

Lattice rotation field around indentation for identifying slip system interactions coefficients in FCC Nickel single crystal

Alexandre Bourceret^a, Jalal Smiri^{b,*}, Yves Gaillard^b, Arnaud Lejeune^b, Sergio Sao-Jao^a, Guillaume Kermouche^a, Fabrice Richard^{b,**}

^a*Mines Saint-Étienne, Univ Lyon, CNRS, UMR 5307 LGF, Centre SMS, Saint-Etienne, France*

^b*Université Marie et Louis Pasteur, CNRS, institut FEMTO-ST, F-25000 Besançon, France*

Abstract

This study explores the interest of the misorientation angle field surrounding an indent as an observable for identifying plastic parameters in Face-Centered Cubic (FCC) Nickel single crystals using an inverse method. This misorientation angle field, derived from lattice rotations, is directly linked to slip system activity within a crystal plasticity framework. The ten parameters to be identified belong to a Meric–Cailletaud-type crystal plasticity model, governing both slip system interactions and hardening mechanisms. Previous approaches, such as nanoindentation load–displacement curves, often suffer from poor conditioning of the inverse problem associated with identifying the 10 crystal plasticity parameters, while residual topographies typically require multiple crystal orientations to achieve an acceptable conditioning. In contrast, the present work provides a numerical proof of concept, through an identifiability analysis, that a single crystallographic orientation of an FCC Nickel single crystal is sufficient to well-condition the inverse problem, when the three-dimensional misorientation angle is used as the observable.

Keywords: Crystal plasticity, Slip system interactions, Lattice rotation, Berkovich nano-indentation, Identifiability analysis

1. Introduction

Plastic deformation in face-centered cubic (FCC) crystals is mainly accommodated by crystallographic slip along specific crystallographic planes and directions that define slip systems. The associated slip activity governs hardening behavior [1, 2], plastic anisotropy [3–5], and therefore controls the macroscopic mechanical response [6, 7]. By explicitly describing the kinematics of crystallographic slip and slip-system interactions, crystal plasticity models enable the prediction of the mechanical response of crystalline materials. In particular, this study employs the Crystal Plasticity Finite Element Method (CPFEM) as

*Corresponding author

**Corresponding author

a continuum mechanics framework to simulate the behavior of FCC Nickel single crystal by accounting for grain-scale slip activity. Reliable identification of slip-system interaction coefficients is thus essential, as these parameters allow such models to reproduce realistic plastic deformation and support both fundamental studies and engineering applications [8, 9]. This requirement calls for the development of simple and cost-effective experimental techniques capable of delivering suitable observable(s) to identify these parameters by minimizing the discrepancy between experimental measurements and crystal plasticity simulations through an inverse method. Nanoindentation is particularly advantageous, owing to its precise position control, high resolution load control, accurate displacement measurement and non-destructive nature [10–12]. Drawing upon these capabilities, recent contributions in the literature have sought to identify the plastic parameters of different constitutive models from nanoindentation by means of inverse methods [13–17].

In these approaches, the predicted load–displacement (P – h) curve (or normalized (P – h) curve) is adjusted by modifying the plastic properties until it correspond to the experimental nanoindentation response. However, as Cheng et al. [18] first pointed out, relying on the indentation curve is generally insufficient to uniquely identify the plastic parameters. Solutions are frequently non-unique and unstable [19] for various indenter tip geometries (conical, pyramidal, or spherical), even when simple elastic–plastic laws with only two parameters are employed—the yield stress σ_y and the work-hardening exponent n of a power hardening law, a limitation also emphasized in [20]. Consequently, such approaches are typically regarded as providing a calibration of a mechanical test model to fit the observed response rather than an identification of the intrinsic constitutive material parameters.

In line with these insights, Renner et al. [21] demonstrated, through an identifiability analysis (based on an Identifiability index, I_{index}), that using the P – h curve from Berkovich indentation is not an information-rich observable and is therefore unsuitable to simultaneously identify crystal plasticity parameters (including slip system interaction coefficients) of a Méric–Cailletaud-type (MC) law [22], which leads in practice to non-unique solutions for the material parameters.

