilayer pad	Single layer pad
Impressing time *t*, s	10	10
Pressure *P*, N/m^2	303900	303900
Vibration frequency *f*, kHz	12.91	5.2
Temperature *T*, ˚C	148	148

5. Replicas quality examination techniques

The quality of replicas was evaluated using an indirect optical method - measurement of the diffraction efficiency. Periodical microstructures are manufactured from optic materials, thus optical evaluation techniques are used for quality analysis.

Diffraction efficiency of replicated microstructure was evaluated by non-destructive optical laser control method (Fig. 11). Laser ($\lambda = 632.8$ nm) and photodiode BPW-34 were used to register diffraction spectrum. Photodiode is connected to ammeter.

The laser beam is directed to the microstructure. As the beam passes through the microstructure, it is being diffracted into particular amount of maxima, which reach the photodiode. The electric current, which passes through photodiode is registered with ammeter. Electrical current, which passes through the photodiode linearly depends on the lighting, thus no additional calculations are needed in order to compare results. Diffraction maximas are scattered, so they are measured by changing the position of photodiode so that desired maxima would pass through photodiode.

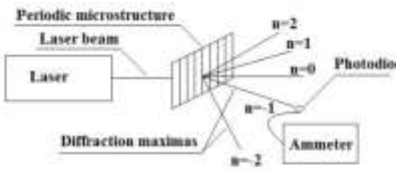


Fig. 11 Principal scheme of diffraction efficiency measurement stand

Optical microscope “NICON Eclipse LV 150” with CCD camera was used in order to magnify and examine defects.

Optical microscopy was used for qualitative surface analysis. The main purpose of this investigation is to magnify and calculate defects per area of 2400 μm^2.

Analytical evaluation of geometrical parameters of surface of periodical microstructures was performed by using atomic force microscope NANOTOP-206 (AFM). Investigation of this type is capable to show profile of surface view, as well provide with information about surface parameters, like: maximum and average height; skewness etc.

6. Results and discussions

During the investigation with Atomic Force Microscope was focused on finding out how precise master mold is being replicated on the surface of polymer. Profile view images of master mold and periodic microstructures, created with single layer vibroactive pad and multilayer vibroactive pad are compared (Fig. 12).

From Fig. 12 can be stated, that high frequency excitation with multilayer actuator allowed obtain more similar to master mold microstructure. Average depth of master mold is 264 nm, depth of microstructure, made with single layer pad is equal to 230 nm, whereas depth of microstructure, made with multilayer is 245 nm.

Diffraction efficiency of +1 and -1 maxima is the most significant criteria, which determines optical quality of the periodical grating. Higher values of these maxima are strongly desirable in many applications [25]. The main attention is being paid to these maxima.

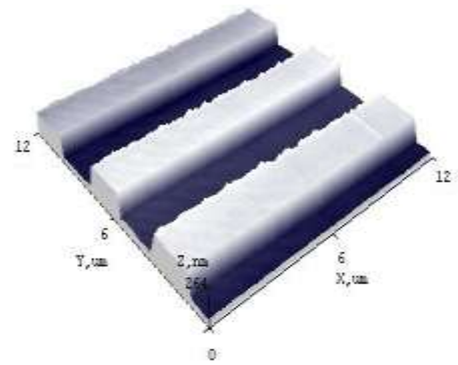
The calculation of diffraction efficiency is being performed by using formulas:

$$RE_{i,j} = \frac{I_{i,j}}{I_j}, \tag{4}$$

$$I_j = \sum_i I_{i,j}, \tag{5}$$

where I_j is sum of currents at every maxima; $I_{i,j}$ is magnitude of current at particular maxima; $RE_{i,j}$ is relative diffraction efficiency.

First of all sum I_j of all currents (different diffraction maxima)- intensity of the transmitted maxima is being calculated, then current value, obtained at particular maxima, is being divided from the sum and the relative diffraction maxima value in percent is obtained. The relative efficiency allows neglect optical properties of material, thus allowing evaluate the geometry of microstructure, produced from different materials.



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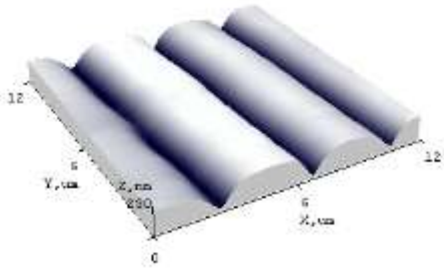

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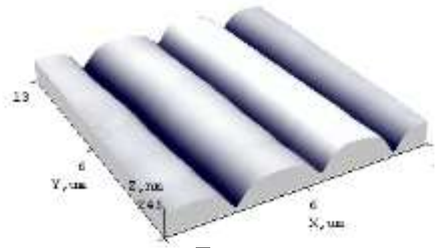


c

Fig. 12 Atomic force microscope images: a - master mold; b - microstructure, made with single layer vibroactive pad; c - microstructure, made with vibroactive pad, based on stack type piezoactuator

Measurement of diffraction maxima results (Fig. 13) show that the high frequency vibration excitation by using multilayer actuator as a basis of vibroactive pad during the process of mechanical hot imprint increases the diffraction efficiency of the first order maximum 3 times, when comparing with microstructure, created with single layer vibroactive pad (1.24% vs 0.43%) and 3.65 times, when observing -1 maxima (0.84 % vs 0.26%). Results show a positive trend for future research, when having purpose to get periodic microstructure with higher diffraction efficiency.

