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Review on Numerical Modeling of Instrumented Indentation Tests for Elastoplastic Material Behavior Identification

J. Marteau · S. Bouvier · M. Bigerelle

Abstract The impacts of the parameters controlling the finite element simulation of instrumented indentation tests and their consequences on numerical results are reviewed in case of homogeneous materials and functionally graded ones. Through a comparative study of the results of different finite element models, the effects of model dimensions (two-dimensional vs. three-dimensional) and its characteristics (boundary conditions, element choice, mesh refinement) on the numerical results are analyzed. Effects associated with rate-independent material behavior, surface roughness, friction, residual stresses and indenter tip bluntness are discussed. It is shown that depending on the material behavior and the maximum indentation depth, the previous conditions can strongly affect the numerical results of indentation tests. The choice of the simulation conditions should be carefully thought as it affects the numerical results. This is also important when building inverse approaches, i.e. methods that extract the material properties using indentation test data, as they are often based on numerical results. Even if the simulation conditions are carefully chosen, some differences may remain between the experimental and numerical results. The last part of this review analyzes the two main sources of remaining differences between the results of finite element simulation and experimentation: the determination of the reference point and the Indentation Size Effect.

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1 Introduction

The needs for knowledge on material properties at finer and finer scales led to the development of new devices and methods. At the same time, the development of new materials such as property graded materials as well as the development of thin films, showed the limit of conventional testing techniques, such as tensile or compression tests. These events led to the development of new techniques such as the instrumented indentation test, also referred to as depth-sensing indentation. Instrumented indentation is similar to standard hardness tests. In standard hardness tests, hardness is determined by forcing a given indenter into the surface of a material: the load is increased until it reaches a user-defined value. Then, it is either held constant for a short period of time before removing or immediately removed. After unloading, the surface area of the residual indentation is measured using a microscope. Hardness is defined as the maximum load P_{max} divided by the residual surface area of the indentation. In the instrumented indentation test, the indentation load P and the displacement h are continuously recorded during the loading and unloading cycles. The instrumented indentation can be performed accurately using depths in the nanometer range as well as in the micro- and macro-meters ranges.

This technique offers many advantages such as the relative simplicity of the experimental setup, the small size of the samples and its global non-destructive aspect. However, this apparent simplicity is counterbalanced by the difficulty of construing the recorded data. Indeed, instrumented indentation tests induce complex stresses (a mixture of compressive and tensile stresses), which remain poorly understood. Moreover, the calculation of mechanical properties, such as hardness or Young's modulus, is based on an estimation of the area of contact. When the examined material work-hardens,

the estimation of the contact area is usually inaccurate thus giving false mechanical properties. It is also difficult to determine the first contact between the indenter and the surface. A false determination of this point leads to inaccurate calculations of mechanical properties.

The interpretation of instrumented indentation data remains a major mechanical issue. Until recently, test interpretation was essentially based on the use of empirical or semi-empirical formulae determined from experimental observations, as proposed by the pioneering work of Tabor [1]. Recent progress in computer sciences and engineering has provided new tools to study mechanical phenomena: numerical simulations. It enables the visualization of the tests, the resulting stress fields while providing an important flexibility for the material behavior (elastic, elastoplastic, viscoplastic...).

Finite element simulations of the instrumented indentation test are widely used. This fact is highlighted by the variety of the investigations and studied materials: polymers [2,3], composites [4–6], ceramics [7,8], bones [9,10], metallic glasses [11,12], single crystals [13,14] ...

The present paper proposes an extensive literature review on how instrumented indentation tests are simulated using continuum mechanics and finite element approach. Only the materials having an elastoplastic behavior will be examined. Indeed, a substantial body of research is based on these conditions (e.g. [15,16]). Furthermore, specimens having elastoplastic behavior are the most commonly examined when building inverse approaches i.e. methods that extract material properties using indentation test data (e.g. [17,18]). The simulation conditions, such as the boundary conditions, behavior laws..., are compared and analyzed in order to assess their influences on the numerical results and consequently on the results of inverse approaches. The first six sections are dedicated to this analysis. The first section aims at investigating the influence of the simulation dimensions (two-dimensional versus three dimensional models) on the results. Then, the second and third sections describe the model, the mesh characteristics, the behavior laws and plasticity criteria used in the simulation of the instrumented indentation test. The fourth and fifth sections are dedicated to the influence of the friction coefficient on the indentation results and to the characteristics of the simulated indenter. The sixth section presents the most common strategies for the simulation of materials showing roughness or residual stresses, as well as their effects on the results. A careful examination of all the previous elements enables to more closely emulate the real conditions of the indentation test. However, differences between the simulated and experimental results usually remain. This is why the last part of this paper is devoted to the most common sources of differences: the determination of the reference point and the Indentation Size Effect.

2 Simulation Dimensions: 2D Versus 3D

First, numerical simulations of the instrumented indentation test were conducted using two-dimensional (2D) models, thanks to simplified geometrical representations and geometrical symmetries. It was mainly motivated by the limitations of memory systems and computing power environments. Then, technical progress enabled the use of the third dimension (3D) to get more realistic models [19]. However, as reflected by recent publications (e.g. [20–22]), 3D models have not replaced 2D models. This may be explained by two factors. First, 3D simulations remain memory and time-consuming. The second factor is that they are pointless in some configurations. As an example, conical and spherical indenters can be modeled using 2D simulations without requiring any simplifying assumptions provided that the examined material is isotropic or that its behavior can be modeled using rotational symmetry (e.g. plastically graded properties along the axis of symmetry or bi-axial stresses). On the contrary, pyramidal indenters such as Vickers or Berkovich indenters require the use of simplifying assumptions. They are modeled using a cone having an equivalent contact area (i.e. a cone with an angle equal to 140.6°). This raises the question of the impact of this assumption on the results of the simulation. Several authors showed that the substitution of conical indenters having equivalent contact areas for pyramidal indenters does not modify the load versus indentation curve (P–h). An example is given in the work of Lichinchi et al. [23] related to the characterization of the properties of a hard film, deposited on a soft substrate. The behavior is assumed to be elastic perfectly-plastic. Lichinchi et al. [23] compared the P–h curve obtained with a 3D model using a Berkovich indenter with the one given by a 2D model using a conical indenter having an equivalent contact area. The P–h curves are nearly identical, thus indicating that the simplified 2D model is valid at least in terms of indentation curve simulation. More recently, Ruan et al. [24] followed the same approach to confirm this assumption. They simulated the indentation of a bulk material having an elastic perfectly-plastic behavior using similar conditions as Lichinchi et al. [23] for the axisymmetric model (i.e. 2D model). For the 3D model, Ruan et al. [24] adopted the numerical model proposed by Larsson et al. [25]. The indentation loading and unloading curves showed a nearly perfect match. However, the cases studied by Lichinchi et al. [23] and Ruan et al. [24] only concerned basic material behaviors: the material work-hardening was not taken into account. Moreover, the authors did not take into account other factors such as friction or an imperfect shape of the indenter that can have a non-negligible influence on the P–h curve. Tunvisut et al. [26] simulated the indentation of an elastoplastic material with a power-law work-hardening and compared the results obtained with an axisymmetric model to the experimental results obtained