The MC single crystal plasticity framework relates the slip evolution $\dot{\gamma}^s$ on each of the 12 slip systems to the resolved shear stress τ^s by a Norton-type viscoplastic flow:

$$\dot{\gamma}^s = \left\langle \frac{|\tau^s| - \tau_0 - R^s}{K} \right\rangle^n \frac{\tau^s}{|\tau^s|}, \quad (1)$$

where τ^s correspond to the resolved shear stress, τ_0 is the critical resolved shear stress, R^s the work hardening, and while K and n characterize the viscous effect. The work hardening process is assumed to be purely isotropic, with each slip system accounting for both its self-interaction as well as its interactions with all other slip systems, and is expressed as:

$$R^s = Q \sum_r h^{sr} \left(1 - e^{-b|\gamma^r|} \right), \quad (2)$$

where Q drives the saturation level of the hardening, h^{sr} is the interaction matrix coefficients, containing the interaction coefficients $\{h_1, h_2, h_3, h_4, h_5, h_6, h_7\}$, and b drives the saturation rate. All slip systems reach the same saturation value ($Q \sum_r h^{sr}$) after a certain amount of slip, around 10 %, given the value of b

[23]. This phenomenological crystal plasticity model is inspired by classical macroscopic constitutive approaches, while incorporating the basic mechanisms of plastic deformation in single crystals, i.e., the presence of slip systems [22, 24]. For a comprehensive description of the single crystal framework for finite strain elasto-viscoplastic behavior, especially regarding the MC model, the reader is referred to [23–26].

Within this constitutive framework, Renner et al.[21] also showed that post-indentation residual topographies offer a significantly richer source of information. In particular, pile-up patterns were shown to be highly sensitive to crystallographic orientation and hardening behavior, with latent hardening coefficients exerting a strong influence on the surface morphology.

Building on this, Renner et al.[27] performed a quantitative analysis using identifiability indices and demonstrated that combining residual topographies is essential for identifying all the MC plastic parameters.

More recently, Bourceret et al.[23] confirmed the relevance of combining residual topographies for improving parameters identifiability. On the other hand, using both the indentation curve and residual topographies data does not enhance identifiability and may even dilute the information content. Their study led to the identification of a new set of parameters values related to the MC hardening law, including the slip system interaction coefficients. Using the Crystal Plasticity Finite Element Model Updating method (CPFEMU), they identified all the 10 plastic parameters $\{\tau_0, Q, b, h_1, h_2, h_3, h_4, h_5, h_6, h_7\}$ of the model using a reduced yet optimized couple of simulated topographies. While promising, this study underscored the limited conditioning of the inverse problem even when combining multiple residual topographies from very different relative tip/crystal orientations and suggested the necessity of exploring other types of observables.

In the context of observables that can complement or even replace classical observables such as indentation curves or residual topographies, recent study by Juran et al.[28] suggested that "EBSD measurements should be an interesting way to determine new experimental data for further development of indentation-based reverse methods". Owing to the mutual dependence between crystallographic slip and lattice rotation investigated by Hestroffer et al. [29], lattice rotation is expected to contain rich information on the interactions among slip systems. Building on this perspective, the present work investigates the information content of the volumetric misorientation angle field.

The misorientation angle field describes the local deviation of lattice orientation relative to the mean orientation of the grain (single crystal). Under the assumption of an initially homogeneous microstructure, these local deviations are purely deformation-induced and directly results from the nanoindentation process. The misorientation angle serves as a scalar representation of the cumulative lattice rotation tensor $\mathbf{R}_e$. The representative misorientation angle θ is defined by :

$$\theta = \arccos \left(\frac{\text{trace}(\mathbf{R}_e) - 1}{2} \right). \quad (3)$$

The tensor $\mathbf{R}_e$ is derived from the elastic deformation gradient, $\mathbf{F}_e$, which arises from slip gradients, with the slip carried by the plastic deformation gra-

dient $\mathbf{F}_p$. These slip gradients introduce strain incompatibility. In response, $\mathbf{F}_e$ adjusts through both lattice rotation and elastic distortion to restore local compatibility.

The misorientation angle can be extracted from post-indentation measurements using either destructive or non-destructive approaches. Destructive methods allow for local stress relief as surfaces are sequentially exposed for measurement, such as serial sectioning by Focused Ion Beam (FIB) followed by Electron Backscatter Diffraction (EBSD), while non-destructive techniques include methods such as three-dimensional X-ray microscopy (3DXM).

