

Senin, Nicola and Leach, Richard K. (2018) Informationrich surface metrology. Procedia CIRP . ISSN 2212-8271 (In Press)

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ScienceDirect

Procedia CIRP 00 (2016) 000-000



15th CIRP Conference on Computer Aided Tolerancing - CIRP CAT 2018

Information-rich surface metrology

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Abstract

Information-rich metrology refers to the incorporation of any type of available information in the data acquisition and processing pipeline of a measurement process, in order to improve the efficiency and quality of the measurement. In this work, the information-rich metrology paradigm is explored as it is applied to the measurement and characterisation of surface topography. The advantages and challenges of introducing heterogeneous information sources in the surface characterisation pipeline are illustrated. Examples are provided about the incorporation of structured knowledge about a part nominal geometry, the manufacturing processes with their signature topographic features and set-up parameters, and the measurement instruments with their performance characteristics and behaviour in relation to the specific properties of the surfaces being measured. A wide array of surface metrology applications, ranging from product inspection, to surface classification, to defect identification and to the investigation of advanced manufacturing processes, is used to illustrate the information-rich paradigm.

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Peer-review under responsibility of the Scientific Committee of the 15th CIRP Conference on Computer Aided Tolerancing - CIRP CAT 2018.

Keywords: Surface metrology; areal topography characterisation; information rich metrology

1. Introduction

Information-rich metrology (IRM) is a term that is introduced here to refer to the use of any type of additionallyavailable information to improve a measurement process [1]. Information may come from knowledge of the manufacturing process, knowledge of the object to be measured, and/or knowledge of the physical interactions/principles underlying the measurement technology itself. Information may either come from pre-existing knowledge (i.e. "a priori"), from mathematical modelling or simulation, or from other measurement processes, even performed concurrently to the measurement one is aiming to improve. An overview of how information sources and information flow change when the IRM paradigm is adopted is provided in Fig. 1. The idea of using available information related to the product, or process, product-measurement-instrument interaction, or makes intuitive sense because metrology in manufacturing takes place in controlled and very predictable conditions, with a sensible amount of information which is known in advance.

1.1. Information about the measured object and the manufacturing process

When a part or product is manufactured, in particular when using digital manufacturing methods, a large amount of information is typically available about the object being produced. For example, CAD data provides information about the nominal form. Analogously, a significant amount of information is available, or can be easily acquired, about the manufacturing process, in terms of its capability, the features and defects it generates, the materials it is designed to operate with, and the types of geometries and surfaces it typically produces. Most of such information is generated and exploited through product design and manufacturing process planning. In IRM, the aim is for such information to be used to improve metrology, for example, in the inspection and verification of part quality, or in manufacturing process monitoring.

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1.2. Information about the measurement instrument and the instrument-surface interaction

One of the most promising paradigms for IRM is based on using additional information about the manufacturing process and the object that is produced, to develop improved mathematical models that describe the interactions between the measured object and the measuring instrument. In practice, mathematical models that describe physical principles and phenomena underlying many measurement technologies are already available, although one has to be careful that over-simplifications are not abused. In optical measurement, for example, many models have been developed over the last decades [2], to support the theory of variation microscopy, coherence focus scanning interferometry, confocal microscopy, fringe projection, photogrammetry, etc.



Figure 1. Additional sources of information and changes in information flow when shifting from (a) conventional metrology to (b) the IRM paradigm.

It is safe to say that the totality of current commercial optical measurement systems is already making use of complex mathematical models to interpret raw data acquired through their probes. However, because such models aim to be general, which means that they must be applicable with little prior knowledge of the measurement scenarios, they can make very few assumptions about the nature of the surface which will be measured, the material properties that will be encountered, and other factors. Thus, such models are limited in the information they can provide. A typical example is the interpretation of signals originated by light captured by the detector after multiple reflections and scattering. Trying to reconstruct what determined the patterns captured by the detector implies the solving of complex (often non-linear) inverse problems, which are typically unsolvable or ambiguous without resorting to additional sources of information.

The advantage of working in the scenarios typically encountered in manufacturing metrology is that such additional information is often readily available: at the macroscopic scale, there is information about part shape and expected dimensions, at the microscopic scale, there is information about the expected surface texture, and about signature features left by the manufacturing processes. All such information is exploited to a small extent in conventional manufacturing metrology, but is rarely used to develop a better understanding of how measurement instruments interact with surfaces, useful in turn to achieve a better interpretation of measurement raw data.

