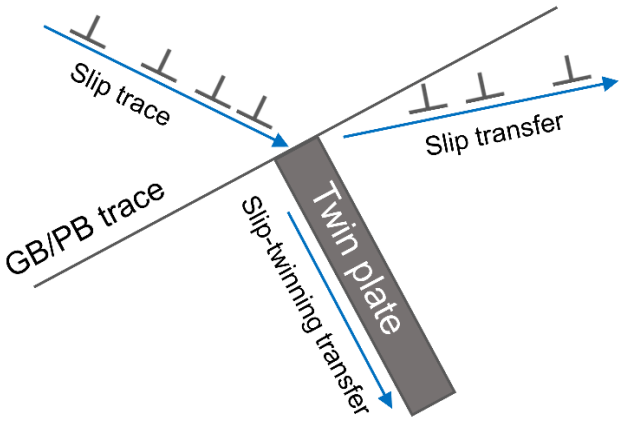
Slip Trace Crystallography Toolbox (STrCryst V1.0)

User Guide



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May. 2021

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Chapter 1. Preface

Metals and alloys undergo plastic deformation once the external load exceeds their yield strengths. One of the conspicuous features resulting from this, are the surface steps produced by various deformation micro-events, such as dislocation slip, mechanical twinning, or displacive phase transformations. In a microscopic viewpoint, these surface steps are the intersections between crystallographic planes on which plasticity mechanisms take place and the sample's surface plane. This kind of intrinsic correlation motivates the design of this *STrCryst* toolbox, in a sense to enable quantitative crystallographic analysis of plastic deformation micro-mechanisms.

The current *STrCryst* (V1.0) toolbox developed in MATLAB includes two major functions: (1) distinguish operative deformation module by trace calculation; and (2) analyze deformation compatibility considering slip transfer incident between adjacent grains. Follow-up version of it will incorporate more functions based on the inputs and feedbacks from users. Please feel free to reach out to the developer (slwei@mit.edu), if you have any question or suggestion.

STrCryst will always be free, and please kindly cite S.L. Wei et al., Acta Mater., 2021, 206: 116520, so your colleagues may know about this toolbox. Thanks!

Chapter 2. Installation environment and important instructions

2.1 Download and installation

Download *STrCryst* Version 1.0: https://github.com/shaolouwei

STrCryst was developed in the App designer environment of MATLAB R2019b and has been tested on R2020a, and R2020b. *STrCryst* has *NOT* been tested on MATLAB versions prior to 2019b.

-***Required:*** R2019b

-Recommended: R2019b or later version

Please also make sure that MATLAB App designer has been properly installed. Once downloaded the *.mlappinstall* file, double click, and an automated installation procedure will be activated in MATLAB. Manual installation can also be carried out in the MATLAB APPs panel by clicking "Install App" (Fig. 2.1 (a)). Once being successfully installed and activated in the "My Apps Panel" the program will navigate to the main panel shown as Fig. 2.1 (b).

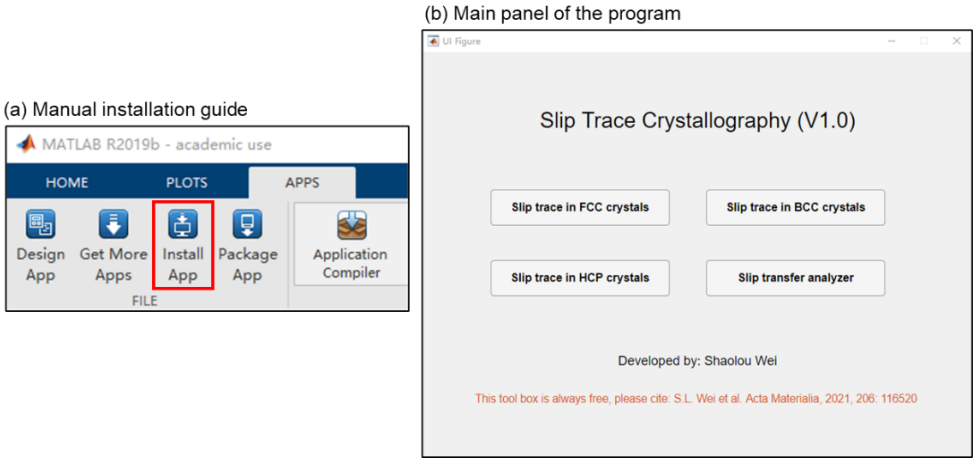


Fig. 2.1 | Manual installation and main panel of *STrCryst*.

