PTB news
Scientific Newsletter
1
2019

Three times a year, PTB News provides topical information from the varied spectrum of activities of the Physikalisch-Technische Bundesanstalt (PTB) consisting of fundamental research, legal metrology and PTB's various activities in the service of the economy.

SCIENTIFIC NEWS

TECHNOLOGY TRANSFER

MISCELLANEOUS

Natural constants as the main protagonists

The General Conference on Weights and Measures (CGPM) adopts revision of the International System of Units

Especially interesting for
- metrology institutes
- high-tech industry
- schools and universities

On the occasion of their 26th General Conference on Weights and Measures (CGPM) in November 2018 in Versailles, the signatory states of the Metre Convention decided to fundamentally reform the International System of Units (SI). This resolution stipulates that, in the future, all SI units will be based on the numerical values laid down for seven selected natural constants. In passing this resolution, the General Conference has followed a recommendation issued by the International Committee on Weights and Measures (Comité international des poids et mesures, CIPM) – the world's supreme expert committee on metrology. The new definitions of the units will come into force on 20 May 2019, World Metrology Day.

In principle, the idea of defining units of measurement on the basis of natural constants is not new. What began 50 years ago with the definition of the second by means of atomic clocks, and continued over 30 years ago with the definition of the meter with the aid of the speed of light, will now continue for all of the units in the International System of Units (SI). In this context, four other fundamental constants will be playing the leading roles: Planck's constant, h, the Avogadro constant, N_A, the Boltzmann constant, k, and the charge of the electron, e.

In the major national metrology institutes, elaborate experiments have taken place over the past several years to measure these very constants as accurately as possible. The target measurement uncertainties set for these experiments have been achieved and the requirement that the experiments take place independently of one another has been fulfilled. It was therefore possible to determine the numerical values attributed to the fundamental constants concerned with very high accuracy.

With this fundamental revision, the system of units does away with the old system's deficiencies in terms of definitions. One particularly noticeable deficiency was that the mass of the international prototype of the kilogram and its copies varied by up to half a microgram per year. The new system now has a decisive advantage: natural constants are valid anywhere in the universe and at any time. They lend the new SI a universal

In the new International System of Units (SI), seven fundamental constants will be determined as defining reference entities. The seven base units – arranged in the outer circle of the diagram – will lose their prominent role. (Diagram: BIPM)

character. In contrast to standards such as the international prototype of the kilogram or the triple point of water, the realization of units based on fixed numerical values of natural constants is not restricted to a particular graduation on a unit scale. The SI is thus intrinsically open to technological innovation. ■

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Publications
Decisions of the 26th meeting of the General Conference of Weights and Measures, Versailles, 13–16 November 2018, published at: https://www.bipm.org/en/worldwide-metrology/cgpm/

The International System of Units, 9th edition, Bureau International des Poids et Mesures (BIPM), published at: https://www.bipm.org/en/publications/si-brochure/

Quantitative magnetic resonance imaging

Fast and accurate procedure for improved diagnosis of cardiac diseases

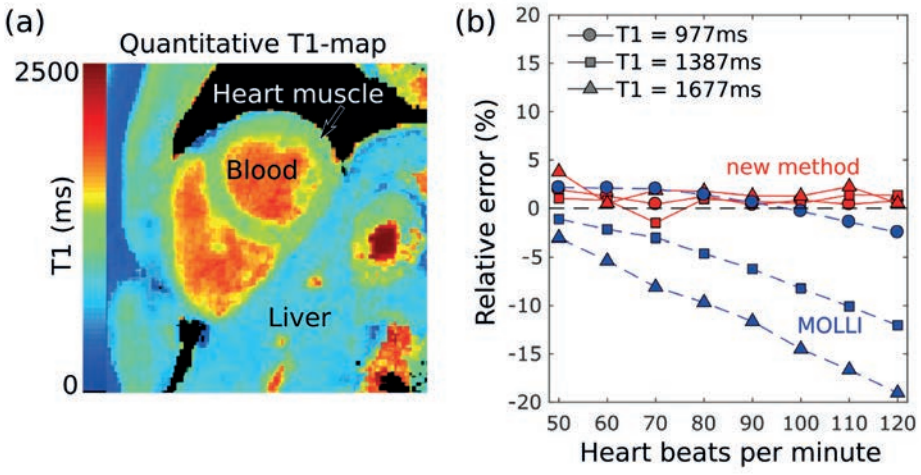
Especially interesting for
- medical research
- manufacturers of medical imaging devices
- cardiology

