New Approaches to High-Tech Materials: Nondestructive Testing and Computer Simulations in Materials Science and Engineering

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Alexander I. Melker
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Introduction

The first International Workshop on New Approaches to High-Tech Materials: Nondestructive Testing and Computer Simulation in Materials Science and Engineering, NDTCS-97, took place 9–13 June 1997 in St. Petersburg. Roughly 200 scientists, including graduate students, from Belarus, Czech Republic, France, Germany, Poland, Russia, United States, and Ukraine attended. The workshop continues a set of All-Union specialized symposia in this active area of research. The symposia were established by St. Petersburg State Technical University and quickly expanded throughout the former Soviet Union. These migrating symposia operated with success from March 1976, when the first Symposium on Computer Simulation of Radiation Damage in Solids began, until 1991, when most of them ceased all activity with the splitting of the Soviet Union. Under these new conditions, the NDTCS-97 organizers tried to give impetus to the reconstruction of the science of CIS with wide international participation. As a result, NDTCS-97 may be considered as a phoenix appearing from ashes at its place of birth.

There were a total of 127 scientific contributions to the workshop program that were organized into eight oral sessions:

1. Laser, Optical, and X-Ray Technologies
2. Electronic and Optical Properties of Condensed Matter
3. Nanotechnology: Smart Materials and Soft Condensed Matter
4. Surfaces, Amorphization, and Ion Beam Technology
5. Computer Technologies: Molecular Dynamics, Visualization, and Cognitives
6. Defects and Mechanical Properties of Condensed Matter
7. Phase Transition and Fracture
8. Mechanics of Continuum Media

Most of the sessions were supplemented with an invited tutorial lecture. A total of 54 papers were accepted for publication in these proceedings, mostly from Sessions 1–5. In addition, 16 papers from Sessions 6–8 have been submitted for publication in the journal *Modeling and Computer Simulation in Materials Science and Engineering*.

A large portion of Session 1 is related to laser, optical, and x-ray techniques and measurements. These contributions are supplemented by papers on computer simulation, which permits an increase in the efficiency of experimental models. Other papers consider the effect of laser beams on materials.

Session 2 deals mainly with theoretical aspects of interactions between external fields, photons, fast electrons, and condensed matter. Photoionization, polarization, absorption, and scattering, as well as formation of regular spatial temporal structures and critical dynamics are discussed.

Session 3 pertains to soft condensed matter (polymers, membranes, polymer liquid crystals, etc.) and shape memory alloys. In spite of their different origins, these materials have much in common, operating as functional devices at a nanoscale level. The focus of the papers presented is the development of models predicting materials behavior.

In reality, many devices are made and/or operate in severe conditions or extreme environments. The fabrication process and service are tightly connected with surface phenomena. These questions are considered in Session 4.

Session 5 concerns the problems of developing new algorithms of computer simulation for complex systems that permit an increased calculation rate. In addition, considerable attention is given to visualization and cognitives. It should be emphasized that visualization of the results obtained is the Achilles heel of modern computer simulation.

Much important research presented at the workshop has not been included in these proceedings, e.g., fullerenes, amorphous materials, quasi-crystals, etc., but can be found in the abstract book. As mentioned earlier, some of the papers from Sessions 6–8 will be published elsewhere. We apologize to the reader for not reviewing those contributions.

In a time of decreasing resources, organizing this meeting was more difficult than anticipated. In this regard, we would like to acknowledge the following institutions that made significant contributions.

- St. Petersburg State Technical University as a whole and the Departments of Metal Physics and Computer Technologies in Materials Science in particular
- NPO Special Materials
- Polytest Company, Ltd.
- SPIE Russia Chapter

The organizers particularly sought to assist CIS scientists from outside Russia who had no financial freedom. These outreach efforts were also extended to some graduate students. The latter recipients of assistance contributed to the workshop in the form of papers and labor (copying, registration, chauffeuring, etc.). This facilitated such amenities as low-cost registration fee, airport transportation, etc. We hope that the experiences gained will help improve the next workshop, planned for June 1998 in St. Petersburg.