Operating system requirements: Windows OS. Note that *STrCryst* was developed on Windows 10 and has *NOT* been tested on Mac OS.

Screen display preference: *STrCryst* operates the best with 100 % scaling (without zooming) of your screen. Manual adjustment of the screen scaling might cause display error in *STrCryst*.

2.2 Important instructions

(1) Current version of *STrCryst* follows the sample frame convention of a **TESCAN MIRA 3 SEM**, as schematically shown below.

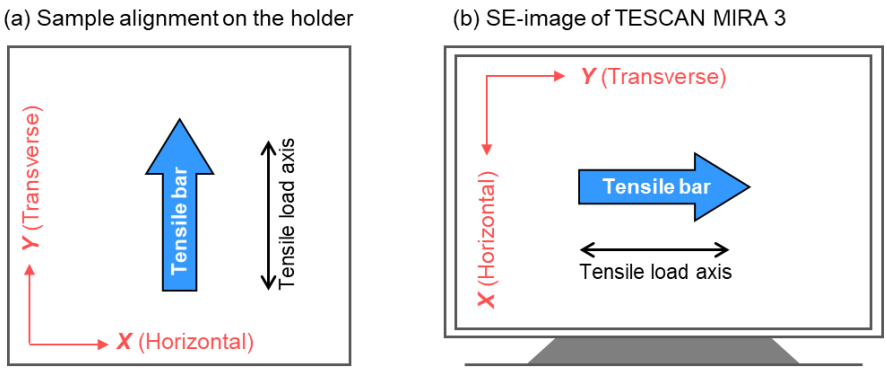


Fig. 2.2 | Sample frame alignment convention of TESCAN MIRA 3 SEM

Because of this, in **ALL** the calculations that will be detailed below, the default loading axis has been pre-set as $\boldsymbol{F} = [0\ 1\ 0]$, and the observational direction $\boldsymbol{N} = \boldsymbol{X} \times \boldsymbol{Y} = [0\ 0\ 1]$ (sample frame, capitalized letters). If you are trying to perform calculation using images taken from different SEM systems than **TESCAN MIRA 3**, it is crucial to firstly verify your sample frame convention, and make sure to always verify your loading axis when conducting Schmid factor calculations.

(2) The Euler angles definition in the current version of STrCryst follows the Bunge's convention [1], and thus the coordinate transformation tensor is computed as:

$$\mathbf{G} = \begin{bmatrix} \cos\varphi_1\cos\varphi_2 - \sin\varphi_1\sin\varphi_2\cos\phi & \sin\varphi_1\cos\varphi_2 + \cos\varphi_1\sin\varphi_2\cos\phi & \sin\varphi_2\sin\phi \\ -\cos\varphi_1\sin\varphi_2 - \sin\varphi_1\cos\varphi_2\cos\phi & -\sin\varphi_1\sin\varphi_2 + \cos\varphi_1\cos\varphi_2\cos\phi & \cos\varphi_2\sin\phi \\ \sin\varphi_1\sin\phi & -\cos\varphi_1\sin\phi & \cos\phi \end{bmatrix} \tag{2.1}$$

While most of the EBSD systems are accord with the Bunge's convention, there are cases where the Roe's or the Kocks' convention is adopted. While exporting Euler angles, please make sure that your data are in line with the Bunge's convention. This can be easily achieved in commercial EBSD software such as OIM:

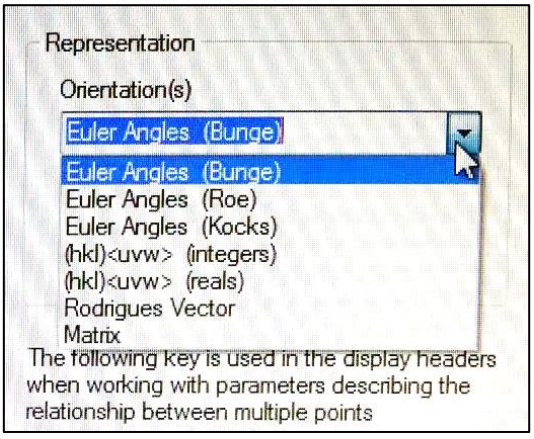


Fig. 2.3 | Verification of orientation representation in the OIM EBSD post-processing software

(3) All the calculations in the present version only take into account crystallographic-based plastic deformation behavior (strain-dominant). In various cases, atomic shuffle can also lead to (sometimes dominate) deformation features similar to strain-dominant ones, for example the $\{10\bar{1}2\}\langle\bar{1}011\rangle$ twin in HCP-metals [2–4]. Please be extract careful to interpret calculation results for these situations, as their atomistic procedures may not be fully in line with the crystallography presumption applied here. Please also refer to Appendix A1 for more details.

Chapter 3. Theoretical slip trace alignment calculation

This chapter concerns about slip trace analysis of plastically deformed metallic samples. Crystallographic fundamentals of this calculation has been discussed in detail in the literature [5]. As summarized in **Tab. 3.1**, the current version of *STrCryst* incorporates typical plastic deformation responses FCC, BCC, and HCP-structured crystals.

Tab. 3.1 | Summary of compiled slip trace calculation module in *STrCryst*

Calculation module	Slip systems	# of plane trace	Plot in STrCryst
FCC	$\{111\}\langle 110\rangle$	4	Slip trace
BCC	$\{110\}\langle 1\bar{1}1\rangle$	6	110 trace
	$\{112\}\langle 11\bar{1}\rangle$	12	112 trace
	$\{123\}\langle 11\bar{1}\rangle$	24	123 trace
HCP	$\{0001\}\langle 11\bar{2}0\rangle$	1	Basal trace (light blue)
	$\{10\bar{1}0\}\langle 11\bar{2}0\rangle$	3	Prismatic trace
	$\{10\bar{1}1\}\langle 11\bar{2}0\rangle$	6	Pyramidal-I <a> trace
	$\{11\bar{2}\bar{3}\}\langle 11\bar{2}\bar{2}\rangle$	6	Pyramidal-II <c+a> trace
	$\{10\bar{1}2\}\langle\bar{1}011\rangle$ (twin)	6	10-12 twin trace (brown)

The following snapshot provides an exemplary calculation conducted for HCP-structured Ti.