In this work, we aim to develop a strategy that provides a well-conditioned inverse problem of plastic parameter identification in Ni FCC single crystals using nanoindentation. This study is conceived as a numerical proof of concept. Several possibilities are evaluated, including the use of a single orientation or selecting optimal combination of crystallographic orientations, either to employ a single observable (misorientation angle field or residual topography) or incorporate both observables (misorientation angle field and residual topography). To understand how the crystallographic orientation (see Fig. 1) and the choice of observables affect the conditioning of the problem, we perform finite element simulations (see Fig. 2) for 13 different crystallographic orientations, each yielding surface topography and misorientation angle field data. Ultimately, the present analysis highlights the crystallographic orientation(s) that merit special attention for future nanoindentation experiments. The resulting real experimental data from these orientation(s) will subsequently feed into the parameter identification process (e.g. via Finite Element Model Updating method (FEMU)), which are beyond the scope of the present work.

2. Method of designing nanoindentation experiments guided by observable richness across FCC crystal orientations

Table 1: Values of the MC plastic model parameters $\zeta = \{\zeta_j\}_{j=1}^{10} = \{\tau_0, Q, b, h_1, h_2, h_3, h_4, h_5, h_6, h_7\}$ for Ni single crystals, identified by [23]. The corresponding units are provided when applicable.

Parameter	τ_0 (MPa)	Q (MPa)	b (-)	h_1 (-)	h_2 (-)	h_3 (-)	h_4 (-)	h_5 (-)	h_6 (-)	h_7 (-)
Value	69.13	152.2	29.4	0.21	0.46	0.69	0.28	0.15	1.05	0.10

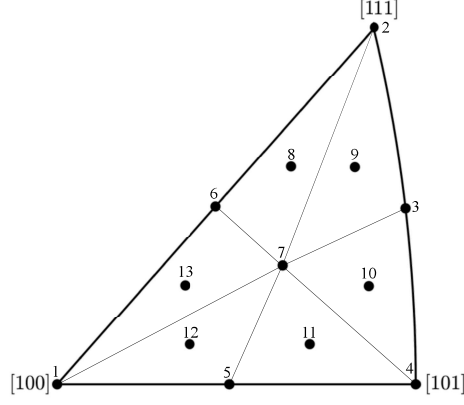


Figure 1: Partitioning of the FCC-(IPF) bounded by the $[100]$, $[110]$, and $[111]$ directions. The 13 selected crystallographic orientations are shown: orientations 1–7 correspond to the vertices of the sub-triangles, while orientations 8–13 represent their centroids.

Table 2: List of the 13 selected crystal orientations for an FCC single crystal, defined by their Euler angles (ϕ_1, ψ, ϕ_2) in degrees and corresponding Miller indices. The (hkl) notation indicates the crystallographic plane orientation, while the $[uvw]$ notation specifies the crystallographic direction. The orientations are listed in the same order as shown in Fig. 1.

Number	Euler Angles			Miller indices			
	ϕ_1 (°)	ψ (°)	ϕ_2 (°)	(hkl)	[uvw]		
1	90.00	90.00	90.00	1 0 0	0	0	1
2	90.00	54.74	45.00	1 1 1	-1	-1	2
3	90.00	72.37	45.00	9 9 4	-2	-2	9
4	90.00	90.00	45.00	1 1 0	0	0	1
5	90.00	90.00	67.50	12 5 0	0	0	1
6	90.00	69.94	68.58	5 2 2	-3	-1	9
7	90.00	76.97	60.45	7 4 2	-2	-1	10
8	90.00	66.52	58.41	8 5 4	-3	-2	8
9	90.00	67.54	50.53	11 9 6	-4	-3	12
10	90.00	79.79	50.18	12 10 3	-1	-1	8
11	90.00	85.71	57.50	11 7 1	-1	0	12
12	90.00	85.45	72.58	12 4 1	-1	0	12
13	90.00	78.64	73.03	10 3 2	-2	-1	11