Alexander I. Melker

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SESSIO

Laser, Optical, and X Technologies

RING LASER FOR CONTROL AND MEASUREMENT

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ABSTRACT

In the ring laser,multiple passage through an active medium may be provided, in contrast to the linear laser, by a running wave.Each of the running waves may be provided generation.Generally, counterpropagating running waves are not similar in the ring laser.They differ in intensity, phase,frequency,polarisation.This distinctions are called nonreciprocity .Features of the ring laser for various applications.They allow the development of frequency standards,laser giro,goniometer,analytical instruments. Ring laser offer advantages for linear-angular measurements and measurements of parameters of moution. Ways to optimize the parameters of ring laser are indicated.

1. INTRODUCTION

The first investigations of ring lasers used gas active media and adressed realizing the Sagnac experiment.As a result the term laser gyro appeared.We consider ring laser for measurements of angles.The period of radiation travel in a rotating ring resonator depends from length and area of resonator perimeter,angular velocity of ring laser.The nonzero difference of periods of counterpropogating waves means that the frequencies of counterprorogating waves of the resonator differ.This difference is determinated by intensities of counterpropogating waves.Some our books and rewiews [1-5] are devoted to this question.

2. MEASUREMENTS OF ANGLES AND ANGULAR VELOCITY

The frequency difference is equal:

$$\Delta\nu=\sum \kappa_n \omega^n \qquad (1)$$

where k-coefficients, ω -angular velocity. This expression is valid far from the region in which locking of frequencies of counterpropogating waves take place.Three terms of this expression

$$\Delta\nu=\kappa_1 \omega+\kappa^o+\kappa_{-1} \omega \qquad (2)$$

are sufficient to describe most of practical problems. Here, $k_1 = k(1+k_A)$ is a scale factor. $k_1=k$ for an empty resonator,and k_A is the contribution made by the active medium. For the He-Ne laser, the latter quantity is equal to 10-3.Expression (2) is the output characteristic of the rotating ring laser.It is used a_ _he basic to derive formulas for determinating the angular velocity and the angle of rotation.

The scale factor k can be determinated experimentally using the sum of the numbers of periods of the beat frequency of a ring in the one revolution [4,6,7].

$$N= 0{,}5\ (N_+ + N_-) \qquad (3)$$

where N_+ and N_- are the numbers of periods for rotation in opposite directions.For this purpose,one should build up a set of N for different periods of rotation T, plot the dependence N(T), extropolate it to point T=0, and obtain k_1 - N(0). Of particular interest is the component k_A of the scale factor. It is determinated by different extrapolations [6,7].

The second term k_o in the right-hand side of expression (2), which characterizes nonreciprocity, determines the zero shift of the output characteristic.Nonreciprocity in a ring laser is caused by the effects of Fizeau-Frenel (the distinction of refractive indices of a moving medium for counterpropagating beams results in a distinction of frequencies of counterpropagating waves in a ring laser),Langmuir(atomic motion induced by the discharge current), Faradey, and by diffraction [8]. . The zero shift in a ring laser can be determined experimentally by rotating the laser in opposite directions.It satisfies the expression k_o T=N.

The coefficient k_{-1} ,which allows linear coupling of counterpropagating waves, determines the degree of nonlinearity of output characteristic.Coupling of counterpropagating waves in a ring laser is conditioned by propeties of the resonator and the active medium.When radiation reflects from elements found inside the resonator,it scatters.As this take place, a portion of radiation returning in the backward direction affects the intencity of a counterpropagating wave[9].

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It is usual to neglect scattering in the active medium of a ring laser because the interaction of counterpropagating waves caused by the overlap of Bennet holes is more efficient. Due to the presence of atoms participating in the generation of counterpropagating waves,this interaction leads to competition between these waves.