using a Vickers indenter. Again, an excellent agreement was found between the numerical and experimental curves. Warren et al. [27] completed a more comprehensive comparison of 2D and 3D models. The material behavior was modeled using an elastic–plastic behavior with a power-law work-hardening. The authors also considered the effects of friction and the influence of the tip defect of the Berkovich indenter. The comparison of von Mises contours calculated with the 2D and 3D models revealed the limitations of the 2D model simplifications: noticeable differences were observed in the stress fields and the shape of the indentation imprint. Sakharova et al. [28] also showed that the indenter shape can significantly influence the indentation results. By juxtaposing the results given by conical, Berkovich and Vickers indentation tests, they pointed out the fact that, depending on the material behavior, the indenters may not be interchangeable: they gave significantly different P–h curves and thus different hardness results. Sakharova et al. [28] systematically investigated the h_f/h_{max} ratio where h_f is the residual indentation depth after unloading and h_{max} is the maximum indentation depth (with $0.2 < h_f/h_{max} < 0.98$). For materials having low h_f/h_{max} ratios (i.e. hard materials), the results obtained with a Vickers indenter were closer to the ones found using a conical indenter than the ones calculated using a Berkovich indenter. On the contrary, for materials having high h_f/h_{max} ratios (i.e. for soft or medium-hard materials), the indenters gave similar results. The simplifying assumption required to replace pyramidal indenters with conical indenters has thus limitations. Depending on the studied material, one may need to use a 3D model if the indentations are practiced using a pyramidal indenter (e.g. Vickers or Berkovich indenters).

Geometrical simplifications should also be considered with care when indenting surfaces having complex geometries, such as rough surfaces. Walter et al. [29] investigated the effects of surface roughness on the indentation results by comparing data given by 2D and 3D models. Indentations with a spherical tip were conducted on CrN coatings having an arithmetic surface roughness (R_a) ranging between 2.6 and 11.2 nm. The results of both models indicated that an increase of roughness led to an increase of the scatter of the P–h curves. However, larger scatter was observed for the curves given by the 2D model. Furthermore, in this model, the loading curves showed deviations from both sides of reference curve (i.e. the curve standing for the smooth sample) while all the loading curves given by the 3D model laid to the right of the reference curve. Walter et al. [29] argued that this difference was due to the symmetry of the 2D model. When the latter was swept for visualization, the line profile of asperities was transformed into a set of concentric rings. This set of concentric rings provided a stiffer antibody for a spherical tip than a set of randomly distributed asperities, corresponding to the 3D model. Walter et al. [29] also detected that the calculated mean contact area of the 2D model tended to be

higher than the one calculated with the 3D model. This effect became more and more pronounced with increasing surface roughness. They concluded that the error introduced by the simplified representation limited the validity of the 2D model to samples having an arithmetic surface roughness R_a lower than 3 nm. The previous works emphasized the fact that, for pyramidal indenters, the 2D model assumptions (i.e. axisymmetric models with a cone having a contact area equivalent to the studied pyramidal indenter) require some considerations. If one is only interested in the indentation curves, 2D models are sufficient. The small differences observed between the results of 2D and 3D models are usually largely compensated by experimental errors associated with test reproducibility. Though, if strain or stress distributions are examined or if the indentation imprint is observed, then a 3D model should be used. Similarly, if the studied material has a complex structure (e.g. anisotropic or a lack of symmetry of the properties) or a complex surface (e.g. rough surface) then a 3D model should be preferred, whatever the indenter shape.

3 Model and Mesh Characteristics

3.1 Boundary Conditions

Several types of boundary conditions can be used when simulating the instrumented indentation test. The boundary conditions of the indenter are always the same: they prevent rotation and promote normal translation to the specimen surface.

For 2D models, axisymmetric models are inevitably used, with roller boundary conditions along the symmetry axis of the substrate (i.e. the indented material). For the other faces, several types of conditions can be used. The most basic conditions are:

- (i) totally fixed nodes,
- (ii) nodes with roller boundary conditions,
- (iii) unrestrained nodes.

Usually, the nodes at the bottom of the mesh have roller conditions or are completely fixed while the nodes at the sides of the mesh remain unrestrained (e.g. [30–38]). Fixing the nodes at the bottom and sides of the mesh is rarely used when simulating indentation tests because it increases the model rigidity, even if this effect tends to disappear if the model dimensions are large enough (e.g. [39]). In some cases, the boundary conditions that are used are not mentioned or not completely described and their choice is justified by saying that the model was tested and is insensible to the boundary conditions (e.g. [40,41]). In other cases, the lack of effects of the choice of the boundary conditions is justified by indicating that the model dimensions are large enough compared

to the studied contact area, which enables to assume that the substrate is semi-infinite and thus insensible to boundary conditions (e.g. [42–44]). In summary, if the substrate dimensions are large enough compared to the indentation depth, then the simulation of the indentation test is globally unaffected by the boundary conditions.

When the substrate dimensions are limited (e.g. a large number of degrees of freedom are required), the boundary conditions should be examined with great care. For instance, Walter et al. [29] reproduced surface roughness measured with an Atomic Force Microscope onto the surface of a 3D model. The authors had to use very small spacing between the nodes of the surface of their model in order to faithfully reproduce the measured roughness. In order to limit computing time, they modeled a small volume equal to $6 \times 6 \times 6 \mu\text{m}^3$. Because of the model size, Walter et al. [29] had to select boundary conditions that would not reduce the accuracy of the calculated results. To assess the impact of the boundary conditions, Walter et al. [29] examined different scenarios:

- (i) All the nodes belonging to the side and bottom faces are fixed in the normal direction,
- (ii) Only the nodes at the bottom of the mesh are fixed in the normal direction while the nodes of the side faces can move unrestrained,
- (iii) The movements of the nodes of the side and bottom surfaces are described according to the equations derived by Boussinesq, which enable to determine the displacement of an arbitrary point inside a semi-infinite body loaded with a centered force,
- (iv) Sub-modeling: first, the solution is computed for a larger model having larger elements. Then, the calculated solution is used to describe the boundary conditions of a smaller model having smaller elements. This refinement is repeated several times in order to obtain the boundary conditions of the chosen model (here, the $6 \times 6 \times 6 \mu\text{m}^3$ model).

In order to assess the impact of the previous scenarios of boundary conditions, Walter et al. [29] compared the numerical P–h curves given by the indentation of a smooth surface with the indentation curves given by Hertz’s theory of contact mechanics. As expected, the first scenario gave a model that is too stiff due to the constriction of all sides. Its indentation curve lied far from the exact solution. The second scenario gave better results but the behavior remained too stiff compared to the theoretical solution. The best results were obtained with the fourth scenario, which was thus applied to the simulation of indentation tests on rough surface. These studies highlight the importance of boundary conditions as they can particularly affect the accuracy of the results when the model dimensions are small (e.g. 3D simulations).

3.2 Element Type and Mesh Size

Simulation of indentation tests with 2D models requires the use of axisymmetric elements. The most employed ones are quadrangles being either four-node bilinear elements (e.g. [45,46]) or eight-node elements with quadratic interpolation (e.g. [24,47]). For 3D models, eight-node hexahedrons are preferred: the latter can be either isoparametric (e.g. [25,48]), with linear interpolation (e.g. [29,49]) or with quadratic interpolation (e.g. [50]).