1.3. Smart aggregation of information

The IRM paradigm requires a fundamental re-design of the data analysis processes that are typically adopted in conventional metrology applications. The addition of a potentially high number of heterogeneous information streams raises a whole series of challenges regarding how such information should be homogenised, aggregated and finally exploited towards achieving a better measurement result overall. Recent work on multi-sensor data fusion provides and overview of the challenges and approaches for sensor data aggregation [3, 4]. Challenges are in how to handle of large amounts of data in increasingly shorter times (possibly verging towards Big Data issues), in how to data mine the relevant relationships between variables, and finally in how to obtain mathematical and statistical models that ultimately support what can be referred to as the "smart" measurement paradigm, as opposed to the conventional metrology pipeline of "blind" processing (i.e. where knowledge is extracted exclusively from the raw data provided by the measurement instrument, with no help from any other sources of information). As in many other applications involving Big Data, a fundamental role in such a paradigm shift may be covered by artificial intelligence (AI) technologies. Machine learning in particular, can provide significant support to the development of the smart measurement solutions of the future (for example, see [5]).

1.4. The IRM advantage

Central to the IRM paradigm is the aim to improve measurement quality. Quality is here intended as a generic term encompassing multiple facets: improving quality may mean reducing measurement times, improving measurement performance indicators (accuracy, precision, etc.), expanding the range of covered scales (spatial resolution and range), and improving coverage, intended as the capability to reach surfaces which may be harder to reach, for example measuring beyond the maximum permissible slope for a given measurement technology. Improving coverage and metrological quality of measurement is a key strategic objective in manufacturing metrology, as many emerging measurement applications (for example, in additive manufacturing), are creating new challenges related to geometric complexity and lack of uniform material properties [6-9]. Improving measurement speed is almost as essential in many in-process and in-situ measurement applications [10-13], as well as the need to overcome the fundamental limits of individual measurement technologies [14]. The idea of

overcoming the above limitations by manipulating the acquired data (as opposed - or in addition - to creating new measurement technologies) is not new (see [15-20] for examples of adaptive or intelligent data reduction and sampling techniques), and is the fundamental conceptual paradigm that defines IRM.

A final note must be reserved to consider that IRM is not only about improving the quality of a measurement, as the information-rich paradigm may also lead to an improved interpretation of the same measurement result. Thanks to an information-rich approach, more advanced conclusions or further insight on the system under observation can be gained, for example, by being able to look at the same data with a new set of eyes provided by the information-rich paradigm. A typical example of this is the incorporation of information about a process or product, to implement advanced statistical models for quality monitoring and/or process control [21-24].

2. Information-rich surface metrology

Whilst the previous considerations are general to any metrology application, this paper focuses specifically on the measurement of surface topography, and on what it means for surface metrology to embrace the information-rich paradigm in terms of challenges and new opportunities.

2.1. The paradigm shift illustrated through an example

The conventional data processing pipeline adopted by surface metrology is shown in Fig. 2. The pipeline is based on ISO 25178-2 [25] terminology, but equivalent concepts also apply to the older ISO 4287 standard [26]. A form operator (F-operator) is used to de-trend the signal (i.e. level) and to remove any trace of the underlying form of the part. An Sfilter is used to remove high frequency noise, and an L-filter is used to separate and remove the waviness component. Data processing is designed to make the resulting scale-limited surface (SL-surface) as close as possible to a stationary random signal, suitable to be described by texture parameters that are for a significant part derived from sample statistics.



Figure 2. Information processing pipeline adopted in conventional surface metrology: example on profile data (adapted from [27]).

Very little information is required to apply this procedure: some knowledge of the surface nominal form is required for the F-operator, and previous information about relevant spatial frequencies (typically coming from the manufacturing process and the measuring instrument) is required to choose suitable nesting indices for the S and L filters (cut-off frequencies in the ISO 4287 terminology). The paucity of information requirements is an advantage, as it makes the procedure of very general applicability. But generality is also the main limitation of the procedure, as further case-specific information cannot be exploited to delve deeper into the analysis of measurement data.

An example application of the information-rich paradigm is shown in Fig. 3 for a simple case of profile measurement in cylindrical turning. In this case, the expected topography is modelled using a geometrical construction from the literature [28], which relates the spacing, depth and shape of the machining grooves to process parameters, such as feed rate and tool tip geometry. Whilst measurement can proceed in the same way as in the conventional method, what changes is the way the data is analysed: the simulated, expected topography can be subtracted from the measured profile, and then the residuals can be characterised, again possibly with the conventional means of isolating a stationary random signal. The advantages are immediately visible: it is possible, for example, to investigate aspects, such as the regularity and geometric properties of the machining marks (i.e. how much they deviate from the expected results) and in turn identify effects of machining error at multiple scales (chatter phenomena, oscillations of the workpiece, worn tool, etc.). The price to pay for a potentially much more in-depth investigation is that the method is not generic (it only applies to cylindrical turning), knowledge of nominal manufacturing parameters is required, the whole process of fitting to a nominal geometry, and investigating the residuals requires more preparation and is more challenging to implement.