To diminish light scattering,it is customary to decrease the number of optical elements and enterfaces inside the resonator of a ring laser and eliminate radiation reflected from external objects backward into the resonator. The interaction of counterpropagating wavesin the active medium is reduced by broadening the profile of the radiation power and thus reducing the overlap of Bennet holes.In a ring He-Ne laser, this is achieved using a mixture of neon isotopes.

In view of expression (2), the coeffisient k_{-1} can be represented in the form

$$\kappa_{-1}=\omega[N(I)-\kappa_{-1}]T^{-1} \qquad (4)$$

and easily determined from experimental data.

The first term in the ridht-hand side of expression (2) makes the dominant contribution. A typical contribution of counterpropagating waves does not exceed 10^{-4} in a ring He-Ne laser and sometimes it is possible to reach a level of 10^{-6}. If a nonreciprocal elements is absent, a typical value of the zero shift corresponding to the first term does not exceed 10^{-5}.

The principle of angular-velocity measurements is contained in expression (2). A ring laser is mo-unted on a rotating platform whose velocity must be measured.The coefficients of output characteristic are determined using the given method, the beat frequency of counterpropagating waves is measured,and angular velocity is calculated.The accuracy of angular-velocity measurements is determined,first of all, by the error in determination of the coefficients of the output charactiristic and their stability.As a result,the angular velocity can be determined with a relative accuracy of 10^{-5} to 10^{-6} by the expression

$$\Delta\nu=\kappa_1\,\omega \qquad (5)$$

Parameters of rotating He-Ne lasers for which the angular velocity is measured with the given accuracy are given in [6,7,10].Expression (5) may be used to advantage for angular velocities corresponding to beat frequencies of 100 to 200 kHz and more.One should also mention that the model of a ring He-Ne laser described by expression (2) is constructed for the case where the beat frequency of counterpropagating waves is considerably less than the width of operating neon transition(8-10 MHz). Therefore, expression (2) is not accurate for beat frequencies above 1 to 2 Mhz and terms with ω .etc., should be including in this case. This restricts the use of expression (5) for high angularvelocities.

At low angular velocities when the nonlinearity of the output characteristic caused by coupling of counterpropagating waves must be taken into consideration,expression (5) as well should not be used. To get out of the nonlinear section of the output characteristic of a ring gas laser,nonreciprocal elements used.In this connection,two terms in the right-hand side of expression (2) must be used instead of (5). This imposes additional requirements on the stability of factors providing nonreciprocity.Moreover,most of nonrecirpocal elements enhance coupling of counterpropagating waves and,thus,increase the nonlinearity of the output characteristic, which sometimes prohibits neglecting the term with k_{-1}. At pr--ent, a number of devices constructed on the basis of ring laser are available for angular velocity measurements,from primary standards in definite ranges to operating measuring instruments, including laser gyros. The angular velocity is measured in the following way.Coefficients of the output characterictic of a ring laser are determined,the beat frequency of the rotating device is measured,and then the rotation velocity is calculated .In practice,calculations are performed during the calibration of the measuring device,that is, during the constraction of the output characteristioc in the given range of angular velocities,but not during measuring procedure.

A ring laser can be used to measure the angle and the angulae velocity simultaneously. The integration of expression (5) with respect to time gives the number of periods N of the frequency during the measurement

$$N_\varphi = k_1\,\varphi \qquad (6)$$

It is proportional to the angle through which the platform with the laser rotates in this time. In particular, when $\varphi=2\pi$, we have

$$N=k_1\,2\pi \qquad (7)$$

It is customary to use an inherent standard,an angle of 360 °,and measure the number of periods of the beat frequency and not the beat frequency itself.In this case,the frequency meter operates in the pulse counting mode The performance of goniometer on the basis of a ring laser is described by the formula

$$\varphi=2\pi N_\varphi/N \qquad (8)$$

obtained from expressions (6)and (7).