Another influential parameter in the simulation of indentation tests is the size of the elements in the indented area i.e. the area where the largest deformations occur. This area should be meshed with special care for two main reasons: (i) to facilitate the detection of contact and (ii) to allow an accurate description of the material stresses and strains. In finite element computation, contact detection involves the definition of two elements: the master (the indenter) and the slave (the indented substrate). In order to have an accurate detection of the contact between these two elements, the mesh of the indented area must be fine enough. If the mesh is too coarse, then the contact between slave and master elements may not be detected before indenting the surface, which generally leads to divergent calculation.

In general, sensitivity to mesh size is investigated observing the indentation curves, even if different methods are employed by the authors. Liu et al. [51] assessed the effects of the refinement of the elements of the indented area by quantifying the maximum deviations occurring between P–h curves obtained with different element sizes. The tested elements are either 10 % smaller or 10 % bigger or 50 % bigger than the elements of a mesh used as a benchmark. The authors observed that, with a coarser mesh (10 and 50 % bigger elements), the indentation curve had large oscillations. The indentation curves given by the mesh having 10 % smaller elements showed only small differences compared with the results of the reference mesh. Using these results, they confirmed their choice of element size and checked the model convergence. Bressan et al. [52] also examined the impact of the size of the elements of the indented area but they preferred comparing the values of the achieved maximum load and the global aspect of the curves (e.g. referred to as “rough” when numerous oscillations are observed). The mesh quality can also be assessed by observing the hardness values calculated using the obtained indentation curves (e.g. [53]).

Other authors validated their mesh refinement by comparing the results of their finite element model with an analytical one. For instance, Beghini et al. [36] compared the stresses calculated with their finite element model to the analytical solution given by Hertz theory. Beghini et al. [36] also observed the maximum indentation depth at the onset of plasticity. This comparative study is however limited to the study

of the elastic behavior as no analytic solutions are known for plastic behavior.

Mesh refinement is also of primary importance when sink-in or pile-up effects are studied because of the sensitivity of these phenomena to element size [54]. The reason behind this is the contact detection algorithm. For instance, Lee et al. [55] validated their mesh refinement by observing pile-up changes with the increase of the number of elements in the indented area. To do so, they divided the final indentation depth including the pile-up height by the nominal depth, measured using the original surface level.

To sum up, the number of elements in the contact zone and the size of the refined area are important parameters for the simulation of indentation tests. They ensure that the numerical results are not affected by the selected mesh. In many published works, the description of the mesh characteristics is rarely complete. Some authors limit their description to the number of elements in contact with the indenter during the test (e.g. [41,56,57]) while others only give the total number of elements (e.g. [58–60]). This makes it difficult to carry out comparative studies of the different models.

4 Behavior Laws and Plasticity Criteria

In the present work, the review of the behavior laws used to simulate indentation tests is restricted to rate-independent laws. The main behavior laws and plasticity criteria identified in the literature are divided into two categories. The first one, entitled “homogeneous materials”, gathers behavior laws used to describe bulk materials or films while the second category, entitled “functionally graded materials”, gathers materials whose properties gradually vary with depth.

4.1 Homogeneous Materials

In the majority of the laws identified in the literature, the authors considered uniaxial behavior and assumed that the material is isotropic. Quadratic plastic criteria are mainly used. The equivalent quantities are mostly obtained using the classical von Mises criterion. Some studies used Hill criterion, which is particularly relevant when the material behavior is anisotropic. For the sake of simplicity, the following assumptions are generally made:

- The material remains perfectly elastic during the deformation (e.g. [45]),
- The material is perfectly plastic (e.g. [23,24]),
- The material behavior can be described using a bilinear law in which the elastic part is described using Hooke’s law while the plastic part is described by the tangent modulus E_t (e.g. [61]).

The most commonly used behavior law for the simulation of indentation tests, particularly when developing inverse approaches (i.e. methods for identifying the material properties from the indentation curve), is Hollomon’s law. The latter is expressed as follows:

$$\bar{\sigma} = K\bar{\varepsilon}_p^n, \quad (1)$$

where $\bar{\sigma}$ is the equivalent stress, $\bar{\varepsilon}_p$ is the equivalent plastic strain, n is the strain-hardening exponent and K is a constant depending on the material characteristics. In practice, most authors prefer writing the previous equation as follows:

$$\begin{cases} \sigma = E\varepsilon_e & \text{pour } \sigma < \sigma_y \\ \sigma = R\varepsilon^n & \text{pour } \sigma \geq \sigma_y \end{cases}, \quad (2)$$

where E is Young’s modulus, ε_e is the elastic deformation (assumed to be small compared to the total deformation), R is a material parameter, σ_y is the yield stress (which can be considered as constant for elastic perfectly plastic behavior or evolving with accumulated plastic strain in order to take into account the material hardening) and ε is the total strain. Equation (2) assumes that the material is isotropic, has isotropic linear elasticity (Hooke stress–strain relation is used in finite element simulation) and that the stress field is uniaxial (the second relation in Eq. (2) is written using von Mises equivalent quantities). Based on small deformation theory, the total strain can be written as follows:

$$\varepsilon = \varepsilon_e + \varepsilon_p. \quad (3)$$

Considering the mathematical continuity between the first part and second part of Eq. (2), the following equations can be obtained (e.g. [36,40,44,48,62–69]):

$$\sigma = \sigma_y \left(\frac{E}{\sigma_y} \right)^n \varepsilon^n \quad \text{ou} \quad \sigma = \sigma_y \left(1 + \frac{E}{\sigma_y} \varepsilon_p \right)^n. \quad (4)$$

It is worth noting that, although this expression is mathematically exact, it assumes that there is a correlation between the elastic properties and the plastic ones (through the writing of constant K), which remains debatable from a mechanical point of view. This correlation is sought in inverse approaches as it enables to reduce the number of material parameters that have to be identified but it can also lead to identification errors due to the imposed correlation. Besides, the hypotheses on which this expression is based usually do not match reality: stress fields are not uniaxial and the levels of plastic deformations that are reached during indentation tests are usually large and require the use of the large deformation approach.

Ludwik’s law is another power-law used to describe the material behavior in the simulation of indentation tests (e.g. [47,70]):

$$\bar{\sigma} = \sigma_y + k\bar{\varepsilon}_p^n, \quad (5)$$

where k is a material parameter. In Eq. (5), σ_y is the initial yield stress (i.e. at the beginning of plastic strain). The term

$k\bar{\varepsilon}_p^n$ describes material work-hardening. Other groups used the power-law described by Swift's law (e.g. [28,53]):

$$\bar{\sigma} = \sigma_y + C (\varepsilon_0 + \bar{\varepsilon}_p)^n, \quad (6)$$

where C and ε_0 are material parameters. The initial yield stress σ_y is equal to $C\varepsilon_0^n$.

Finally, other authors used the Ramberg–Osgood relationship. For instance, Haj-Ali et al. [71] wrote this law for a 1D case:

$$\varepsilon = \frac{\sigma}{E} + \frac{\sigma^n}{F}, \quad (7)$$

Where E is Young's modulus and F is a material parameter.

In order to describe material behaviors that exhibit stress saturation, Voce law is more suitable (e.g. [72,73]):

$$\bar{\sigma} = \sigma_y + R_{inf} (1 - \exp(-b\bar{\varepsilon}_p)), \quad (8)$$

where R_{inf} and b are constants depending on the material properties.

