* Use of crystal plasticity approach to facilitate constitutive models development for sheet metal forming

# Research background

## Sheet metal forming and constitutive model

Over the past years, it has become very customary to perform finite element (FE) simulations in order to predict failure of a raw blank metal sheet before actually forming it into a desired shape. The mechanical behaviors of such a blank metal sheet are usually characterized based on simple experiments such as uniaxial tension, disc compression, and simple shear tests. The constitutive characteristics are usually simplified into a certain set of parameters, for example, yield stress, anisotropic coefficients, hardening parameters and so on. The material characteristics in FE model are defined by such constitutive parameters. Depending on the choice of constitutive model, the kind of parameters to obtain varies. Some constitutive model assumes the material behavior as a known priori, e.g., isotropic hardening for mild steels, which reduces the number of insignificant anisotropy associated parameters. For that reason, only proper choice of constitutive model may lead to cost-effective FE simulations. On contrary, there are cases where existing constitutive models are not able to manifest what is experimentally observed. In this case, it is necessary to develop a new constitutive model with a reasonable accuracy but without introducing too many parameters to determine. In what follows, contemporary issues, which existing constitutive model fail to predict or reproduce, are discussed.

## Contemporary issues

* Springback:
  + Die design often requires an iterative try-and-error process in order to fulfill final product dimension, which is expensive and time consuming
  + Need of an accurate constitutive model on springback phenomena (elasticity driving problem: high accuracy of prediction is required)
* Presence of multi-phase and unconventional source of plastic accommodation (TRIP and TWIP)
  + Unconventional material behaviors attributed to complex microstructure and related phenomena
  + Microstructure-based modeling is necessary.
* Importance of multiaxial characteristics
  + Stretching is dominant deformation mode in sheet metal forming process
  + Some triaxiality-dependent behavior is observed for some AHSS steels (TRIP anisotropic hardening).

## Multi-scale approach

Why multi-scale?

* Advanced continuum constitutive model needs experiments that are very difficult or tedious to actually perform.
  + Barlat’s yield function that requires through-thickness anisotropy coefficients;
  + Some cases that requires multi-path changes
* Each scale has its own merits (Atomic, Molecular, Granular, and so on)
  + Examples!!! (Groh et al., IJP 2009)
* Extension of a constitutive model increases not only the predictive accuracy but also the number of parameters to be experimentally characterized.
* Interactive modeling strategy (bridging results from different scales)
  + What would be suitable scale for sheet metal forming constitutive model? (A: crystal plasticity)

## Application of crystal plasticity

Advantages of crystal plasticity for sheet metal constitutive modeling

* Anisotropy: representative statistical texture (grains)
* Granular scale: characteristics originated from granular scale may easily be extended
* CP may provide physically more meaningful insights on macroscopic behavior of the polycrystal in terms of single crystal frame.
* Research areas where use of crystal plasticity is beneficial
  + List of such examples

During this study, four different cases of crystal plasticity application are performed. These studies are individually independent, however, they are quite closely related.

a) Optimization tool development that is associated with proper use of crystal plasticity model with cautions that may influence the model prediction accuracy.

b) An assistive application of crystal plasticity for experimental biaxial tests

c) Provision of a virtual testing frame to facilitate the continuum-based constitutive model development

d) Extension of a chosen crystal plasticity framework to model thermo-mechanical constitutive behaviors for phase-transforming steels

# Crystal plasticity

Brief chronicles on crystal plasticity development

## Classical models

Taylor & Sachs (static) bounds

Brief introduction on intermediate approach

## Mean field Self-consistent models

### Visco-Plastic Self-Consistent model (Lebensohn-Tomé)

[Deal details on the development of VPSC with introducing important papers]

Rate dependent single crystal constitutive law

Eshelby tensor and Mura’s inclusion and equivalent inclusion method, and its solution for visco-plastic medium

### Elasto-Plastic Self-Consistent model (Turner-Tomé)

Hutchinson’s self-consistent solution fro elasto-plastic medium and its implementation by Turner and Tomé

Find applications of this model: in particular Bjorn’s papers on internal lattice strain measurement to find a relevant diffraction peak for lattice strain measurement. May need to mention difficulties in multi-phase modeling [Private communication with Tomé]

### Elasto-Visco-Plastic Self-Consistent (Wang-Tomé … )

[Inform briefly how the elasticity is incorporated]

May need to mention the issues associated with elasticity (Bauschinger, TRIP, internal lattice strain…)

## Full field models (FFT, CPFEM)

CPFEM, FFT on for inhomogeneous granular scale.