Figure 3. Information rich surface metrology example: use of a topography model from the literature [28] to investigate a measured profile from cylindrical turning.

2.3. Introduction to feature-based representations

The use of modelling to predict topography from manufacturing process parameters, as exemplified in the previous section, introduces the concept that, in IRM, additional information layers pertaining to topography can be added to the characterisation pipeline, for example, where topography itself is described in terms of its constituent features. For the cylindrical turning example, such features are the machining marks, but in general multiple higher-level information overlays can be added to represent additional viewpoints. For example, in Fig. 4, an areal topography dataset acquired by an atomic force microscope (AFM) is shown, again representing a cylindrical turned surface, where further overlays (in addition to machining marks), are used to identify scratches from functional life, or artefacts from the measurement process.

Feature-based representation is the term introduced in IRM to refer to the use of additional, higher-level information overlays where topography is partitioned into regions, and the relevant ones are mapped to classes defined within some userdefined ontology. As ontologies may be case-specific (i.e. referred to a specific manufacturing process, application or measurement technology), once again, IRM sacrifices generality for depth and breadth of investigation possibilities.



Figure 4. Feature overlays for a cylindrical turning surface measured with AFM.

2.4. The feature-based characterisation pipeline and examples

For "feature-aware" topography characterisation, a new data processing pipeline is introduced within the informationrich surface metrology paradigm [29]. This is summarised in Fig. 5, and is comprised of the phases of feature identification (the features of interest are identified through template matching of their shape and size properties to those defined in the ontology of reference), feature extraction (the features of interest are isolated through a partitioning/segmentation of the original dataset, and then extracted as independent geometric entities); and feature characterisation (the feature of interest are described in terms of their relevant shape and size properties).



Figure 5. The feature-based characterisation pipeline.

Feature-based overlays are a core concept of informationrich surface metrology, as they allow mapping of low-level topography information (point cloud or structured grid of height values) to multiple layers of higher-level information, each designed to allow some type of context-specific reasoning, for example, to investigate manufacturing signature features, measurement artefacts or elements of structured surfaces.

An example application of feature-based characterisation is shown in Fig. 6 for a metal laser powder bed fusion (LBPF) surface measured with coherence scanning interferometry (CSI). In Fig. 6.a, spatter formations are algorithmically identified in the measured dataset; in Fig. 6.b and Fig. 6.c, some of such formations are isolated and characterised in terms of footprint area and protruding height from the surroundings [30].



Figure 6. Identification, isolation and characterisation of spatter formations on metallic surface fabricated via laser powder bed fusion. Measurement obtained via CSI (adapted from [30]); a) identified features; b) footprint area properties; c) feature height properties.

In Fig. 7, a similar feature-based characterisation pipeline is used to isolate and characterise LPBF weld tracks and weld ripple spacing [30]. In Fig. 8, the feature-based characterisation pipeline is used to quantify the regularity of the cross-section of a manufacturing artefact specimen, designed to study the process capability of ink-jetting to fabricate micro-conductor lines made of metal particles in a polymer matrix [31].



Figure 7. Characterisation of weld tracks and weld ripples on metallic surface fabricated via laser powder bed fusion. Measurement obtained via CSI (adapted from [30]); a) identified weld tracks; b) cross-section width regularity analysis on isolated weld track; c) detail of weld ripples; d) ripple spacing analysis.

In Fig. 9, unit dimples from a regular pattern designed to reduce friction in bearing applications are algorithmically identified and isolated [32]. In addition to the characterisation of their diameters, the regularity of the pattern layout is investigated by reconstruction of the network of distances between feature centroids.



Figure 8. Characterisation of cross-section regularity of manufacturing sample artefact fabricated via ink-jetting. Measurement obtained via focus variation (adapted from [31]); a) original measurement; b) investigation of cross-section width uniformity across length.

Depending on the degree of determinism of the studied identification topography, different feature and characterisation solutions may be adopted. For example, high variability of shape and size of feature instances suggest the use of statistical modelling tools for shape representation and comparison, the main goal being to pursue robustness to intrinsic variability of feature instances, while still ensuring discrimination of features belonging to different classes. Additional challenges for shape-based reasoning are related to possible lack of information due to sub-optimal sampling density, occlusions, re-entrant portions or too steep to measure portions of the features, all of which being typical issues of micro-scale topography measurement.