The goniometer operates in the following way. A ring laser is mounted on a rotating platform. The signal at the beat frequency is separeted by a photodetector,then goes to frequency meter. To measure angles between fasets of aprism, it is mounted and rotated on the same platform. They are determined using a photoelectric autocollimator.At instants corresponding to the coincidence of optical axes, electric pulses deter-ming the unknown anle are recorded. The number of periods of the frequency of the ring laser in the interval between pulses N is measured by the frequency meter. In addition, the first pulse from the output of the autocolli-matoris used to trigger and turn off the frequency meter,which thus counts the number of periods of the beat frequency N in one complete revolution. The output device devides N_φ by N and multiplies by 2π.As a result,we have the unknown angle φ at the goniometer output.

Self-calibration performed in every revolution of the rotating platform reduces requirements imposed on the stability of ring laser parameters and the rotation period.It will suffice to hold them constant during one revolution. Moreover, it is possible to choose the rotation velocity of the platform such that theinter-action of counterpropagating waves is minimum. This can not be realized in system of angular velocity measurements. However,high accuracy of angular measurements reqires a high precision system to record the angular position.

The advantages of the goniometer on the basis of a ring laser are a high measurement accuracy, a small step of discreteness, a wide range of angles accessible for measurements,sell-sufficiency and a digital output signal allowing a rather simple automation of measurements.An automated goniometer on the basis og a ring gas laser is described in detail in [11].

In relation to angular measurements,one should mention marking angular scales using a ring laser.For this purpose, the beat frequency is supplied to an actuating mechanism making a scale mark, which corresponds to a defenite angle, on the side surface of the rotating platform. Mechanical, optical, magnetic and other types the scales can be formed. In [6] the procedure used to calibrate rotating magnetic drums using a ring He-Ne laser is described.The scale division of one angular pulse was equal to 0.7". Because the recording density istoo high in this case, the signal at the beat frequency can be supplied to the actuating mechanism by a frequency divider.

A ring laser can also be used to determined the angular distance between distant object [12],which is of interest in geodesy and astronomy. We don't consider other applications here.Note in conclusion,that the application of expression (5) is restricted

$$N=\kappa_1\,\varphi+\sum_{n\neq 1}\int\kappa_n\,\omega^{-1}\,dt \qquad (9)$$

and must be written instead of (6) in the general case.

In view of (5), one may use, in the majority of cases for currently available accuracities, the expression

$$N=\kappa_1\,\varphi+\int\kappa^{o}dt+\int\kappa_{-1}\,\omega_{-1}dt \qquad (10)$$

The most comprehensive study of accuracy of a goniometer on the basic of a ring He-Ne laser was performed in [6]. These investigations were continued in [11].`It is our opinion that the papers cited contain most of questions related of the accuracy of a laser goniometer.Let us briefly run through the subject. The accuracy of angular measurements performed with a ring laser is limited by errors of the laser and recording devices. The first group of errors is determined by the level of technical fluctuations of the ringlaser, and the instability of the scale factoris the main one. The second group includes errors of the scheme recording the angular position, the error of frequency meter quantization, and the error associated with the width of running interference fringers.Let us consider them separately.

The level of technical fluctuations determines the error introduced to angular measurements by the ring laser. It was mentioned above that expression (5) will be used as the output characteristic. The main reason for the measurement error is the variation of coefficients of the output characteristic of the ring laser in time. If the coefficients k_o and k_{-1} are time - independent,their contribution to the error is caused only by the variability of the laser rotation velocity. If all the three coefficients vary in time, the angular measures of the period of the beat frequency during calibration and measurement are different. Therefore, it is important to shorten the time interval between these procedures. Because the angle φ being measured always lies within the angle of 2π, the best way is to perform calibration and measurements simultaneously.Such calibration is termed continuous. In this case, the error of angular measurements depends on the time of fluctuations of coefficients of the output characterictic. For the case where coefficients of the output characteristic undergo harmonic variations with identical frequencies and phases, the formula for the angle being measured is derived in [6].