Magnetic resonance imaging (MRI) is an important imaging procedure in cardiology. To date, only qualitative imaging has been possible with MRI, since the measuring time is limited due to heart movements and breathing. A new image reconstruction procedure has now been developed at PTB. This method quantifies the biophysical parameters of the cardiac muscle with high spatial resolution and thus enables an objective diagnosis.

In conventional diagnosis, the images recorded are interpreted visually, so that the diagnosis depends on the doctor examining the image and on external influence quantities such as the manufacturer of the device and its place of installation. Quantitative imaging is a new field in biomedical research and clinical diagnostics. It consists in acquiring biophysical parameters of the tissue. This leads to more objective diagnoses and improved comparability between images. Developing these parameters allows the course of the therapy to be appraised.

In MRI, the tissue-specific relaxation time T_1 is used as a quantitative marker. T_1 describes the time-dependent behavior of the nuclear spins after they have been excited by means of a magnetic AC field. Cardiac T_1 imaging has great potential for clinical application since it allows pathologies of the heart to be diagnosed without radiation and without contrast agents. However, the major challenge is the heart's movement due to breathing and the heart beating, which limits the measuring time and, thus, the spatial resolution of the images. Furthermore, systematic measurement errors may occur due to simplified signal models.

A novel measurement procedure has now been developed at PTB: it provides T_1 maps of the heart with high spatial resolution in only 16 seconds. For this purpose, an iterative, model-based reconstruction procedure has been developed that can be used to determine T_1 values from very few measurement values. This has allowed the spatial resolution of the T_1 maps to be increased from (1.4×2.1) mm² to (1.3×1.3) mm² without changing the measuring time. Furthermore, the measurement provides information on the contraction of the heart during a cardiac cycle. This makes another important clinical parameter on the heart function available without requiring any additional measurement. The patient is thus examined more efficiently. The procedure was evaluated both in a T_1 phantom and in healthy volunteers. In contrast to methods that are already available, the accuracy of the T_1 values is independent of the heart rate and, with a difference of -0.3 % ± 2.5 %, it is in excellent agreement with the result of a four-hour reference measurement. The procedure is currently being tested on patients within the scope of a cooperation project with the Charité hospital in Berlin.



a: T_1 map of the heart of a healthy volunteer. b: Evaluation of the accuracy of the T_1 values in a phantom for different heart rates (bpm). The accuracy of the T_1 values (red) is independent of the heartbeat, whereas MOLLI – the most widely used T_1 imaging method – underestimates T_1 values at high heart rates (blue).

This measurement procedure paves the way for quantitative cardiac MRI for both hospitals and research; it is expected to contribute to improving diagnoses and making measurements performed at different hospitals easier to compare. ■

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Scientific publication
K. M. Becker, J. Schulz-Menger, T. Schaeffter, C. Kolbitsch: Simultaneous high-resolution cardiac T_1 mapping and cine imaging using model-based iterative image reconstruction. Magn. Reson. Med., 81(2), 1080–1091 (2019)

A precise view of the Sun

UV array spectroradiometer to measure the thickness of the ozone layer of the Earth's atmosphere

Especially interesting for
- climate resvearch
- meteorology

Within the scope of a cooperation project involving PTB and the Gigahertz-Optik company, a new compact array spectroradiometer was developed, characterized and field-tested. This new device can measure the direct spectral irradiance of the Sun on Earth with very little effort and at short intervals, thus allowing conclusions to be drawn as to the total ozone column of the Earth's atmosphere.