All the material laws introduced so far describe an isotropic hardening which is suitable for monotonic loading. In order to consider a possible plastic behavior during unloading, the previous models can be extending to non-monotonic loading using the kinematic hardening based on the formulation of Armstrong and Frederick [74]. The kinematic hardening is described by a second order tensor, \bar{X} , whose evolution law is given by:

$$\dot{\bar{X}} = \frac{2}{3}C\dot{\bar{\varepsilon}}_p - \gamma\bar{X}\dot{\bar{\varepsilon}}_p, \quad (9)$$

where C and γ are material parameters and $\dot{\bar{\varepsilon}}_p$ is the plastic strain rate tensor. The combination of hardening given by Eqs. (8) and (9) is usually called the Lemaitre and Chaboche's model [75], and is used when cyclic loadings are modeled (e.g. [72,76]).

When studying phenomena taking place during the indentation of crystals (slip activities, dislocation arrangements...), constitutive meso-plastic models are used. For example, Liu et al. [77] developed an approach based on crystal plasticity, with the isotropic hardening model developed by Peirce et al. [78] and Hutchinson et al. [79].

4.2 Functionally Graded Material

Functionally graded materials can be divided into two main categories: the materials having a variation of elastic properties and the ones having a variation of plastic properties.

Suresh et al. [42] studied the behavior of a material showing a gradient of elastic properties along the depth. The gradient was described by the following exponential law:

$$E = E_0 \exp(az), \quad (10)$$

where E_0 is the Young's modulus at the surface of the material, z stands for the depth and a is a constant enabling to describe the gradient variation.

Different strategies are used to model a gradient of plastic properties. Few studies have been published on this subject. Overall, three main strategies are used to describe the gradient of plastic properties. In the first strategy, the gradient is described by modifying only one parameter of the behavior law: the yield stress changes with an increase of the depth. For instance, Choi et al. [46] chose to use a behavior law similar to Hollomon's but in which the yield stress varies with depth, as follows:

$$\sigma_y(z) = \sigma_y^{surf} (1 + \beta z), \quad (11)$$

where σ_y^{surf} is the yield stress at the material surface, β is a factor describing the gradient and z is the depth.

The second strategy is based on the use of a volumetric mixing law. For example, Nakamura et al. [32] described the variations in the composition of a metallic–ceramic mixture through the use of an idealized power-law:

$$V_c = \left(\frac{z}{t}\right)^n, \quad (12)$$

where t stands for the thickness of the layer containing the metal–ceramic mixture, z is the depth and the exponent n is a constant characterizing the mixture. The volume fraction of the ceramic phase V_c is then used in a modified rule of mixture [80] to determine the effective modulus E_f and the effective yield stress σ_{yf} of the composite.

The gradual variation of material properties in Moussa et al. [81] is described using three layers of different thicknesses. For the first layer having a thickness of e_1 (surface), the stress is homogeneous through the thickness. For the second layer (transition layer) having a thickness of e_2 , the stress exhibits a linear relationship along the thickness. For the third layer (substrate), the stress is again homogeneous through the thickness. In the transition layer, the properties are described by mixing the behavior laws of the substrate and the material surface:

$$\begin{cases} \sigma = \sigma^{surf} & \text{pour } z > e_1, \\ \sigma = \sigma^{sub} + \frac{\sigma^{surf} - \sigma^{sub}}{e_2} (e_2 + e_1 - z) & \text{pour } e_1 < z < e_1 + e_2, \\ \sigma = \sigma^{sub} & \text{pour } z > e_1 + e_2 \end{cases} \quad (13)$$

where σ^{surf} and σ^{sub} are respectively the stress of the hardening law of the surface and the substrate, and z is the depth.

The third strategy directly implements the gradient by modifying the behavior law of the concerned layer. For instance, Giannakopoulos et al. [43] modified Ramberg–Osgood equation by including a local variation of the elasto-plastic properties through the thickness:

$$\bar{\varepsilon}_p = \left(\frac{\bar{\sigma}}{J}\right)^n \left(\frac{z}{e}\right)^m, \quad (14)$$

Where $\bar{\varepsilon}_p$ is the equivalent plastic strain, $\bar{\sigma}$ is the equivalent stress, J is the characteristic stress, n is the strain-hardening coefficient, m is an exponent describing the gradient intensity and e is the thickness in which the elastoplastic properties vary with the depth z .

As a conclusion, the previous research works indicate that there is a non-negligible number of ways of describing functionally graded materials, even if the study of these materials is recent. The graded properties concern either the elastic or plastic behavior. There are smooth gradients as well as step gradients displaying more or less abrupt transitions in material properties between the discrete layers.

5 Friction Coefficient

Friction is part of the parameters whose effects on the results of the numerical simulation of indentation tests are still discussed. Some research groups assume that friction is equal to zero, by arguing that:

- (i) friction effects on the results of the simulation of the indentation test are negligible [35,40,69],
- (ii) friction influence is low for the studied material [23],
- (iii) when friction is not considered, convergence is facilitated [36],
- (iv) the studied surfaces are smooth therefore friction effects can be neglected [26].

Overall, friction effects on the results of the numerical simulation of indentation tests remain poorly understood. Several researches in this field share two common goals: to quantify the influence of friction on the indentation test results and to find the most relevant value for the friction coefficient of the finite element model, in order to faithfully reproduce experimentations.

Most of the finite element models were built using different conditions and hypotheses (i.e. different indenter shapes, maximum indentation depths, behavior laws, etc) and remain thus difficult to compare. Despite these differences, some main trends can be identified.

Most of the examined papers used Coulomb's law for the description of friction (e.g. [82,83]). The paper of Gao et al. [84] stands out among the other studies as it compared Coulomb's law to the friction stress model. Gao et al. [84] indicated that the friction stress model gave better results than Coulomb's law for the calculation of the correction factor β defined by Oliver and Pharr [85]. Nevertheless, Coulomb's law remains the most used method for the description of friction due to its simplicity.

Tabor [1] described the evolution of the normal force W as a function of the friction coefficient μ (Coulomb's friction coefficient) and the semi-angle α of a conical indenter using the following equation:

$$W = P \left(1 + \frac{\mu}{\tan \alpha}\right) \frac{\pi d^2}{4}, \quad (15)$$

where d is the contact diameter (i.e. the diameter of the imprint) and P is the mean yield pressure, which is assumed to be independent of the indenter shape according to Hankins [86]. Equation (15) indicates that for large values of the semi-angle α , the ratio $\frac{\mu}{\tan \alpha}$ is small compared to 1. Consequently, for Berkovich and Vickers indenters (having both an equivalent semi-angle equal to 70.3°), the effect of friction on normal forces can be neglected. In order to get an in-depth knowledge of this relation, Bucaille et al. [40] simulated the indentation of a substrate using a conical indenter having a semi-angle equal to either 42.5°, 50°, 60° or 70.3° with a friction coefficient ranging from 0 to 0.3. The comparison of normal loads enabled Bucaille et al. [40] to quantify the influence of the value chosen for the friction coefficient as a function of the indenter angle. They found that, for large values of semi-angles (60° and 70.3°), a variation of the friction coefficient from 0 to 0.3 only induced a 3% change of the normal force, for a given indentation depth. The influence of friction is greater for low semi-angle values: for the semi-angle standing for the cube-corner indenter (42.5°), a 20% increase of the maximum force was observed when the friction coefficient μ was increased from 0 to 0.2. When changing the value of the coefficient of friction, Bressan et al. [52] observed a slight increase of the maximum force needed to indent a material with a cone having a contact area equivalent to a Vickers indenter. This observation enabled them to conclude that the effect of friction was negligible with the examined simulation conditions. Antunes et al. [87] examined the influence of the friction coefficient value (μ was equal to 0.08, 0.16 and 0.24) on the shape of the P-h curves given by a 3D simulation of an elastoplastic material indented with a Vickers indenter. As no differences were distinguished between the curves, Antunes et al. [87] concluded that the influence of friction could be neglected. Sakharova et al. [28] confirmed these results by using similar hypotheses in their simulation and widened the conclusions to the conical, Vickers and Berkovich indentations of composite materials. Other studies, such as the one published by Warren et al. [27], highlighted the fact that friction could have small influence on the loading part of the indentation curve while no effects were detected on the unloading part or on the shape of the indentation imprint. Overall, research in this field investigated the effects of friction in specific cases and do not permit to draw general conclusions relative to the effects of the friction coefficient in numerical modeling of the indentation test.

Similar analyses were performed for spherical indenters. For a given indentation depth, Lee et al. [55] noticed a slight increase of the load with an increase of the value of the friction coefficient. However, this increase was not quantified. Through the use of an elastic–viscoplastic behavior law, Berke et al. [88] showed that the value of the friction coefficient affected the P–h curve obtained with a spherical indenter. When friction is taken into account, there is an increase of the load required to reach the same indentation depth as the one obtained without friction. Berke et al. [88] also found that the first part of the curve tended to be stiffer after an indentation depth equal to 20 nm and that this effect tended to amplify when increasing the indentation depth. No friction effects were detected during the unloading. The dependence of the indentation curve on the value of the friction coefficient was also noted by Mesarovic et al. [89] and confirmed by the work of Cao et al. [68,90]. Cao et al. further indicated that, for elastic perfectly-plastic materials, friction effects can be large for high h/R ratios (where h is the indentation depth and R is the indenter radius). They also underlined the fact that this effect can be large for materials having low strain-hardening coefficients. For a given h/R ratio and a given strain hardening coefficient, Cao et al. noted that a large E/σ_y ratio can also increase the impact of friction on the indentation results. As a consequence, Cao et al. concluded that either a large strain-hardening coefficient or a small E/σ_y ratio was required in order to neglect the influence of friction when indenting elastoplastic materials with a spherical indenter.

It should also be noted that several authors showed that, above a certain value of the friction coefficient, the indentation curves become indistinguishable from one another. For elastic viscoplastic materials, using a spherical indenter, Berke et al. [88] showed that the limit value of the friction coefficient was approximately equal to 0.3. Similar results were obtained by Habbab et al. [91] when indenting elastoplastic materials with a spherical indenter and by Bucaille et al. [40] when indenting elastoplastic materials with sharp indenters.

To sum up, in the numerical simulation of the indentation test, friction effects are highly dependent on the conditions or hypotheses of the finite element models. The friction coefficient affects the results obtained with sharp indenters if the indenter angle is low ($<50^\circ$), otherwise this effect can be neglected. Friction effects are more pronounced when indenting elastic perfectly-plastic materials or materials having a low strain-hardening coefficient with a spherical indenter. Friction can have non-negligible effects for large h/R ratios, too. Finally, a “saturation effect” is observed for sharp and spherical indenters: when the friction coefficient is larger than 0.3, the indentation curves become indistinguishable from one another.

Friction effects on pile-up heights and on the indentation depth were also investigated. The term pile-up means that the

contact area tends to be deformed upward (the indentation imprint has a crater shape) and is the opposite of the sink-in phenomenon. Liu et al. [51] observed that an increase of the friction coefficient from 0 to 0.4 tended to reduce the pile-up height obtained with a spherical indenter. Indeed, friction prevented any gliding of the material and thus pile-up building. Similar trends were observed by Bucaille et al. [40] with sharp indenters having different angles. Bucaille et al. [40] showed that pile-up was greater when using sharp indenters having small angles and that it reduced with friction. Guo et al. [92] found similar results and underlined the fact that, when the semi-angle of conical indenters was sufficiently high ($\theta \geq 80^\circ$), friction became predominant, i.e. there was nearly no gliding at the interface between the material and the indenter. They found that there was also a saturation effect of the increase of pile-up or sink-in with an increase of the friction coefficient (for values higher than 0.3). Mata and Alcalà [56] also examined the influence of friction when indenting materials having a power-law behavior, with sharp indenters. They concluded that if no pile-up or sink-in occurred during the indentation then friction had no effect on the indentation curves. It is, for example, the case for materials having a high strain-hardening exponent. By contrast, friction effects should be carefully examined and taken into account in finite element simulations for materials that harden a lot during the indentation. Similar results were found by Taljat et al. [67].

Finally, Antunes et al. [53] observed that the friction coefficient value affected the equivalent plastic strain distribution. When indenting an elastoplastic material with a Vickers indenter, they found higher maximum equivalent deformations with lower values for the friction coefficient. The location of the maximum equivalent deformation also depended on the value of the coefficient of friction. Globally, Antunes et al. [53] noted that an increase of the value of the coefficient of friction tended to smooth the deformation gradient.

All these observations show that it is important to study the effects of friction to accurately identify the material parameters, especially for materials that tend to pile-up or sink-in, as well as when using spherical indenters.

6 Indenter Modeling

6.1 Indenter Behavior

Pyramidal or conical indenters are mainly simulated as perfectly rigid bodies (e.g. [52,93]). In some cases, the authors corrected a possible elastic deformation of the indenter (e.g. [23]) using the following formula:

$$\frac{1}{E_r} = \frac{1 - \nu^2}{E} + \frac{1 - \nu_i^2}{E_i}, \quad (16)$$

where E and γ are the specimen Young's modulus and Poisson's ratio, respectively, while E_i and γ_i are the indenter Young's modulus and Poisson's ratio, respectively and E_r is the system reduced modulus. This correction enables to minimize the bias due to a possible deformation of the indenter.

In general, spherical indenters are modeled with an elastic behavior (e.g. [33,47]). They are usually less stiff than pyramidal or conical indenters as they are often made of tungsten carbide, contrary to sharp indenters, which are usually made of diamond or sapphire. Yet, some authors prefer to assume that the studied spherical indenter is perfectly rigid (e.g. [90]). It is worth noting that the deformation of spherical indenters should be considered in order to minimize calculation errors, particularly if the investigated specimen is hard compared to the indenter material.

6.2 Indenter Tip Defects

Whatever the manufacturing process, real indenters display manufacturing imperfections in their shape or their tip. Sharp indenters have blunt or rounded tips while spherical indenters have imperfect spherical shapes. These defects are caused by machining difficulties and are usually exacerbated with use. Particular attention should be paid to these defects as they can introduce errors in the estimation of the contact area and can thus affect the indentation test results.