Previously we assumed that fluctuations of all three coefficients of the output characterictic have similar frequencies and phases. It was assumed that the error of measurements of angle was a random quantity.In practice,correlation with rotation of ring laser is possible. Because of this, the stability of parameters of the ring laser.the decrease of contributionsof the zero shift and nonlinearity of the output characteristic, and the stability of rotation velocity are the topical problems. It is nessary to independently stabilize a number of parameters of a ring laser,primarily the radiation frequency and the discharge current. The accuracy of angular measurements can be substantially improved by locking the beat frequency of a ring laser with intermode beats.However,this leads to considerable complication of the equipment. The radiation frequency of a ring laser can be stabilized using the emission profile, the absorption cell, and the difference of intermode beats in the three-mode regime.

3. OPTIMIZATION OF PARAMETERS OF RING LASER

Ring laser used in precise measurements must have a sufficiently high stability of frequency and radiation power. For thus purpose, parameters of an active medium and resonator must be chosen in such way that the change of environmental conditions has aminimum effect on the power and frequency of radiation.

Spatial distributions of the field in a laser resonator and the population inversion in an active medium are nonuniform. The region of overlap determines the power and, hence, the frequency of radiation. Therefore,an optimum relation between components of an active medium depends on resonator parameters (for example [3]).

Various overlaps of the field with the population inversion can be realized using cylindrical,conic, parabolic and sectional geometry of active elements. Different cross section of active elements, namely, circular, rectungular, elliptic, etc. give differentavarige gains and transverse spatial distributions of a gain. The rectangular cross section provides a diffuse distributionof gain for which resonator misalignment has a minimum effect on laser parameters. Because of this, it is best matched to a ring laser. Further studies [3] gave new cross section of an active element that are optimum from different points of views.

A new chapter of the search for optimum laser parameters is assosiated with investugation of oscillation and waves in a discharge of a gas laser [3,13-15]. Investigations in this line continue and the problem deserves a separate direction.

4. CONCLUSION

A consideration of some properties of ring laser showed it efficiency in measuring technique and plenty of new problems that should be solved to improve the measurement accuracy. Some types of measurements in which ring laser is used and many questions were not considered here(see [3-5]). Ring laser is used for measuring the Earth's rotation [16,17]. The work is continued.

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LIDARS FOR CONTROL AND MEASUREMENTS

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ABSTRACT

Laser radiation has a wide application in molecules Raman lidar control and its concentration measurement in atmosphere under industrial regions for creation people good living conditions. Back scattering vibration Raman lidar equation computer simulation for iodine molecules and its heavy isotopes with YAG - Nd, cuprous vapor and eximer lasers have been made to choose optimal lidar system for studied molecules monitoring in atmosphere. Background stray sunlight power were calculated to determine the minimum molecules concentration at ranging distance up to 6 km.

1. LASERS PARAMETERS

YAG - Nd laser radiation and essentially its second, third and fourth harmonics were widely used in monitoring systems [1] and allows to get the pulses with energy up to 100 mJ of time duration 10 ns at pulses repetition rate to 50 Hz. Such a laser harmonics radiation can be served in Raman lidar I_2 monitoring in atmosphere. Rubin laser second harmonic have been pointed for comparing due to widely used in lidar studies [1] though pulse repetition rate in this case is about 0.1 Hz only.

Cuprous vapor pulse laser can be taken in wide application for molecular iodine monitoring in atmosphere Raman lidar studies. Peak power value of 130 kW at 510.6 nm wavelength and second harmonic in UV spectrum at 289.1 nm wavelength power of 75 mW at first harmonic power of 1 W (conversion efficiency is 7.5 %) have been reported in [2]. Thus it can be achieved laser pulses duration of 10 ns with repetition rate up to 20 kHz at 510,6 nm, 255.3 nm (second harmonic), 578.2 nm, 289.1 nm (second harmonic) and 271.2 nm (sum frequency) with peak power of 130, 9, 150, 11 and 10 kW. Above this, N pulses integration regime applying to lidar signal recording allows to have range distance as at effective power is equal to $P N^{1/2}$ [2].