CPFEM (Kalindindi) or VPSC-FEM for macroscopic scale while some representative volume elements are assigned to the individual element. (Application is confined mostly to academia)

# A brief on the following sections

Current Ph. D project focuses on finding applications of VPSC and EVPSC models and aims at providing good reference case studies. Four different topics are discussed:

[The thesis consists of the three topics: 1) VPSC optimization tool development 2) Biaxial state behavior observed by NIST’s MK tooling and the in-plane biaxial tester (Kuwabara), 3) EVPSC-RGVB, and 4) EVPSC extension to account for TRIP phenomena

# Reference

* Part I: Development of the optimization tool for VPSC (The MSMSE paper)

# Research background

Flow curves of 304 austenitic stainless steel show that isotropic hardening does not hold even for monotonic strain path. This may be attributed to

* A) Initially anisotropic texture and, possibly, its consequent anisotropic development as the material deforms,
* B) or martensitic transformation that is triggered by plastic deformation.

Diverging trend in the flow stress curves are not explicable by the ‘isotropic’ phase volume transition. [Show a) the magnetic field based result and b) the work of Allison M. Beese and Dirk Mohr, and also show the phase volume fraction change does not show notable difference according to the direction of tensile direction.]

Although given crystal plasticity model (VPSC) does not possess elastic response of crystal thus inappropriate for transformation investigation, it has been predicting textures development of cubic materials successfully. VPSC frame is expected to capture texture-driving phenomena in such and such … [citations]. Therefore, in this study, it is assumed that only initial austenite’s texture causes such anisotropic hardening.

Constitutive modeling processes based on crystal plasticity usually consists of 1) obtainment of representative discrete model grains and 2) determination of associated constitutive parameters. It is found that constitutive modeling based on rate dependent crystal plasticity framework per se inherits certain ambiguities originated from what follows:

## Texture measurement and OD representativeness in model grains (number of grains)

Discrete nature of the crystal plasticity

Discrete grains from OD and its calculation based on PF.

The statistical representativeness of discrete model grain is checked to find sufficient number of grains.

* Discuss PF measurement from X-ray
  + X-ray is cost-effective
  + Correction techniques based on X-ray’s incomplete pole figures are readily available in the literature
* OD calculations (may be in appendix)
  + OD calculation methods: mention Harmonics and discrete OD methods.
  + Discrete method is taken and its result is based on a particular angular resolution (so is PF)
* Discrete grain sampling is should be checked for representativeness.
  + How to take discrete model grains? (may need to put in appendix)
    - Introduce the interpolate of OD weights in the Euler space
    - Indicate possible error possibly caused by PF->OD calculation. [citation, Delannay group]
    - Mention some better ways of getting discrete representative model grains
  + Show grain number sensitivity due to the statistical nature of discrete model grain input for crystal plasticity simulation
  + Critique some works based on too little number of discrete model grains like (NUMISHEET benchmark problem!)

## Proper linearization method for the power law

By introducing the visco-plastic law, ambiguity in active slip system selection is bypassed. [fact, cite some relevant papers]

The power law, typically with the exponent of 20, has successfully captured flow behavior of slip system. [citation]

In order to facilitate the computation of such highly non-linear response, this relation between slip system shear yield stress and slip shear rate is linearized [cite, secant, tangent, affine, neff=10 and Tomé’s MSMSE paper]. Often, consideration of different linearization method is disregarded when investigating one-dimensional stress state behavior. However, either for multi axial problem or systematic usages for different loading condition, influence of linearization method is significant. [shows the yield locus for different linearization method predicted by VPSC]

# Optimization tool based on Python-SciPy package

Need of optimization tool

Slip-system’s hardening-associated parameters are usually taken as known priories or subject to educative-guess or even fitting based on macroscopic response. This is mostly due to difficulties in direct experimental observations.

It is often seen that many research papers in the literature fit the hardening parameters based on trial-error with the initial educative guess. Here, an optimization tool is developed based on Simplex method.

This tool may be very useful in case one wants to fine-tune the microscopic parameters. In addition, given the multiple options for linearization strategy as discussed before, the optimization tool may provide best suitable linearization method.

* Python-SciPy tool and simplex method
* Configuration of the inputs

# Experimental procedure

Often, verification of constitutive response predicted with crystal plasticity framework focuses on uniaxial state due to experimental difficulties or to the fact that biaxial state is quite different from what is observed in uniaxial [Steglich et al., IJSS]

Since biaxial stretching is more frequently observed during sheet metal forming processes, a correct constitutive model should be capable of predict both uniaxial and multiaxial states. The optimization tool may suggest the best linearization method and provide fine-tuning of slip system hardening parameters.

Therefore, here a number of experimentations are carried out. Uniaxial tension along different angles are performed to find the most suitable linearization scheme. In addition, samples are also biaxially stretched using in-plane biaxial (Kuwabara) and Bulge tests in order to assess predictive capability of the fine-tuned parameters. The details on each experiment are given in what follows.

## Uniaxial tests

## Biaxial tension tests

Specific details on biaxial test system are given in part II.

Uniaxial tension test frame (MTS) is given.

Information on bulge test is given here, too.

# Experimental results and predictive accuracy of the model

Present the uniaxial and biaxial results.