The ozone layer of the Earth's atmosphere is our most vital protection against harmful UV radiation from the Sun. Climate change and the thickness of the ozone layer are closely interrelated; determining the so-called ozone column is therefore an important part of global investigations on climate change. Measuring the thickness of the ozone layer indicates how much ozone is contained in the air column between the Earth's surface and the upper edge of the atmosphere. Accurate measurements involve considerable efforts, both with regard to equipment and to personnel. To date, it had not been possible to employ easy-to-use compact array spectroradiometers for this purpose because their measurement uncertainties and systematic errors were too high due to the limitations of the spectral resolution, their dynamics and stray light suppression.

An important characteristic of the new device that was developed specifically to measure solar UV irradiance is that it efficiently reduces the stray light – a parameter that is vital for high-quality spectral measurements. Stray light inside the instrument is physically reduced right from the beginning by means of appropriate design adjustments. Moreover, it can be effectively corrected by means of additional measurements. The instrument thus provides accurate and stable measurements of the direct solar UV irradiance. Based on this information, it is possible to deduce the ozone column at the moment of the measurement by comparison with the simulated spectral irradiance of an irradiance transfer model.

At an altitude of 2400 m, the spectroradiometer is facing the rising sun in Izaña.

The instrument was thoroughly tested and characterized at PTB in Braunschweig before being used at the Izaña Atmospheric Research Center (IARC) on Tenerife for an international comparison measurement campaign aimed at determining the ozone column. During the measurement campaign, the comparison measurements showed excellent agreement with conventional – and more time-consuming – measurement procedures involving Dobson or Brewer instruments within the range of the stated measurement uncertainties.

Due to its compact design and its fast, continuous measurement sequence, the spectroradiometer represents an efficient supplement to established measurement procedures. Thanks to these properties, it is now possible to set up, for example, a close-mesh measurement network and mobile measuring stations that enable a partly automated determination of the ozone column worldwide. ■

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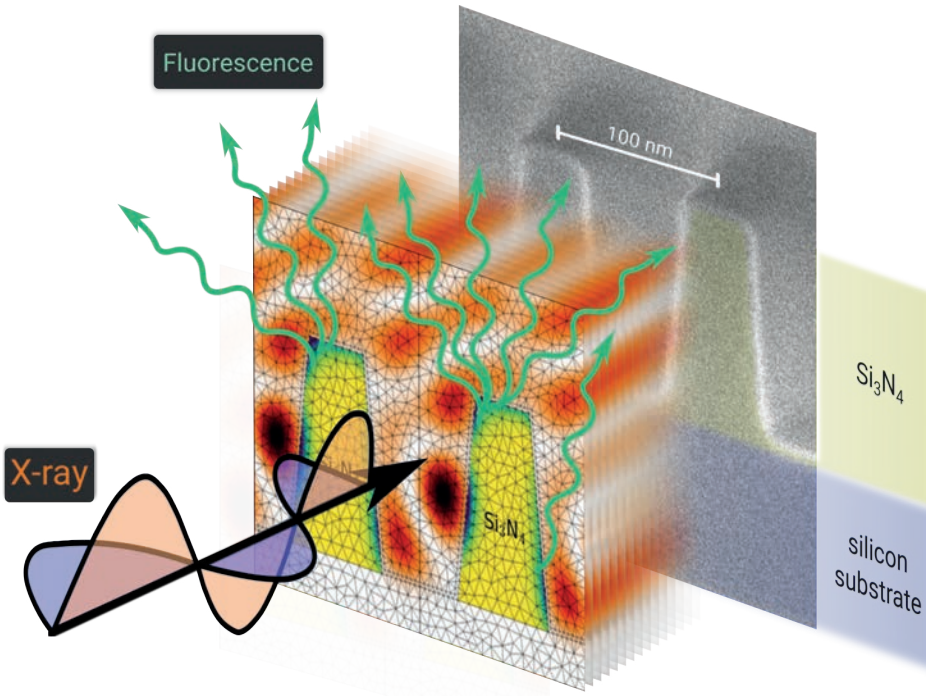
Scientific publication
R. Zuber, P. Sperfeld, S. Riechelmann, S. Nevas, M. Sildoja, G. Seckmeyer: Adaption of an array spectroradiometer for total ozone column retrieval using direct solar irradiance measurements in the UV spectral range. Atmos. Meas. Tech. 11, 2477–2484.