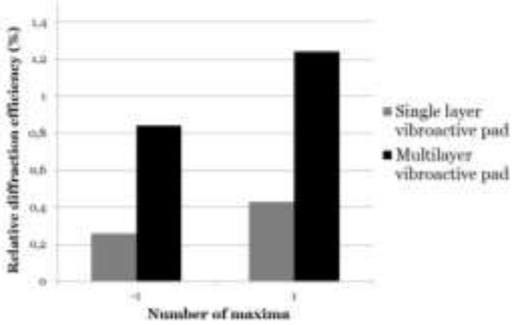
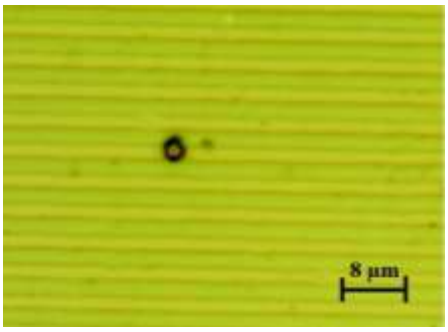


Fig. 13 Distribution of diffraction efficiency

Magnified views (obtained with optical microscope) of the gratings surface are presented in Fig. 14. The main purpose of the comparison between the microstructures is to calculate visible defects.

After the analysis, it was determined, that grating, manufactured with single layer vibroactive pad has 12083.3 defects/mm^2, while grating, made with multilayer pad has 2083.3 defects/mm^2 or 5.8 times less.

Having diffraction efficiency results, can be stated, that multilayer actuator, employed in mechanical hot imprint process allows achieve better results. These results give sufficient basis for future investigations.



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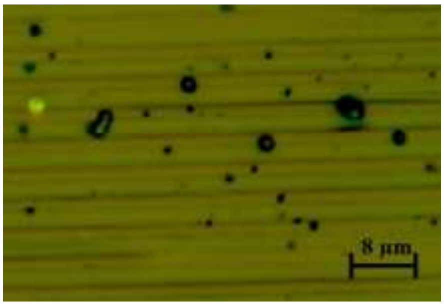

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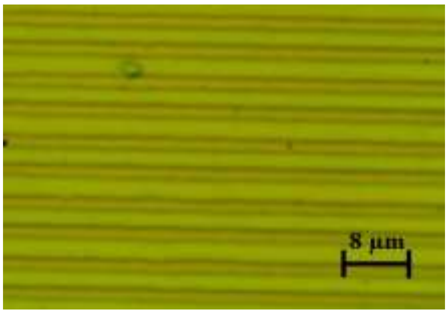

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Fig. 14 Optical microscope images: a - master mold; b - microstructure, made with single layer vibroactive pad; c - microstructure, made with vibroactive pad, based on stack type piezoactuator

4. Conclusions

1. Numerical simulation of eigenfrequencies of vibroactive pad showed, that first vibration mode is obtained under the frequency of 10.500 kHz, experimental results of vibroactive pad 12.910 kHz (difference between modeling and experimental results is 2.71%). Modeling results of second vibration mode – 14.320 kHz, experimental analysis of second vibration mode - 13.600 kHz (difference bet 5.28%).
2. Measurement of diffraction efficiency shows, that first (1.24%) and minus first (0.84 %) maxima in grating, made with multilayer pad are respectively 2.88 and 3.23 times higher than in grating, made with single layer vibroactive pad (0.43% first maxima and 0.26% minus first maxima).
3. Optical microscopy of visible defects showed 2083.3 defects/mm^2 in specimen made with multilayer pad and 12083.3 defects/mm^{2}in specimen, made with single layer pad. Exploitation of multilayer vibroactive pad allowed decrease the number of visible defects by 5.8 times.
4. Average surface depth of master mold is 264 nm, microstructure, made with single layer pad has average surface depth of 230 nm and microstructure, produced with multilayer pad has average surface depth of 245 nm.

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MICROSTRUCTURE, REPLICATED USING HIGH FREQUENCY VIBROACTIVE PAD

S u m m a r y

The paper is dedicated to analysis, practical exploitation of vibroactive pad, whose fundament is multilayer actuator in experiments of mechanical hot imprint. The goal is to compare the quality of microstructures, created by using single layer vibroactive pad and vibroactive pad, based on multilayer actuator. Numerical modelling and experimental analysis is performed in order to find resonant modes of multilayer vibroactive pad. Having operating frequencies, vibroactive pads are applied in mechanical hot imprint process. Microstructures are created on the surface of polycarbonate, the only process variable is type of vibroactive pad. Three types of microstructure quality measurements are performed: measurement of diffraction efficiency, optical microscopy and atomic force microscopy, in order to examine quality of replica.

Keywords: Multilayer actuator, microstructure replication, diffraction efficiency.

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