Several authors investigated the effects of indenter tip defects on the indentation test results and more particularly on the computed P-h curves. Antunes et al. [87] analyzed the effects of Vickers tip imperfection on the indentation test results using a 3D simulation in which the defect is modeled by a flat spot at the end of the indenter. The authors showed that, for a given load, there is a decrease of the maximum indentation depth with an increase of the flat spot size. For instance, for steel, they found that an increase of the flat spot from 0.02 to 0.1 μm induced a 17% decrease of the indentation depth, for indentation depths around 0.25 μm . Similar results were found by Bressan et al. [52] and Bouzakis et al. [94], even if different configurations were used to model the tip defect. Bressan et al. [52] used an axisymmetric model in which the tip defect of a conical indenter was represented using a sphere whereas Bouzakis et al. [94] represented the tip defect using a cone with different height/width ratios. Warren et al. [27] confirmed these results and underlined the fact that the unloading part of the curve is insensitive to the tip defect, as well as the residual indentation depth. Warren et al. [27] extended their analysis to the modeling of a Berkovich indenter having a spherical tip defect with a 150 nm radius. By comparing the total indentation force to the force due to the tip defect, they showed that the tip defect had a negligible effect on the indentation results. Indeed, the maximum indentation depth was equal to 200 nm, which explains why only 2% of the total force was taken by the tip defect. This

effect would have been much larger for smaller indentation depths [95].

Even if the previous studies used different simulation conditions (2D or 3D simulations, indenter tip defects represented either using a sphere, a cone or a flat spot), they all showed that the indenter tip defect changes the indentation curves because of errors in the evaluation of the contact area. These errors can be particularly large for shallow indentation depths. It is worth noting that some authors showed that the tip defect did not affect hardness calculation, Young's modulus determination or the indentation curves when the indenter contact area was corrected [24,53]. However, the tip defect should be carefully modeled if the stress or deformation fields are examined. In this case, the indenter tip defect should match the experimental tip as closely as possible. Antunes et al. [53,87] observed the influence of the indenter tip shapes on the equivalent plastic deformation fields. They found that a Vickers indenter having a flat tip had a behavior similar to a flat punch i.e. the stresses were hydrostatic. Using a sharp indenter tip, the authors observed a higher plastic strain beneath the indenter. However, the differences between the deformation fields disappeared with indentation depths larger than 0.3 μm .

Spherical indenters are also subject to design defects: it is difficult to limit deviations from spherical forms when machining indenters. Some authors (e.g. [96]) pointed out the uncertainties introduced by significant deviations from the ideal indenter geometry when identifying material properties with indentation tests. Even if calibration procedures were created to take into account deviations from spherical forms [97], few studies actually use them in the identification of material properties using a spherical indenter. The studies considering tip defects of spherical indenters usually assume that the defects are predominant only along the axis direction (and not along the circumferential direction), which enables to keep an axisymmetric simulation. For instance, Tyulyukovskiy and Hubert [96] used a neural network to correct the load versus indentation depth curves determined with spherical indenters having non-perfect tips. First, they determined the area function of several spherical indenters having radii ranging from 1 to 10 μm . Then, using the identified area functions, they developed a more general function enabling to describe perfect and imperfect spherical shapes. By varying the indenter area function and the material properties, Tyulyukovskiy and Hubert [96] created a large number of simulations and calculated the corresponding indentation curves. Simultaneously, they calculated the indentation curves obtained for the same material properties but assuming that the indenter is perfectly spherical. Using previous data, they trained their neural network to match the indentation curves obtained with an imperfect indenter to the ones obtained with an ideal indenter. The method developed by Tyulyukovskiy and Hubert [96] is lim-

ited to cases in which the indenter can be considered perfectly rigid during the indentation test and was developed for elastic–viscoplastic materials. Similarly, Brammer et al. [98] showed the effects of spherical indenter defects on the indentation curves for several materials. They developed a corrective method enabling to match a curve obtained with an imperfect spherical indenter to a curve obtained with a perfectly spherical indenter equivalent to the imperfect one. This method was developed for elastoplastic materials and it was assumed that the indenter remained perfectly rigid during the indentation test. Collin et al. [47] expressed the lack of sphericity of the indenter with a function describing the variation of an equivalent radius with the contact radius. This definition seems more complete as it takes into account the indenter elasticity and the variation of the contact radius as a function of the studied load. However, this correction is obtained by fitting the simulated data and is therefore only relevant for the investigated indenter of the study.

The previous studies show that the impact of the defects of the indenter tips on the indentation results depends on the simulation conditions. For sharp indenters, the correction of the tip defects is particularly important when examining shallow indentation depths. By contrast, the deviations from an ideal shape should be taken into for spherical indenters regardless of depth.

7 Simulation of Materials Showing Roughness or Residual Stresses

7.1 Roughness Effect

Experimental observations showed that roughness can strongly disturb the indentation test results and thus the determination of mechanical properties due to distortions of the contact area. For example, De Souza et al. [99] observed a large scatter of results when determining hardness on ion-nitrided titanium having an arithmetic mean roughness R_a ranging from 20 to 240 nm. Roughness particularly affects indentation results at small indentation depths. The European standard EN ISO 14577-1 [100] recommends the use of indentation depths larger than the arithmetic mean roughness R_a . This limit is a problem for the characterization of thin films, which requires shallow indentation depths.

Even if few studies deal with the indentation of rough surfaces, three strategies can be distinguished for modeling topography:

- (i) The first approach gathers studies analyzing interactions taking place between an indenter and a single asperity (peak) or cavity (valley). For instance, Li et al. [101] examined interactions occurring between a conical indenter having a rigid spherical tip and an elastoplastic

material in order to assess the influence of roughness on the scatter of the indentation curves and hardness values.

- (ii) The second approach covers studies with more realistic representations of roughness. Jiang et al. [102] used a quasicontinuum method (coupling finite element modeling and atomic method) to describe the indentation of a rough single crystal copper thin film, using a rigid cylindrical indenter. In the simulation of Jiang et al. [102], the crystal defects appeared as straight grooves. Through the variation of the indenter diameter and the groove width, the authors examined the influence of roughness on the determination of the material hardness and Young's modulus. Berke et al. [88] added four sinusoidal functions having different amplitudes, wavelengths and phases in order to create a profile that would match reality as closely as possible. The created profile was then inserted at the surface of an axisymmetric model to examine the effect of roughness and friction on the determination of the Young's modulus of elastic viscoplastic materials. Walter et al. [45] numerically reproduced AFM profiles measured on CrN thin films (R_a ranged from 2 to 10 nm). The measured profiles were used in axisymmetric models. However, this approach does not adequately describe roughness as it corresponds to the creation of concentric circles in an equivalent 3D model.
- (iii) To the best of the authors' knowledge, the most complex representation of roughness was realized by Walter et al. [29]. In order to investigate the effect of roughness on the scatter of the indentation curves and on the determination of Young's modulus, Walter et al. [29] created a 3D model. In the latter, the heights of the nodes at the surface of the model were interpolated to reproduce AFM measurements made on CrN thin films (R_a ranging from 2.6 to 11 nm). However, this model only described elastic deformations as the indented material remained elastic while the spherical indenter was assumed to be perfectly rigid (the maximum indentation depth was equal to 33 nm).