Taking a closer look into nanostructures

Reconstructing nanostructured surfaces by means of complementary experiments and theoretical modeling

Especially interesting for
- the semiconductor industry
- nanometrology

The increasing complexity of nanostructured surfaces used in technological applications makes their metrological characterization challenging. The importance of highly complex nanostructures consisting of several materials is particularly noticeable in the semiconductor industry. At PTB's laboratory at the BESSY II electron storage ring, it has now been demonstrated on a Si_3N_4 nanostructure on a silicon substrate that a material-sensitive dimensional reconstruction of a nanostructured surface is possible by modeling X-ray fluorescence experiments with synchrotron radiation.



Schematic representation of the combination of the FEM calculation of the electric field strength distribution and the GIXRF measurements carried out on a Si_3N_4 grating structure on a silicon substrate.

X-ray fluorescence analysis is a procedure in which incident X-ray photons excite electrons in inner atomic shells. When these excited states subsequently decay, element-specific X-ray fluorescence is emitted. Quantitative conclusions concerning the composition of the material examined can be drawn based on an energy-selective measurement of the X-ray fluorescence intensities, for which calibrated instruments are used.

Under grazing incidence of the exciting X-ray beam (grazing-incidence X-ray fluorescence, GIXRF), a standing wave field occurs through interference with the fraction of radiation reflected by the sample. This fraction of radiation penetrates locally into the surface structure. By rotating the sample on two axes around the incident X-ray beam, the locations of the maximum electric field strength – and thus the fluorescence emission – can be varied in a targeted way and the structure can be scanned with sub-nanometer resolution.

To assess the data, exact numerical modeling of the spatial field strength distribution is required. To this end, an approach was chosen that had already been developed for experiments on grazing-incidence small-angle X-ray scattering (GISAXS) and that is based on a finite-element method (FEM) to solve the Maxwell equations.

Combining GIXRF with the FEM calculation as well as the quantitative modeling of the emitted fluorescence intensities allows conclusions to be drawn concerning the number and position of atoms of a specific element within the nanostructure.

For future requirements of nanometrology, it is envisaged to combine this experimental theoretical approach with data obtained by means of GISAXS. These data may not contain any information related to the specific material, but they allow a very accurate dimensional reconstruction of the nanostructures. ■

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Scientific publication
V. Soltwisch, P. Hönicke, Y. Kayser, J. Eilbracht, J. Probst, F. Scholze, B. Beckhoff: Element sensitive reconstruction of nanostructured surfaces with finite elements and grazing incidence soft X-ray fluorescence. Nanoscale 10, 6177–6185 (2018)

Mercury compounds in water – a hidden threat?

Analytical method for the determination of mercury compounds in water in the ng/kg range developed

Especially interesting for
- environmental analysis companies and laboratoriesh

Mercury is toxic for many organisms. In the environment, mercury occurs everywhere and in various chemical forms. These mercury compounds are then absorbed by organisms via food, water and air. To assess the risks exhaustively, all forms of mercury as well as their possible conversion products must be known and determined. A traceable analytical method has therefore been developed to enable the quantitative determination of methylmercury and inorganically bound mercury down to the ng/L range.

Taking a water sample from the River Oker in Braunschweig

Mercury occurs in various forms and is very mobile. Most of the mercury comes from natural sources such as volcanic eruptions. But anthropogenic sources such as the combustion of fossil fuels also lead to concentrations that can be very high locally. Due to various conversion processes, the toxicity of mercury can increase further. This is, for example, the case for methylmercury. Methylmercury finds its way into the body via water and food (in particular fish) and may damage the nervous system and the kidneys.

For this reason, the "Minamata Convention on Mercury" was created in 2013, with the aim of reducing worldwide mercury emissions and establishing comparable analytical and control mechanisms.

At PTB, an analytical method has now been developed to determine organic methylmercury and inorganic mercury in water. This method consists in preparing the samples by derivatization into a form that is more easily accessible for separation and extraction into an organic solvent.

This extract is subjected to separation in a gas chromatograph. The analytes are then detected by means of mass spectrometry. With the aid of the species-specific isotope dilution method, the respective concentrations can be determined down to the ng/L range.