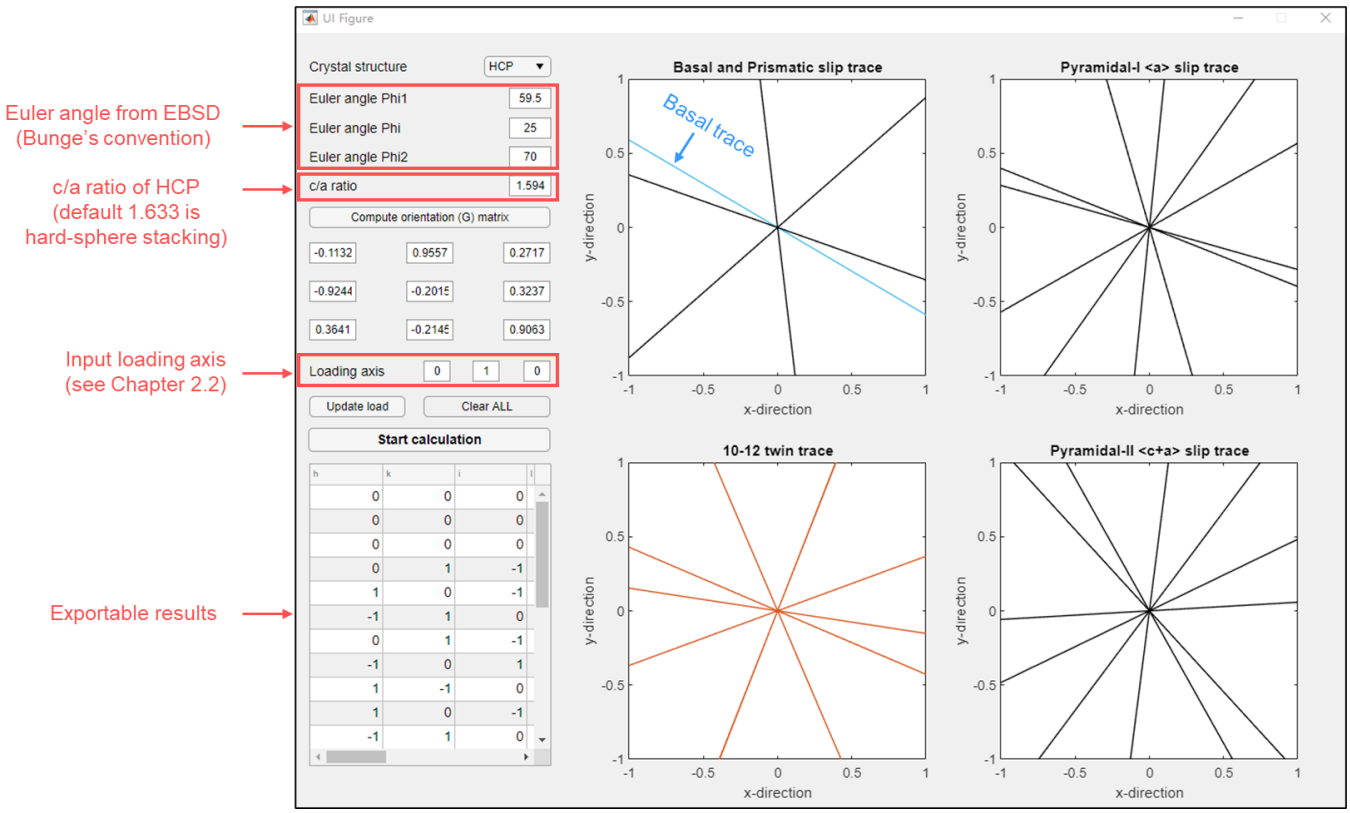


Fig. 3.1 | Exemplary calculations conducted for an HCP-structured Ti alloys with c/a ratio 1.594

By matching the theoretically predicted slip trace alignment with the experimentally measured ones, the activated slip system(s) can be easily identified. Please note that, the presumption of identifying activated slip directions that belong to the same plane family, e.g. $[110]$ versus $[101]$ in $(\bar{1}11)$, is based on the magnitude of their Schmid factors. While this convention has been adopted in appreciable literature, it is always more rigorous to provide all the calculation results.

NOTE: the same calculation is also applicable to distinguish operative planar/wavy slip mode during ECCI experiment.

Chapter 4. Slip transfer analyzer

This function in *STrCryst* enables compatibility analysis between two vicinal grains that exhibit deformation transfer incidents. Crystallographic fundamentals of the calculation are available in the literature [5]. Depending on crystal symmetry, the current version of *STrCryst* concerns about three slip transfer modules: Cubic-to-Cubic, Hexagonal (Hex.)-to-Cubic, and Hex.-to-Hex. transfer. Detailed intergranular compatibility parameters incorporated in the present version are summarized in the following Table.

Tab. 4.1 | Intergranular compatibility parameters compiled in *STrCryst*

Parameter	Definition	Reference
Luster-Morris m′ factor	$m' = [(\mathbf{G}_1^{-1} \cdot \boldsymbol{s}_1) \cdot (\mathbf{G}_2^{-1} \cdot \boldsymbol{s}_2)] \cdot [(\mathbf{G}_1^{-1} \cdot \boldsymbol{n}_1) \cdot (\mathbf{G}_2^{-1} \cdot \boldsymbol{n}_2)]$	[6]
Misorientation angle	$\theta = \arccos[(\mathrm{tr}(\mathbf{G}_1\mathbf{G}_2^{-1}) - 1)/2]$	[7]
Slip direction misalignment	$\kappa = \arccos\,[(\mathbf{G}_1^{-1} \cdot \boldsymbol{s}_1) \cdot (\mathbf{G}_2^{-1} \cdot \boldsymbol{s}_2)]$	[6,8]
Slip plane misalignment	$\psi = \arccos\,[(\mathbf{G}_1^{-1} \cdot \boldsymbol{n}_1) \cdot (\mathbf{G}_2^{-1} \cdot \boldsymbol{n}_2]$	[6]
$SF_1 \cdot (m') \cdot SF_1$	Multiplying Schmid and m′ factors	[9]

The following snapshot is an exemplary calculation conducted for basal-to-basal slip transfer in an HCP-structured Ti alloy.