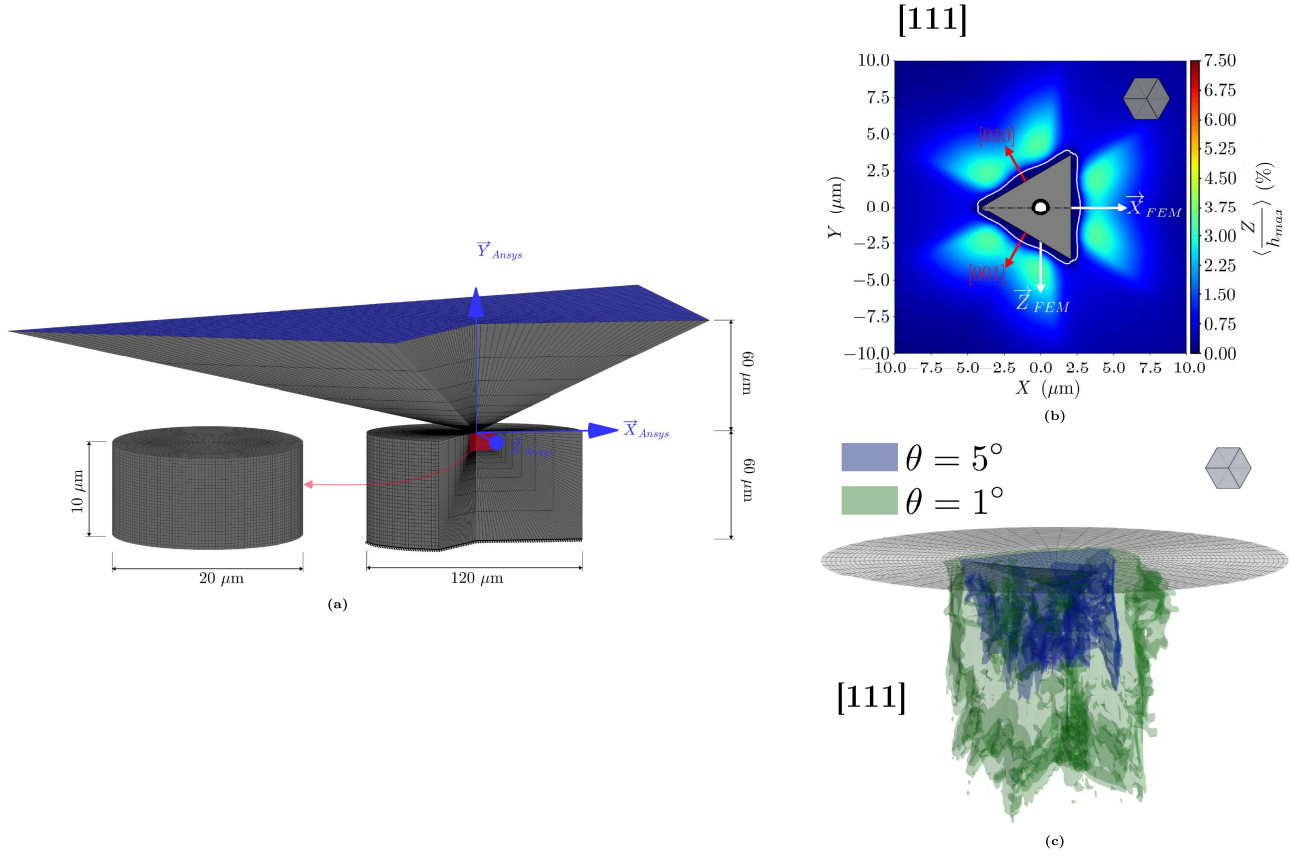


Figure 2: The FE model and typical results are shown here for the [111] crystallographic orientation. **(a)** Right panel: FE model of the nanoindentation test featuring a cylindrical specimen with a 120° opening, meshed using linear hexahedral elements. The coordinate system used in ANSYS [30] is shown in blue ($\vec{X}_{Ansys}, \vec{Y}_{Ansys}, \vec{Z}_{Ansys}$). The Berkovich indenter is positioned above the specimen. The finely meshed area is highlighted in red in the full model and shown in enlarged view in the left panel. **(b)** isocontours of the residual surface topography for the [111] crystallographic orientation over a $20 \times 20 \mu\text{m}^2$ area. A top view of the Berkovich indenter, shown in grey, is included along with the projected crystallographic axes ($\vec{X}_{crystal} = [010], \vec{Y}_{crystal} = [001]$) onto the indentation plane shown in red. A white line marks the zero topography level in the contact area, and at the top right, a cubic crystal shape in grey illustrates the crystallographic orientation. The white axes labeled $\vec{X}_{FEM}$ and $\vec{Z}_{FEM}$ correspond to the same directions as $\vec{X}_{Ansys}$ and $\vec{Z}_{Ansys}$ shown in **(a)**, right panel. The color mapping represents the value of $\langle Z/h_{max} \rangle$, where $\langle \cdot \rangle$ are the Macaulay brackets. **(c)** Reconstructed isocontour from the full-field misorientation angle, showing areas where the misorientation angle equal to 1° in blue and those equal to 5° in green. For **(b)** and **(c)** results is corresponding exclusively to the finely meshed region.