In the European Water Framework Directive, mercury compounds are classified as priority hazardous substances, even though the currently valid Environmental Quality Standards (EQS) of 0.07 µg/L in surface waters and 20 µg/kg in biota (fish, bivalve mollusks, algae, etc.) relate exclusively to the total mercury content.

The new method developed within the scope of the European Metrology Research Programme (Project ENV51) complements the requirements of the directive. It provides a sensitive and comparable measurement method to determine mercury species in water, which can be used to perform a full risk assessment taking the species distribution as well as possible conversion processes into account. ■

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Radiating materials processing

X-ray dose measurements on laser materials processing machines

Especially interesting for
- manufacturers and users of lasers for materials processing
- radiation protection

In the laser materials processing of workpieces unwanted X-rays can occur. Their dose rate and spectral distribution have now been accurately determined for the first time.

Materials processing by means of laser radiation is a long-used technique. More recently, ultrashort pulsed laser radiation has been increasingly used for this purpose. By using the high peak intensities of up to more than 10^{14} W/cm² in the laser focus, unwanted X-rays are generated which were measured for the first time in an application environment of industrial laser materials processing.

For this purpose, a thermoluminescence detection (TLD) based spectrometer was used. The penetration depth of the X-ray radiation in the spectrometer depends on the energy, so that the energy-resolved spectrum of the radiation can be calculated from the dose values in the TLD layers by means of mathematical methods (Bayesian deconvolution).

The resulting dose rate depends on the processed material and its nature and was in the order of 1600 mSv/h to 7300 mSv/h in terms of the radiation protection quantity $\dot{H}'(0{,}07)$, 16 mSv/h to 71 mSv/h in terms of the quantity $\dot{H}'(3)$ and 1 mSv/h to 4 mSv/h in terms of the quantity $\dot{H}^*(10)$, in each case per materials processing time. Such high dose rates would exceed legal dose limits within a few minutes to one hour (for the local skin dose, as estimated by $\dot{H}'(0{,}07)$, and the eye-lens dose estimated by $\dot{H}'(3)$) or a few hours (for the effective dose of the whole body, estimated by $\dot{H}^*(10)$). The spectral distribution was in the range of a few keV up to 30 keV. The dose contribution of photons above 30 keV was negligible.

These measurements, traceable for the first time, not only provided manufacturers and users of ultrashort pulse lasers with important information for the design of the machines with regard to radiation protection, but already influenced the current legislative procedure in the field of radiation protection. At the same time, machines with even higher laser intensities are already being developed. Therefore, the presented measuring method will become even more important in the future. ■

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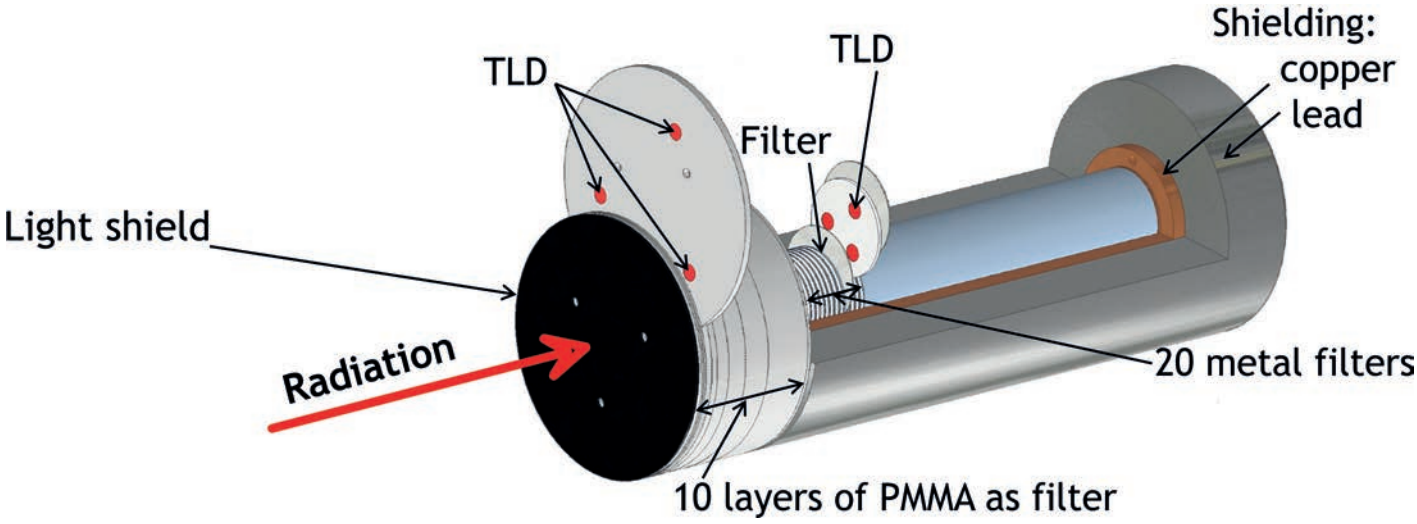
Scientific publication
R. Behrens, B. Pullner, M. Reginatto: X-ray emission from materials processing lasers. Radiat. Prot. Dosim. (2018)
DOI: 10.1093/rpd/ncy126