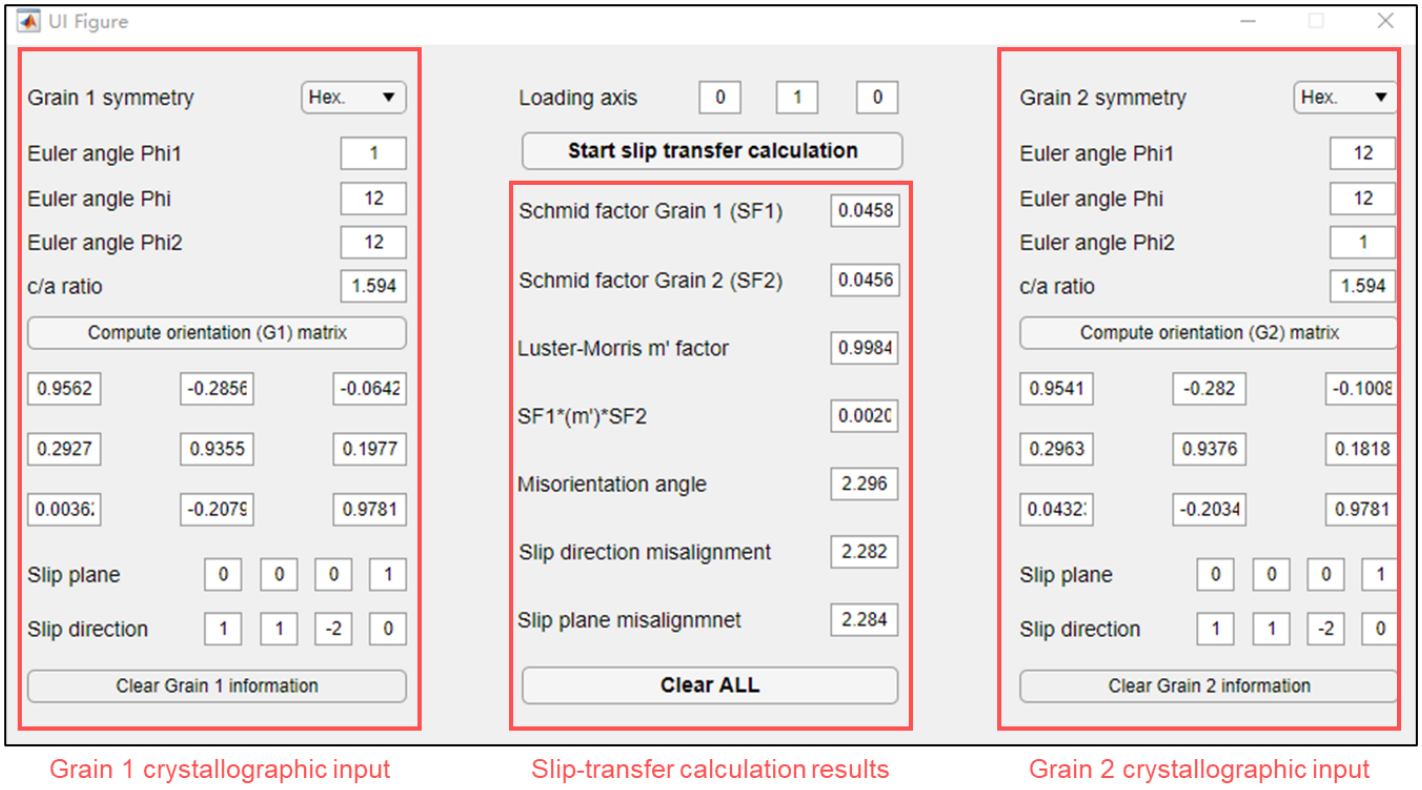


Fig. 3.1 | Exemplary calculations conducted for basal-to-basal slip transfer in an HCP-structured Ti alloy with c/a ratio 1.594

NOTE: this kind of analysis is better to be carried out after identifying the operative slip mode from slip trace (Chapter 3).