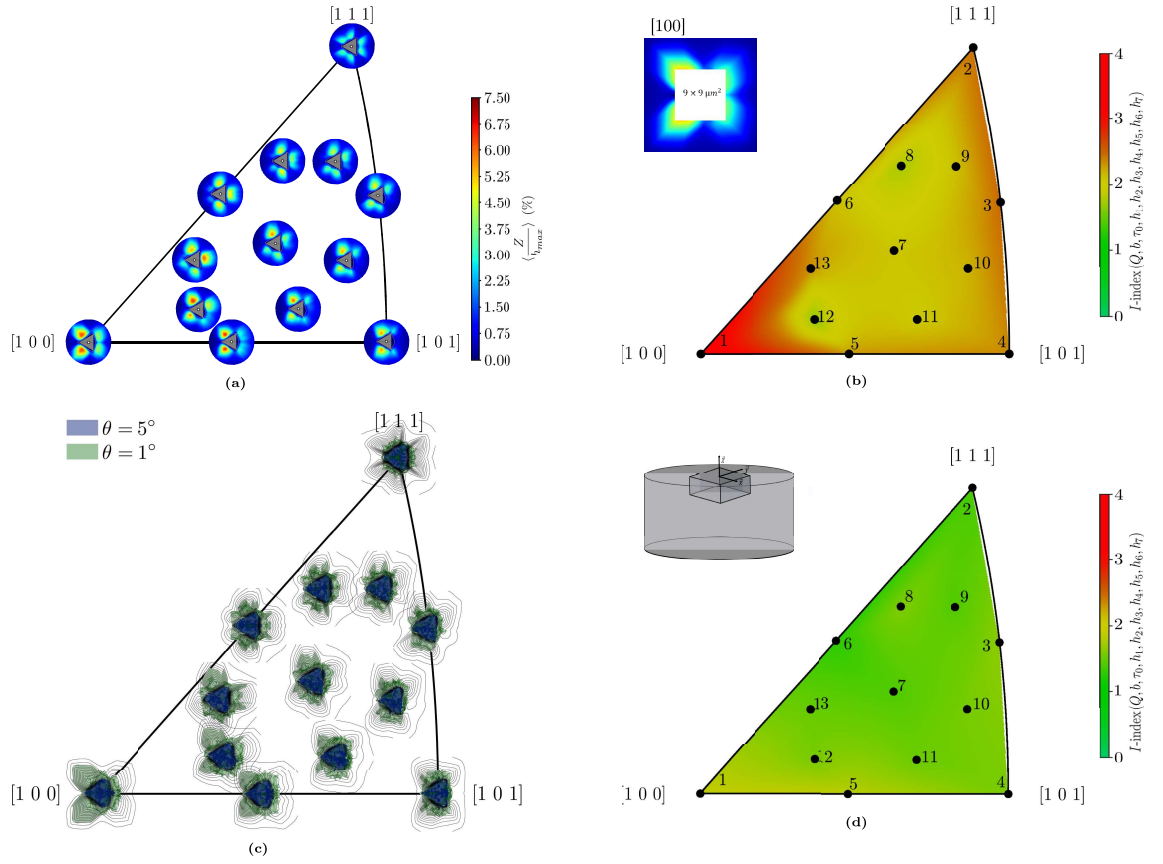


Figure 3: Investigated nanoindentation observables for 13 selected crystallographic orientations represented on the FCC-IPF. **(a)** Dimensionless residual topographies with the indenter tip at the center of the imprint. Top-view of dimensionless residual topographies with the indenter at its center; the displayed topographies correspond to a circular area of radius $10h_{max}$ around the imprint, with h_{max} is the maximum indentation depth. **(b)** Identifiability index (I_{index}) computed from the residual topographies, with inset showing the square ($9 \times 9 \mu m^2$) mask used for all crystallographic orientations to exclude the imprint core data during the analysis. The inset shows only the resulting masked residual topography for the $[100]$ orientation, as illustrating all 13 orientations would be overly cumbersome. **(c)** Top-view misorientation contours are shown with overlaid topography contour lines, highlighting regions where the misorientation angle equal to $\theta = 1^\circ$ (blue) and $\theta = 5^\circ$ (green). **(d)** Identifiability index computed from the 3D misorientation angle fields, with the inset showing the corresponding truncated volume in form of box ($9 \times 9 \times 3 \mu m^3$) used for the analysis. For (b) and (d), identifiability index values are interpolated over the IPF using a regular grid and visualized with a color bar ranging from 0 to 4 (Lower identifiability index values indicate a well-conditioned inverse problem).