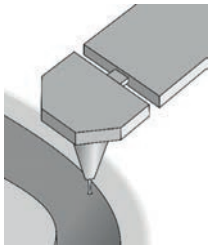


Sketch of the TLD-based spectrometer. Basic principle: The deeper the radiation penetrates the spectrometer, the higher its energy.

3D-AFM: Enhanced 3D sensitivity

Especially interesting for
- manufacturers of scanning force microscopes (AFMs)
- manufacturers of microscope equipment

Today, atomic force microscopy (AFM) is faced with the challenge of measuring 3D structures reliably. State-of-the-art 3D measurements have been prone to errors since commercially available cantilevers (i.e. the measuring pins used in an AFM) do not react equally when exposed to forces from three spatial dimensions. At PTB, this problem has been successfully addressed by developing new cantilevers. These newly structured cantilevers react more sensitively to 3D influences, and they no longer tend to slip when scanning slopes that are not equally steep. (Technology Offer 476) ■



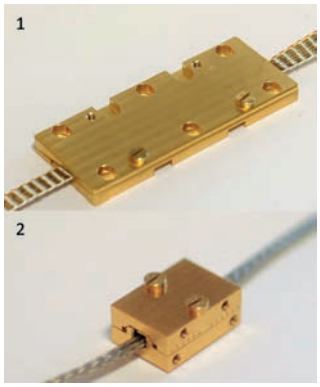
One of the new designs that ensure a well-balanced relation of the stiffness: a modified cantilever with cut-outs in the beam.

Advantages
- enhanced sensitivity with nearly isotropic stiffness
- real 3D probing by means of flexible hinges
- can be integrated into existing atomic force microscopes

Cold cables for "dry" cryostats

Especially interesting for
- providers of equipment for cryogenic technologies such as woven ribbon cables
- manufacturers of cryostats

Modern low-temperature systems increasingly make use of "dry" cryostats whose cooling effect is reached in vacuum solely by direct thermal contact. However, cables and electric wiring may impede the cooling process if they are not coupled thermally at suitable locations between room temperature and operating temperature. At PTB, two new designs have therefore been developed to thermally couple round cables and flat ribbon cables. The heat flow, which propagates through the supply lines to a sensor, can thus be minimized. This is particularly helpful at a temperature below 4 K. (Technology Offers 473 & 483) ■



1: The clamping device for flat ribbon cables, which features an adjustable channel height, is pressed together by means of screwed joints and can also be stacked. 2: Round cables are fixed inside the second cable clamp by means of several spring elements.

Advantages
- low thermal impedance for varying cable sizes
- can easily be integrated into existing cryostats
- connections are easily disengaged

Self-traceable voltage divider

Especially interesting for
- calibration laboratories
- research institutes

Accurate measurements of high voltages in the range of 200 kV require the use of voltage dividers. These devices divide high voltages into smaller ones that can only then be accurately measured. The size of the signal is determined by the scale factor. Up to now, this factor had to be determined by regularly calibrating the voltage dividers against national standards. At PTB, a self-traceable voltage divider has now been developed. It provides testing laboratories with a flexible tool. Its main principle is that series-connected resistors can be connected in parallel and adjusted. In this way, it is possible to save both operating expenses and time since there is no need for transporting the equipment to a metrology institute and setting it up there. (Technology Offer 484) ■

The voltage divider: The Perspex tube contains 99 high-precision resistors that can be connected either in series or in parallel.