The different published works on this topic emphasize the difficulties of calculation involved with the modeling of instrumented indentation tests on rough surfaces. Indeed, simulations of real rough surfaces from 3D measured topography with elastoplastic behavior laws require high performance computing as well as careful consideration of contact. Therefore, the effects of surface roughness on the results of indentation test remain under investigation.

7.2 Simulation of Materials with Residual Stresses

Simulations of the indentation of materials having residual stresses are either dedicated to the observations of their

effects on the results of the indentation test or to the building of methods enabling to identify residual stresses through an analysis of indentation test data. However, because of the complexity of the topic, finite element simulations are mainly based on simple hypotheses:

- (i) The residual stresses are either uniaxial or biaxial (e.g. [103–106]), thus enabling the use of axisymmetric models. For now, only a few models include biaxial stresses having different values (e.g. [107, 108]).
- (ii) The residual stress field is uniform along the indentation depth or more accurately along the depth of influence of the indenter [103].
- (iii) The material behavior is often simple. In most studies, the material is assumed to be elastic perfectly-plastic (e.g. [107–110]). Only a few studies are dedicated to bilinear materials (e.g. [105]) or to materials having a power-law hardening behavior (e.g. [106, 111]).

The importance of integrating residual stresses was first highlighted with experiments in which hardness was measured using conventional indentation testing. The development of modern computer tools enabled to accelerate research on the effects of residual stresses and more particularly on the effects of residual stresses on the material properties identified using the indentation test. One of the first studies is the joint analysis of Tsui et al. [112] and Bolshakov et al. [113], which presented the indentation of an aluminum alloy with a sharp indenter. They analyzed the effects of uniaxial and biaxial residual stresses on the determination of hardness and Young's modulus using experimental results and a finite element model. As a first result, the determination of hardness with the Oliver and Pharr method [114] showed an increase of hardness with the introduction of compressive stresses (or a decrease of hardness with the introduction of tensile stresses).

However, through the observation of contact areas, using an optical microscope, they found that the observed variation of hardness was only an experimental artifact. It was caused by pile-up or sink-in phenomena, which modified contact geometry and thus biased hardness calculations. When using the contact area measured with the microscope, hardness values were not affected by residual stresses. Using finite element simulation, Bolshakov et al. [113] confirmed these results and also showed that the computed Young's modulus was not affected by residual stresses either, as long as the real area was used for calculations.

Several studies followed the works of Tsui et al. [112] and Bolshakov et al. [113]. These studies had two main aims:

- (i) They suggested methods to identify residual stresses by quantifying the variation of certain parameters computed

using numerical simulations of the indentation test (e.g. quantification of pile-up variation).

- (ii) They extended the analysis of the impact of residual stresses on the indentation tests through a variation of the test conditions: they used a larger spectrum of materials [109], more complex behavior laws [106] or changed the indenter shape [115],...

According to the literature, residual stresses can significantly affect the indentation curves and the contact area and, by extension, the mechanical properties determined using the indentation curve. Chen et al. [109] found that, the hardness of elastic perfectly plastic materials was insensitive to the presence of residual stresses if the ratio E/σ_y was larger than 300. For lower ratios, there was a decrease of the computed hardness. Sakharova et al. [104] found the same trends using an elastic perfectly-plastic behavior law. When using a nonlinear hardening, Sakharova et al. [104] noticed that the sensitivity of soft materials to residual stresses depended on the value of the strain-hardening exponent: materials having strain-hardening coefficients equal to 0.3 were more sensitive to residual stresses than materials having strain-hardening coefficients equal to 0.01 (i.e. materials having nearly perfectly-plastic behaviors).

The previous studies show that residual stresses can significantly affect the indentation curves and thus the calculated mechanical properties. However, their "real" effects on the identification of mechanical properties remain uncertain as numerical models greatly simplify reality (e.g. homogeneous residual stress fields, simple behavior laws...). Moreover, interactions of residual stresses with other phenomena are either not considered (e.g. indentations of rough surface in presence of residual stresses) or are not completely understood. For instance, what are the effects of the simplified assumptions (e.g. homogeneous residual stress distribution) on the numerical results? All these issues indicate that much research still deserves to be done on the subject.

8 Remaining Differences Between Finite Element Simulation and Experimental Results

This literature review emphasized the fact that several conditions can be used to model the indentation test (2D vs. 3D, boundary conditions, mesh refinement, friction...). Some of these conditions can significantly impact the simulation results, such as the indentation curve, the residual imprint.... It is worth noting that one of the goals sought by the simulation of indentation tests is to identify the material properties (e.g. hardness, Young's modulus, yield stress, work-hardening coefficient) using inverse approaches. The latter are often based on the fitting of experimental P–h curves with numerical ones. However, the indentation curves are

often subject to significant variations caused by different factors. Among them, there are surface phenomena e.g. attractive or repulsive forces at the material surface, which can induce errors in the initial surface detection. There are also effects linked to sample preparation such as oxidation, contamination or surface hardening because of mechanical polishing. All of these effects affect the accuracy of measured P - h curves. Beyond purely numerical issues, there are two main phenomena left that are responsible for the remaining differences between the results of finite element simulation and experimentation: the determination of the reference point and the Indentation Size Effects. These two issues are discussed in the following sections.

8.1 Contact Detection and Determination of the Reference Point

The difficulty of determining the reference point is directly linked to the difficulty of detecting the moment when the indenter comes into contact with the material surface. Generally, instrumented nano- or microindenters are programmed to monitor the harmonic contact stiffness until reaching a preset value. When the threshold is exceeded, the indentation depth is set to zero, namely the zero position or the reference point. The latter is thus strongly influenced by the material stiffness, surface forces, surface contamination, preset value, and specimen roughness. In an attempt to counteract the zero position uncertainty, several methods were developed.

Fischer-Cripps [116] identified several correction methods in the literature. One of them suggests fixing a force threshold for the detection of contact. Once this force is reached, the indentation depth is set to zero and the P - h curve is recorded. As the zero position remains uncertain, the initial data are described through the fitting of a curve, extrapolated back to $P = 0$ (zero force). This extrapolation provides a value for the initial indentation depth, which is subtracted to the subsequent indentation depths. The indentation curve is then shifted to the right. The main inconvenient of this method is that it requires some knowledge about the material properties to be able to correctly set the force threshold. Similarly, Grau et al. [117] underlined the importance of the reference point and described the initial loading by fitting a second order polynomial to the experimental curve. This fit is then extrapolated back to $P = 0$ to determine the initial indentation depth. Ullner et al. [118] studied the effects of this method on the indentation test results and concluded that its effects were highly dependent on the studied load, the experimental scatter, the uncertainties that can be accepted about the determination of the initial depth, the interval used for fitting the function as well as on the fitting function. Recently, Marteau et al. [119, 120] presented an original method that enables to calculate hardness from the indentation curves without being influenced by the reference point. This method requires the

simultaneous processing of several indentation curves and the comparison of their shape to the one predicted by Bernhardt's law [121].

For spherical indenters, Chudoba et al. [122] and Kalidindi et al. [49] suggested extrapolating the indentation curve near the contact point by fitting the first 30 nanometers using Hertz's theory (P is proportional to $h^{3/2}$). However, this method cannot be applied to all the materials as the elastic part of the curve is quasi-inexistent for some materials.