Our design of optimal nanoindentation experiments is guided by the concept of the observable richness available across FCC crystal orientations. Observable richness denotes the capacity of an observable to yield a convex cost function suitable for minimization during the FEMU process. Here, observable richness for a given orientation is evaluated through a local parametric identifiability index, computed for a specific set of model parameters. The chosen parameters are the plastic parameters of MC model $\zeta = \{\tau_0, Q, b, h_1, h_2, h_3, h_4, h_5, h_6, h_7\}$, identified by Bourceret et al. [23] for Ni single crystals as reported in Table 1.

Local identifiability is evaluated using two complementary metrics : (i) the sensitivity of each observable to variation in model parameters, and (ii) the degree of collinearity among the resulting sensitivity vectors, which reflects the degree of parameter distinguishability. Together, these metrics are summarized in a scalar quantity, the Identifiability index (I_{index}), defined as :

$$I_{index} = \log_{10} \left(\frac{\lambda_{\max}}{\lambda_{\min}} \right), \quad (4)$$

where $\lambda_{\max}$ and $\lambda_{\min}$ are the maximum and minimum eigenvalues of the dimensionless hessian matrix $[H]$ relative to any observable o . In this work, o represents either the indentation force, the residual topography or the misorientation angle computed from the CPFEM simulations,

$$\overline{H}_{ij}^o = \sum_{k=1}^{N_p} \overline{S}_{ki}^o \overline{S}_{kj}^o, \quad (5)$$

with N_p the number of observable sampled points. The normalized sensitivity vector is defined as

$$\overline{S}_{kj}^o = \frac{\zeta_j}{o_{\max} \sqrt{N_p}} \frac{\partial o_k}{\partial \zeta_j}, \quad (6)$$

where $o_{\max}$ is the maximum value of the observable and ζ_j denotes the j -th model parameter.

The I_{index} provides insight into the conditioning of the inverse problem and supports both the *a priori* design of experiment(s) and the *a posteriori* evaluation of the solution stability. As the identifiability index decreases, the inverse problem is said to be better conditioned. For reference, the problem is usually considered well-conditioned when the I_{index} is less than 2, and ill-conditioned when the I_{index} is greater than 3. These bound values are based on the conditioning of the dimensionless hessian matrix and the resulting shape of the cost function. When I_{index} is less than 2, the eigenvalues of the hessian are of comparable magnitude, leading to a convex cost function that is not significantly elongated in any direction. In contrast, for I_{index} is greater than 3 strong eigenvalue disparity produces an elongated cost function, typically associated with solution valleys and poor parameter identifiability.

For details on the mathematical formulation and numerical implementation of the metrics that constitute the I_{index} , refer to [23, 31, 32].

In the present work, we apply this methodology to systematically explore orientation-dependent identifiability based on two post-indentation observables : (i) residual topographies, and (ii) 3D misorientation angle fields.

To this end, a representative set of 13 crystallographic orientations was selected within the FCC inverse pole figure (IPF), bounded by [100], [110], and

[111] directions. Figure 1 illustrates the selection process, where the IPF is partitioned into six sub-regions: orientations 1–7 correspond to the vertices of the sub-triangles, while orientations 8–13 represent their centroids. The corresponding Euler angles and Miller indices for each orientation are listed in Table 2.

For each orientation, nanoindentation CPFEM simulations were carried out using a User MATERIAL subroutine (UMAT) corresponding to the MC model, implemented through the MFront numerical tool [25]. A total of 143 simulations were conducted: one reference simulation per orientation, followed by ten simulations with individual perturbations of each model parameter. All simulations employed identical conditions, including sample and indenter geometry, azimuth angle defined in [27], mesh density, material model, loading protocol, and boundary conditions. Figure 2 illustrates the FE model along with typical results obtained for the [111] crystallographic orientation, provided here as a demonstrative example. These data results were extracted from the finely meshed cylinder shown in Fig. 2 ((a), left panel). Full details of the CPFEM simulation setup are provided in [23].