Advantages
- allows the scale factor of a voltage divider to be checked directly
- fast: traceability is achieved within an hour
- improved measurement uncertainty due to shorter traceability chain

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Awards

Frank Härtig

Dr. Härtig, the head of Division 1 "Mechanics and Acoustics" has been appointed President Elect of IMEKO following a unanimous vote in his favor. In the coming three years, he will coordinate 24 technical committees. In 2021, he will then take over the presidency of IMEKO for three years.

Gisa Foyer, Holger Kahmann

Mr. Kahmann, who works in Department 1.2 "Solid Mechanics" and Dr. Foyer, who previously worked in the same department, have received the György Striker Junior Paper Award for best publication at the IMEKO XXII World Congress in Belfast. Their publication, titled "A finite element analysis of effects on force lever systems under nacelle test bench conditions", was developed within the scope of an EMPIR project on the traceability of torque measurements in wind turbine testing facilities.

Davood Momeni Pakdehi

At Graphene Week 2018, a conference held by the European Graphene Flagship, Davood Momeni Pakdehi, a doctoral candidate in Department 2.5 "Semiconductor Physics and Magnetism" was awarded the best poster prize for his work titled "Stacking order induced sequential doping of epitaxial graphene on SiC" in the category of "Synthesis and Growth".

Elisa Pirovano

The member of Department 6.4 "Neutron Radiation" has obtained the doctoral award of the European Nuclear Education Network (ENEN) for her thesis titled "Neutron scattering cross section measurements with a new scintillator array", which she wrote at the JRC in Geel.

An issue of "maßstäbe" on the new SI

What can we expect from the revision of the International System of Units (SI), which was approved on 16 November 2018 and will enter into force on 20 May 2019? The answer depends on who you ask – an ordinary citizen, a student, a scientist or a metrologist in industry. The editorial staff of maßstäbe has asked this question – and gathered the answers in a new issue that is just as colorful and diverse as the answers obtained (Issue 14, "Maße für alle", only in German). You can order this issue individually or as a classroom set free of charge; alternatively, you can subscribe to maßstäbe.
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Successful excellence initiative

"QuantumFrontiers" is a joint project of Leibniz University Hannover and TU Braunschweig that is realized in close collaboration with PTB. This project will become an excellence cluster and will thus receive several million euros of support within the scope of the excellence strategy of the Federal Republic of Germany and of the German federal states. This excellence strategy aims to promote top-level research at German universities and to strengthen Germany's position as an internationally competitive scientific location. QuantumFrontiers deals with new measurement technologies at the nanometer level. At this small scale, physical fundamental units such as mass, length and time are expected to become more accurate. For this purpose, quantum mechanical effects are exploited to improve measurement accuracies. Experts from the most varied fields of physics, astronomy, geodesy and geoinformatics, semiconductor research, circuits and integrated systems are working together to attain this goal.
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Joint professorship

Dr. Gavin O'Connor was jointly appointed as a university professor by TU Braunschweig and the Physikalisch-Technische Bundesanstalt (PTB). He assumed this post on 1 September 2018. Dr. O'Connor is a 45-year-old chemist who specializes in mass spectrometry, especially in the field of biological measurements and chemical metrology. Prior to his appointment as a professor, Dr. O'Connor worked for the Joint Research Centre of the European Commission in Geel, Belgium. There, he managed a team of scientists who developed analytical methods for food allergens using procedures such as mass spectrometry.

Prof. Dr. Joachim Ullrich (President of PTB), Prof. Dr. Gavin O'Connor with Prof. Anke Kaysser-Pyzalla (President of TU Braunschweig) and Dr. Bernd Güttler (Head of Division 3 "Chemical Physics and Explosion Protection" of PTB) (from left to right; photo: Bernt Erlewein, TU Braunschweig)

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