To limit the effects of a false determination of the zero position, Brammer et al. [123] developed a method to identify the material properties based on the derivative of the indentation curve instead of directly using the indentation curve. Moreover, the authors removed the beginning of the indentation curve which may introduce numerical errors. They showed that the use of the derivative enabled to eliminate any errors due to a false determination of the reference point, when identifying the material properties. Truncating the beginning of the indentation curve remains debatable as it risks deleting local information on the material properties.

Most of the methods developed to correct a false determination of the reference point are based on the use of the indentation curves and their extrapolation. These methods are often developed for particular cases and are difficult to generalize. Removing the first nanometers can be interesting when the global response of the material is examined. However, when studying finer scales, truncating can be an issue as it risks eliminating certain phenomena taking place at the material surface, which can be important to locally characterize the material behavior. Determining the reference point is thus a complex issue and remains a major difficulty when using indentation tests to characterize the material properties or when comparing experimental results to finite element ones.

8.2 Indentation Size Effect

At shallow depths (smaller than one micrometer), conventional and instrumented indentation experiments have repeatedly shown Indentation Size Effects (ISE) i.e. the increase of indentation hardness with the decrease of indentation depth. In some cases, a decrease of hardness was observed (e.g. [124]), it is called inverse ISE. The latter is often attributed to measurement artifacts, thus it will not be discussed hereafter.

Despite the existence of a comprehensive literature on the topic of the ISE, this phenomenon remains misunderstood. Several interpretations were proposed based on intrinsic or extrinsic reasons.

Usually, ISE are observed with geometrically similar indenters (i.e. with conical or pyramidal indenters). It is often difficult to identify what caused the size effect with certainty. Among the extrinsic reasons, there is the false calibration of

the contact area of the indenter, which can induce a miscalculation of hardness. For instance, if the indenter is assumed to be perfectly sharp instead of blunt when treating the indentation test data, then hardness can be overestimated at shallow depths, leading to an “artificial” ISE.

Similarly, samples should be prepared with care to enable an accurate characterization of the material properties using the instrumented indentation test. The following problems can be encountered during sample preparation:

- (i) A modification of the surface properties because of grinding, e.g. hardening of the surface,
- (ii) Surface contamination e.g. oxydation,
- (iii) Surface roughness. Roughness particularly affects the indentation test results when it has the same order of magnitude as the indentation depth. As previously indicated, the European standard EN ISO 14577-1 [100] advises to use an indentation depth larger than the arithmetic mean roughness R_a . Kim et al. [125] developed an ISE model describing the influence of roughness on hardness determination. To do so, they assumed that the deformation of a rough material caused by nanoindentation is the sum of two phenomena: the flattening of the rough part of the surface and the deformation of the flat part of the surface. Through an analytical separation of the work provided to flatten the rough part from the work given to deform the flat part, they suggested a new ISE model.

A false determination of the reference point can also induce an artificial increase of hardness at shallow depths, which can be interpreted as an ISE if it is not corrected.

Recently, Pharr et al. [126] also highlighted the fact that the use of Continuous Stiffness Measurement (CSM) method can give false values of hardness at shallow depths (particularly for soft materials).

ISE were also detected when indenting noble materials (i.e. no risk of surface hardening) in perfectly monitored conditions (e.g. no contamination of the surface). Thus, models were developed to explain such phenomena. These models can be gathered into two categories: physical models, which are based on dislocation theory and phenomenological models, which are based on conventional descriptions of plasticity with the introduction of scale-parameters. The model of Nix and Gao [127] belongs to the most famous physical models. This model explains the observed size effects using the concept of geometrically necessary dislocations. The latter are present in the indented area to accommodate the permanent deformation associated with the volume displaced by the indenter. These dislocations are added to the statistically distributed dislocations which come from the material deformation. This addition gives rise to a hardening phenomenon which is larger for small indentation depths.

The literature survey on ISE topics indicates that many phenomena described above are somehow already incorporated in the simulation of indentation tests (e.g. surface roughness, tip radius, residual stresses and reference point). Physical models based on dislocation theory and advanced phenomenological models with scale parameters are already developed to take into account the ISE. However, in these models, the ISE is explained by one phenomenon, thus it does not describe what is really observed in experimentations. More research is still needed to understand the actual contributions of the mentioned phenomena to the ISE: is it possible to experimentally quantify each contribution in order to prioritize them? What about the interactions of these different phenomena? Future research should concentrate on these different issues.

9 Conclusion

Through the analysis of a hundred articles, the review proposed in this paper focused on how the indentation test is modeled and the consequences on the numerical results.

This review highlighted the lack of homogeneity of the different modeling strategies: 2D versus 3D models, friction modeling, behavior laws, boundary conditions... The impacts of the different modeling conditions were assessed thus enabling to set some general rules on how to “accurately” model the instrumented indentation test for material behavior identification. The following conclusions can be drawn from the present work:

- Simulating a pyramidal indenter with a conical one having the same contact area has no influence on the indentation curve for most materials. This simplified representation cannot be used when studying the stress or strain fields or the indentation imprint.
- Axisymmetric models should be limited to isotropic materials or to materials having a symmetry axis (e.g. materials that exhibit in-depth gradients or materials having residual bi-axial stress fields).
- Boundary conditions should be carefully set when the model dimensions are small: for instance when modeling roughness using a 3D simulation.
- Friction has a large effect on the indentation curves and the indentation imprint when using spherical indenters or sharp indenters having small angles (e.g. cube-corner). For spherical indenters, friction effects are particularly large when examining large ratios of the indentation depth over the indenter radius and for materials having a low strain-hardening coefficient.
- Several investigators highlighted the effects of roughness and residual stresses on indentation curves. However, these two aspects remain difficult to simulate. Roughness should

be examined with a 3D model as a 2D model is not representative of reality. Yet, 2D models are often used in order to limit computation time. Similarly, simplifying assumptions are often made in order to simulate residual stresses with 2D models (i.e. biaxial stresses, homogeneous fields). Such simplifying assumptions degrade the accuracy of the results.

- Finally, even if the simulation conditions are thoroughly studied, other phenomena disturb the comparison of the simulated results with experimentation. Beyond purely numerical issues, phenomena such as a false determination of the reference point of the indentation curve and indentation size effects should be taken into account.

However, as mentioned in this review, one has to keep in mind that the goals sought by the simulation of indentation tests is to identify the material properties using inverse approaches by the experimental data with numerical one. Therefore, the accuracy of material property identification depends on both the accuracy of experimental and numerical data. The accuracy of numerical data depends on different aspects that have been reported before. Research should also be conducted to control the quality of experimental data and to gain in-depth knowledge of the effects of different parameters, such as surface roughness, material behavior, residual stresses... on the experimental indentation curves. An effective tool to tackle these different issues is the use of Design of Experiments. It may enable to separate the different phenomena in order to examine how they individually affect the material response. For instance,

- The effect of surface topography could be assessed on samples having different roughness induced by chemical attack in order to avoid any residual stress related to mechanical polishing,
- The impact of the material behavior could be assessed using different materials having similar Young's modulus and different yield strengths or similar elastic properties with different work-hardening coefficients,
- The effect of residual stresses could be investigated on pre-strained samples (e.g. in compression, in bending) taken from the same material and having the same surface roughness.

This research would contribute to the improvement of existing deterministic models or would lead to the development of stochastic models for indentation tests if necessary.

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