3. Results and discussion

Table 3: Identifiability index values computed for 13 crystallographic orientations. Each row corresponds to one orientation, while the columns report the Identifiability index values based on Force P (P-h indentation curve) $P(\{\zeta\})$, residual topography $Z(\{\zeta\})$, misorientation angle $\theta(\{\zeta\})$. The additional (last two) columns report the Identifiability index values obtained from combining two observables: Force P (P-h curve) with residual topography, and residual topography with misorientation angle. The analysis is performed for the parameter set $\zeta = \{\tau_0, Q, b, h_1, h_2, h_3, h_4, h_5, h_6, h_7\}$, using the values provided in Table 1. Residual topography values are computed from the top surface of the finely meshed cylinder shown in Fig. 2 (a), left panel) within a $20 \times 20 \mu\text{m}^2$ area centered on the indenter tip, excluding the central $9 \times 9 \mu\text{m}^2$ imprint core (see masked region in the inset of the Fig. 3(b)). Misorientation angle values are extracted from the remaining volume of the same cylinder after truncation by a rectangular $9 \times 9 \times 3 \mu\text{m}^3$ region (see masked region in the inset of the Fig. 3(d)). These exclusions remove regions with a high numerical uncertainty (such as those affected by the friction law and contact-induced perturbations in the sensitivity of the observables).

Number	$I_{index}(P(\{\zeta\}))$	$I_{index}(Z(\{\zeta\}))$	$I_{index}(\theta(\{\zeta\}))$	$I_{index}(P(\{\zeta\}) \cup Z(\{\zeta\}))$	$I_{index}(Z(\{\zeta\}) \cup \theta(\{\zeta\}))$
1	4.9	3.3	1.9	3.3	1.9
2	5.9	2.4	1.4	3.1	1.4
3	5.4	2.5	1.7	2.8	1.7
4	5.0	2.4	1.6	2.4	1.6
5	5.5	2.3	1.8	2.9	1.8
6	5.6	2.1	1.3	2.8	1.3
7	5.4	2.1	1.4	2.8	1.4
8	5.0	1.8	1.6	2.5	1.6
9	5.0	2.1	1.4	2.4	1.4
10	5.4	2.2	1.6	2.8	1.6
11	5.3	2.0	1.5	2.5	1.5
12	5.3	1.6	1.6	2.6	1.6
13	5.3	2.3	1.5	2.6	1.5

Fig. 3 (a) illustrates the pile-up distribution around the residual topographies respected to the IPF as in [33].

The topographies are made dimensionless, normalized by the maximum indentation depth, $h_{max} = 1 \mu\text{m}$. The represented region used for the surface analysis is a circular area centered at the imprint, with a radius equal to $10h_{max}$. The number, height, and shape of the pile-ups are strongly dependent on crystallographic orientation, reflecting the plastic anisotropic response of the crystal.

A similar dependence is observed for the misorientation field in Fig. 3 (c), which also captures the anisotropic nature of the crystal's plastic response.

Fig. 3 (b) and (d) show the distribution of the identifiability index within the IPF for the two observables considered. The IPFs annotated with the identifiability index computed separately for each observable, highlight the correlation between the crystallographic orientation of the Ni single crystal and its informativeness. This representation facilitates the interpretation of orientation-dependent identifiability and supports informed decision-making in experiment planning. The contour plots were obtained by interpolating the computed values from the 13 selected orientations over a regular interpolation grid, allowing a continuous visualization of the identifiability variation across all crystallographic directions.

The exact numerical values of the identifiability index for all 13 crystallographic orientations are reported in Table 3, which lists the values obtained from the residual topography, the volumetric misorientation angle, and their combined evaluation in the last three columns, respectively. The second column reports the identifiability index associated with the force P (from the $P-h$ curve), included only as a reference to recall the ill-conditioning of the inverse problem associated with this observable.

In Fig. 3(b), corresponding to the residual topography-based observable, one would see, except for orientations 8 and 12, which exhibit good identifiability ($I_{index} \approx 1.8$ and 1.6 , respectively), the identifiability index of other orientations exceeds 2, ranging from acceptable for orientation 11 ($I_{index} \approx 2$) to ill-conditioned for the [100] orientation, which shows the poorest conditioning among all ($I_{index} \approx 3.3$). The data used for this identifiability analysis is associated with the top surface region, as shown in the inset of Fig. 3(b). This region corresponds to a $20 \times 20 \mu\text{m}^2$ area centered on the imprint tip, with a central $9 \times 9 \mu\text{m}^2$ square excluded to remove the imprint core. This exclusion was applied to remove contact-affected regions characterized by a high numerical uncertainty (arising from the friction law and contact-induced perturbations in the sensitivity of the observables) as well as areas where Atomic Force Microscopy (AFM) measurements are unreliable. Since the position, number, and morphology of the pile-ups depend on the crystallographic orientation, a square mask inevitably excludes a variable, yet limited, amount of information outside the actual imprint core, including portions of the pile-ups. The influence of the mask size was therefore investigated in [34] and an appropriate square mask size was selected on this basis.