Figure 9. Characterisation of individual dimples and regular dimple patterns designed for friction reduction. Measurement obtained via focus variation (FV) (adapted from[32]); a) computation of dimple diameter; b) reconstruction of lattice; c) lattice regularity analysis (left: original, middle: diameters, right: spacing)

Currently investigated approaches for feature identification range from CAD-compare techniques, to the use of a variety of template matching technologies based on shape descriptors (for example, the ring projection transform [33] and the angular radial transform [34]). CAD-compare approaches work well in the presence of highly deterministic structures, for example, when inspecting micro-parts or products (MEMS, microfluidics) and share significant resemblances with the inspection and verification of standard-sized parts (Fig. 10), both in terms of procedural choices and in terms of issues. However, since typical applications of informationrich surface metrology are at the micro-scale, the availability of surface-specific point sets, akin to what is obtainable from a touch probe coordinate measuring machine (CMM), is seldom achievable (because of the low market penetration, and challenges of using micro-CMMs [2, 29]), and thus in most circumstances, characterisation proceeds with blanket measurements (typical of range imaging techniques) that require point set partitioning to isolate the point subsets to fit to each datum [29]. For step-like features, edge detection combined to morphological segmentation methods [35-37]

has also proven effective. For the identification and isolation of feature instances subjected to significant variability, the use of shape descriptors has been explored, for example, applied to super-abrasives (Fig. 11.a) [33] and micro-embossing patterns (Fig. 11.b) [34], or for identifying correspondences between topographies to be aligned [38].



Figure 10. Characterisation of micro-structured elements via CADcompare techniques (adapted from [29]); a) segmentation; b) volumetric comparison between measured and nominal reference.



Figure 11. Feature identification and classification by means of shape descriptors; a) grits in superabrasive (adapted from [33]); b) pattern units in micro-embossing master (adapted from [34]).

2.5. Incorporating knowledge about measurement instruments and instrument-surface interaction

Another primary venue of investigation in the development of the information-rich surface metrology paradigm, pertains to the incorporation of instrument-related information, and in particular, to the use of models that explain instrumentsurface interaction and are thus capable of predicting instrument performance and behaviour when encountering specific topography features. A simple example is shown in Fig 12, where an algorithm is applied, specifically designed to identify and reduce batwing and other spike-like artefacts that appear in CSI measurement in correspondence to abrupt height changes in the topography, as it typically happens when measuring step-like features [39].



Figure 12. Measurement-aware topography data preprocessing example: identification and removal of CSI batwing and spike artefacts from step-like topographic feature (adapted from [39]).

The challenge when incorporating knowledge of a specific measurement technology in the surface data processing pipeline is that, aside from general well-known effects that are clearly recognisable and fairly easy to predict in correspondence of specific topographic features (such as the batwing artefacts mentioned above), a wide range of additional problems are more challenging to spot and handle, as they are related to specific combinations of topographic properties, material properties, and instrument configurations at the time of measurement. In recent work by the authors, it was shown how the assessment of topographic reconstruction error has a key relevance in contemporary surface metrology [40, 41], as measurement error across technologies may sometimes be the same order of magnitude as the features one is trying to measure. The same LPBF region measured via different technologies is shown in Fig. 13; recessed features and high-spatial frequency topographic components are most likely to result in very different reconstructions when acquired with different technologies.



Figure 13. The same topography region reconstructed from single measurement performed with different technologies. Pure 2D imaging results (from optical focus stacking and scanning electron microscopy (SEM) are also shown (adapted from [40]).

Research work is, therefore, in progress, not only to better understand each and every one of the major measurement technologies and how their performance and behaviour is affected by measurement set-up parameters [42-44], but also to investigate instrument-surface interaction by focusing on specific test-cases of interest, such as for example, in the noncontact (optical and X-ray) measurement of metallic, LPBF surfaces [40, 41]. As an example, in Fig. 14 the reconstruction of the topography of an individual spatter formation is shown, as obtained from focus variation and coherence scanning interferometry measurements.



Figure 14. Local height difference in the reconstruction of a LPBF spatter formation by different measurement technologies (CSI: gray against FV: green). Gap colour shown in the cross-section proportional to signed difference (adapted from [30]).