The results for XeCl eximer laser which was widely used in lidars and gives pulses with energy up to 0.1 J, duration of 10 ns at 308 nm wavelength and repetition rate to 50 Hz [1] were demonstrated comparing with other laser results.

Therefore back scattering vibration Raman lidar equation computer simulation for $^{127}I_2$ molecules and its heavy isotopes $^{129}I_2$, $^{131}I_2$ with above mentioned lasers with goal to choose lidar system laser wavelength for detecting minimum iodine molecules concentration is of our interest.

2. LIDAR EQUATION

Back scattering vibration Raman lidar equation computer simulation for $^{127}I_2$ molecules and its heavy isotopes $^{129}I_2$, $^{131}I_2$ with lasers of such a parameters has been fulfilled to choose lidar system optimum variant.

Back scattering Raman lidar equation was written down as in [3] in form

$$P(\lambda,R) = P_0(\lambda_0)K_1\Delta R A_2 T(\lambda_0)T(\lambda)(\frac{d\sigma}{d\Omega})N_a / R^2 \qquad (1)$$

where $P(\lambda, R)$ - Raman signal power from distance R at wavelength λ,

$P_0(\lambda_0)$ - laser power and wavelength,

K_1 - lidar constant,

ΔR - distance step,

A_2 - receiving telescope area,

$T(\lambda_0)$, $T(\lambda)$ - atmospheric transmission corresponding to laser and Raman wavelengths,

$(\frac{d\sigma}{d\Omega})$ - studied molecular Raman differential cross section,

N_A - molecules concentration,

R - range distance to measuring volume.

Studied iodine isotopes molecules Raman lines wavelengths were calculated in accordance to [1] with $^{127}I_2$ studied molecule vibration modes wave number from [4]. Other heavy isotopes wave numbers were calculated by square sum law [5].

Differential back scattering vibration Raman cross section can be determined as [1] changing cycle frequency by wavelength in formula

$$(\frac{d\sigma}{d\Omega})_j \sim \frac{16\pi^4 b_j^2 g_j}{\lambda^4[1-\exp(-hc/\lambda kT)]}\{\bar{\alpha}_j^2 + \frac{7}{45}\bar{\gamma}_j^2\} \tag{2}$$

where b_j - zero point vibration amplitude of j-th mode,

g_j - its degree of degeneracy,

$3\bar{\alpha}_j$ и $\bar{\gamma}_j$ - are trace and anisotropy of the derived molecule polarisability tensor associated with the normal coordinate q_j,

T - molecule vibration temperature,

k, h - Bolzmann and Plank constants,

c - light speed.

Remaining λ dependence only, formula (2) can be rewritten down in form

$$(\frac{d\sigma}{d\Omega})_j = A/\lambda^4 \tag{3}$$

where constant A was determined by known cross section value for argon laser wavelength $\lambda_0 =$ 488 nm $(\frac{d\sigma}{d\Omega})_j = 4.40\ 10^{-28}$ cm^2/ str [6] and it is equal $A = 2.495\ 10^{-17}$ cm^2 nm^4/str. Cuprous vapor laser radiation lies directly in iodine molecule absorption line [7,8] and resonance Raman effect has been taken into account for it and YAG - Nd second harmonic [1]. Constant A was determined by known cross section value for Hg arc lamp radiation $\lambda_0 =$ 546.1 nm $(\frac{d\sigma}{d\Omega})_{jr} = 1.70\ 10^{-24}$ cm^2 /str [1] and for this case it is equal $A = 1.51 \cdot 10^{-13}$ cm^2 nm^4/str. These constants gave possibilities to calculate Raman cross section values for chosen laser wavelengths. Furthermore, our lidar constant K_1 can be rewritten as

$$K_1 = K_2\, \xi_p(\lambda) \tag{4}$$

where $\xi_p(\lambda)$ comultiplier is photomultiplier (PMT) photocathode spectral sensitivity. The another comultipliers in equation (1) have the next values:

- $\Delta R = 7.5$ m for recording time duration of $t_d = 50$ ns,