In contrast, Fig. 3(d), which corresponds to the misorientation angle-based observable, shows generally lower identifiability indices. All orientations exhibit identifiability index values below 2, indicating an improved conditioning compared to the I_{index} computed from the surface topography. The most favorable orientation corresponds to orientation 6 with ($I_{index} \approx 1.3$), while the [100] orientation remains consistently the least favorable regardless of the observable

considered, though with ($I_{index} \approx 1.9 < 2$). The identifiability analysis using of misorientation angle observable was performed on the remaining volume of the finely meshed cylinder after excluding a box-shaped central region centered on the cylinder axis (experimentally more straightforward to remove than a triangular prism-shape), as shown in the inset of Fig. 3(d). This region where EBSD measurement most often fails. The excluded box dimensions are $9 \mu\text{m}$ in width, $9 \mu\text{m}$ in length, and extending $3 \mu\text{m}$ in depth from the top surface ($3h_{\text{max}}$ in depth from the top surface is sufficiently far from the contact-affected regions characterized by a high numerical uncertainty).

	1	2	3	4	5	6	7	8	9	10	11	12	13
1		1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.7	1.7
2			1.4	1.3	1.7	1.1	1.3	1.4	1.3	1.4	1.4	1.4	1.4
3				1.5	1.6	1.3	1.3	1.5	1.4	1.4	1.5	1.5	1.4
4					1.6	1.3	1.3	1.5	1.3	1.4	1.4	1.4	1.3
5						1.5	1.5	1.7	1.5	1.6	1.5	1.5	1.5
6							1.1	1.3	1.2	1.3	1.3	1.4	1.2
7								1.4	1.2	1.4	1.4	1.4	1.3
8									1.5	1.5	1.5	1.6	1.5
9										1.4	1.4	1.5	1.4
10											1.4	1.4	1.4
11												1.5	1.4
12													1.4
13													

Table 4: Identifiability index values based on misorientation angle computed by combining the datasets of every possible pair of crystallographic orientations. The values are presented in a matrix format: only the upper-triangular portion is filled, the diagonal is left blank (corresponding to combinations of an orientation with itself), and the lower-triangular portion is also left blank to avoid redundancy. Values are rounded to one decimal place.

To further evaluate the conditioning improvement obtained when using the misorientation angle as an observable, Table 4 presents the identifiability index values obtained by combining the datasets of every possible pair of crystallographic orientations.

Among these combinations, the pairing of the two most favorable orientations (orientations 2 and 6) stands out. This combination yields an identifiability index of ($I_{index} \approx 1.1$), highlighted in yellow in the Table 4, confirming the very good conditioning achievable with this observable alone. For comparison, combining the two best orientations identified for the residual topography-based observable, namely orientations 8 and 12, the resulting identifiability index ($I_{index} \approx 1.3$), although showing good complementarity, it remains less favorable than the identifiability index obtained from the best orientation in the misorientation-based observable case.

Furthermore, as evidenced by the last column of Table 3, the combined use of residual topography and misorientation angle does not provide complementarity and does not degrade the identifiability for any of the 13 crystallographic orientations.

4. Conclusion

The present identifiability analysis shows that the choice of observable strongly impacts the identification of the 10 plastic hardening parameters of a single crystal Méric–Cailletaud type behaviour law, whereas crystallographic orientation having smaller, but noticeable, effects.

In fact, the volumetric lattice misorientation angle field provides a better conditioning of the inverse problem than the residual topography. The identifiability analyses show that, when using the volumetric misorientation angle field as the observable, a single crystallographic orientation is sufficient to simultaneously identify the ten hardening parameters of a Méric–Cailletaud type law after Berkovich nanoindentation test. Although a single orientation is largely sufficient, the best experimental configuration would be to carry out nanoindentation tests on two different relative tip/crystal orientations and combine their respective misorientation angle data sets. It concerns the two most informative relative tip/crystal orientations (according to the identifiability analysis employing misorientation angle-based observable), that show a good complementarity as well.

These results establish feasibility at the numerical level. Translating this into a physically grounded and reliable identification framework requires the development of experimental techniques capable of measuring full-field lattice rotations with both a spatial resolution comparable to the computational spatial resolution used in the identifiability analysis (approximately 100 nm) and a high angular precision 0.01° [35].

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