Appendix

A1. Important presumptions and limitations of the technique

The following bullet points summarize the important presumptions in the algorithm for the current version of *STrCryst*:

- *Plastic deformation is purely crystallographic*: all calculations presume slip or twinning is only controlled by strain. Atomic shuffle effect is ignored here.
- *Tension-compression symmetry for perfect dislocation slip*: *STrCryst* always enforces positive Schmid factor for calculations considering perfect dislocation slip.
- *Tension-compression asymmetry for* $\{10\bar{1}2\}\langle\bar{1}011\rangle$ *twin*: *STrCryst* does NOT enforce positive Schmid factor for this specific twinning mode because of the well-documented tension-compression asymmetry response.
- *Positive Luster-Morris m' factor*: *STrCryst* enforces positive m' value.
- *Misalignment angle convention*: *STrCryst* enforces the slip direction (also slip plane) misalignment angle in the range of 0-90°.
- *Presence of misorientation: STrCryst* disables any calculation when the orientation inputs are identical for the two vicinal grains.

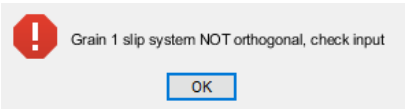
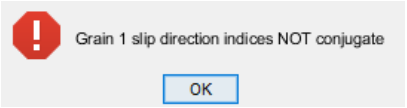
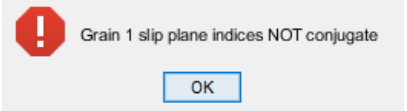
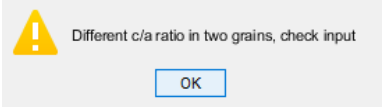
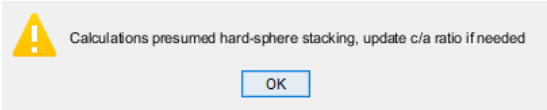
It is always important to keep in mind that this technique also has the following intrinsic limitations.

- *Requirement of high surface quality*: contamination or mechanical scratches will interfere the slip trace imaging.
- *Far-field loading state approximation*: local stress state may be extensively deviate from the uniaxial condition.
- *Misalignment between SE and EBSD*: SE micrograph and EBSD map always exhibit somewhat misalignment.

A2. Error and warning messages

During your calculations, the following listed error and warning messages may come up, reasons and solutions are detailed in the following Table.

Tab. A1 | Intergranular compatibility parameters compiled in *STrCryst*

Error or warning messages	Reasons and solutions
	Dot product of slip plane $[h\ k\ (i)\ l]$ and slip direction $[u\ v\ (t)w]$ is not zero. This violate orthogonality and there must be a typo in your input.
	In HCP slip direction input $[u\ v\ t\ w]$, $u+v+t\neq 0$. This violates the notation convention and there must be a typo in your input.
	In HCP slip plane input $[h\ k\ i\ l]$, $h+k+i\neq 0$. This violates the notation convention and there must be a typo in your input.
	*STrCryst* presume the two adjacent HCP grain exhibits the same c/a ratio. Discard this if you are analyzing slip transfer between two different HCP phases.
	*STrCryst* presumes 1.633 as the c/a ratio considering the hard-sphere HCP stacking sequence. If necessary, update this with the c/a ratio measured for your material.

Acknowledgements

The author (Shaolou Wei) gratefully dedicates this toolbox to Dr. Prof. C. Cem Tasan who introduced him to the field of plasticity micro-mechanics. Special thanks are due to Ms. Jiyun Kang and Dr. Hyunseok Oh for their help with testing the toolbox and valuable suggestions. Discussion with Dr. Feng He is also acknowledged.

Bibliography

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