A series of replicate measurements performed in repeatability conditions over the same portion of surface can be used to investigate precision in local height determination, and possibly may serve as a starting point to explore how such precision may be predicted as a function of the topographic properties of the surface being measured [40, 41]. In Fig. 15, repeated measurements of a metallic LPBF surface with multiple instruments are used to build confidence intervals on local mean height. As the results indicate, some regions of the topography are associated to higher measurement dispersion, which can be used as a starting point to build predictive models of measurement dispersion as a function of local topographic properties, to use in information-rich characterisation approaches.



Figure 15. Local confidence intervals on the mean topography profile extracted from replicate areal measurements with multiple instruments (green: confocal, blue: focus variation, red: coherence scanning interferometry, purple: X-ray computed tomography (adapted from [41]). The width of the confidence intervals can be used as an indication of local precision in height determination.

The same method shown in Fig. 15 can be used to assess statistically relevant discrepancies between reconstructions obtained with different measuring instruments; discrepancies corresponding to the regions where confidence intervals do not intersect [41]. This in turn is equivalent to determining the local bias of the topographic reconstruction of one instrument, if another can be assumed as a more reliable (i.e. accurate) reference.

Statistical modelling of topographies from replicate measurements is a first step towards building a wide array of regression models capable of predicting measurement error from information about the topographic properties of the region being measured. Such predictor models could eventually be extended into simulation tools capable of predicting measurement error and behaviour when confronted with any surface. The incorporation of measurement error models is a first step towards a measurement-aware approach to feature identification and characterisation, as shape/size information pertaining to the relevant features could be modified to accommodate for variability owing to performance and behaviour of the measurement technology used to acquire information. As a minimum, for example, both local bias and precision information arising from statistical topography models could be used to formulate uncertainty budgets associated with topography, which in turn through could be propagated the feature-based characterisation pipeline, ultimately determining the uncertainty of the feature characterisation result. Ultimately, though, the determination of traceability for feature-based characterisation is still fundamentally undermined by the need to establish traceability of surface topography measurement first, a long-time running endeavour [45, 46].

3. Conclusions and outlook

In its attempt to incorporate useful knowledge about the surface, manufacturing process and measurement process within the data processing pipeline, information-rich surface metrology surely loses generality with respect to the conventional approach to surface characterisation, where only minimal information is necessary, and the same data processing pipelines can be applied at least in principle to any surface, measured by any instrument. On the contrary, additional, often significant effort, is needed in informationrich approaches, to collect, understand and appropriately integrate additional data and models into the data processing pipeline. Such effort is typically tied to the specific aspects that define the application, i.e. expected part geometry, the manufacturing process used to produce it, and/or the measurement technologies used to collect data. The methods of conventional surface metrology, the specification standards around it, and even the instruments around it, have been designed to ensure satisfactory results almost in a fool-proof manner, from any surface, with any instrument, and in any operating conditions. On the contrary, it is evident that the information-rich approach requires more preparation, and careful fine tuning, tailored to each and every specific application domain. To make the matter more difficult, as the application changes, it is not unlikely that much additional modelling effort will need re-visiting to adapt to the new circumstances. Manufacturing processes evolve and improve over time, as well as the signature features they generate. Measurement instruments also evolve, and so do their performance and behaviour. Customer specifications on what is relevant to measure and to what accuracies and precisions also evolve, as products with increasingly higher value-added are designed and produced. At each and every iteration, information-rich approaches require significant extra work, to collect extra data, to develop the appropriate support models, and finally to integrate all the sources of heterogeneous information into a coherent pipeline, ultimately aiming at achieving better metrological performance. This process of data gathering and organisation is typically not straightforward.

IRM in general, and information-rich surface metrology in particular, pose a series of challenging issues also from the viewpoint of knowledge representation, as a multitude of heterogeneous sources and many different viewpoints encompassing shape, process and function-related information, must be gathered and merged into a coherent whole. Fundamental challenges of information handling, communication, processing and storage must be addressed, involving a wide array of disciplines and competencies ranging from ontologies, AI, etc.

Ultimately, the application of the IRM paradigm is far from effortless, and far from straightforward, and ultimately may not necessarily be suitable in all manufacturing metrology scenarios. Where it is applicable though, it is asserted that such a significant price to pay is hopefully counterbalanced by the value added to the characterisation results, as dedicated analysis pipelines can be developed that are custom-tailored to specific characterisation requirements, and are capable of providing information that may more directly address specific inspection requests.

Acknowledgements

The authors would like to thank the EPSRC (Grant EP/M008983/1) and the EC (FP7-PEOPLE-MC 624770 METROSURF).

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