Compare the experimental results with model predictions.

# Discussions

* Optimization tool found to be very useful when calculating single crystal hardening behavior based on macroscopic response.
* Stiffness of macroscopic media is open to choose, based on which a certain ambiguity raises when investigating multi-axial constitutive response.
* Lack of phase transformation model in the current approach should be improved -> Requires elasticity to account for phase transformation [Leads to Part IV]

# Reference

* Part II: Comparative study on the two biaxial testing systems with crystal-plasticity-assist approach

# Introduction

* One of the advantages that continuum constitutive model is that it is characterized based on simple uniaxial tests.
* Show schematic view on which stress points are used for characterizing advanced yield functions (like yld2000 characterized by a series of uniaxial tension responses).
* Sheet metal forming processes in general impose multi-axial loadings. Accordingly, some advanced constitutive models require characteristics when multi-axially loaded.
  + Direct measurement for even for monotonous biaxial loading is not an easy task
  + Introduce some works available in the literature (Bulge test, cruciform test, Marciniak test and so on)
  + Some more multiaxial probing tests by combination of shear and tension are reported in the literature (Many D. Mohr groups papers are available)
* Because of difficulties in experimentation, a standard process for biaxial test is not established.
* Results of two biaxial testers are presented and compared with crystal plasticity prediction. The crystal plasticity may provide some valuables insights for the two testers.
* In what follows, details on each biaxial tester are given.

# Biaxial testers

## Marciniak tooling with X-ray goniometer

* Marciniak Tooling with X-ray goniometer
  + System configuration
    - Indirect measurement of non-contact stress (based on elastic lattice strain) and strain measurement (DIC) [cite Iadicola]
      * X-ray goniometer configuration, sample geometry, DIC
      * Digital Image Correlation
  + Stress Calculation
    - Review on correction between elastic lattice strain and stress based on the stress factor by [Thomas, Creuziger, and Iadicola]
    - The linear regression method. The linearity assumption no longer holds according to the observation as plasticity comes into play (texture/grain shape)
  + Experimental stress factor calculation and model predictions
    - Correction based on stress factor – stress factor correlates the internal strain and macroscopic stress based on which experimental internal strain may lead to accurate stress measurement
* In-plane biaxial tester (Kuwabara)
  + Conventional mechanical tester in which stress is based on load cell and strain is measured through two uniaxial strain gauges.
  + Assumption is that the stress and strain is uniform within the squared part of the specimen
  + Sample geometry, system specifications, and the stress and strain measurement tools (load cell and strain gauge)
    - Associated disadvantages
      * Premature instability
      * Uniform assumption? (Determination of strain gauge locations, cite the paper in 2010 metal forming)
  + Cite works based on Kuwabara’s system
* Put a table that briefly compares the two testing systems in terms of 1) Strain measurement method, 2) Stress measurement method, and 3) Measurable strain ranges

# EVPSC prediction and correction

## EVPSC-assist biaxial flow stress determination

* Slip system hardening parameter characterization based on uniaxial tension results
* Show biaxial flow stress behavior

## Discrete model grains

* Pole figures obtained from neutron diffraction (cube sample)
* Slip system hardening parameters (BCC)

## Stress factor calculation based on EVPSC simulations

* Extension of the subroutine dif\_plane for multi-phase
* Explains details on how diffraction-based lattice strain is calculated in the discrete model polycrystal (Cite one of Bjorn’s papers)

# Experimental conditions and results

Balanced biaxial + two plane strain states for a) mild steel and b) dual phase steel

Its analysis… and comparative report on the final experimental data

# Discussion

Discuss pros and cons of both experimental systems.

# Reference

* Part III: Dislocation density-based hardening model incorporation to an Elasto-Visco Plastic Self-Consistent framework

# Research backgrounds

* Needs for more accurate strain hardening model that captures strain path sensitive flow behaviors
  + Metal forming involves many different, either gradual or drastic, strain path changes
  + Blank sheet may experience inhomogeneous loading paths (Bending and unbending) through thickness direction that complicates microscopic state (dislocation cell structure and local inhomogeneity).
  + Advanced hardening model that accounts for the strain path dependency is necessary
* Review on RGVB ([2007](#_ENREF_4_1)) and the recent work in which implementation to VPSC framework is presented. Here in this study, RGVB is implemented to EVPSC that captures elasto-plastic transition

# Incorporation of RGVB into EVPSC

--- Why EVPSC is more suitable frame than VPSC?

Previous study by Kitayama et al predicts the flow behavior of RGVB in VPSC framework on the transient plateau region when loading path is reversed. However, the flow behavior on elasto-plastic region was not captured in their model since VPSC assumes the polycrystal is rigid-plastic. It is apparent that early plastic yielding upon change of loading path is not pure plastic. For this reason, EVPSC may provide a better crystal plasticity framework.

# Verification of the model

## Yield criteria

* Plastic yielding is multi-dimensional response. However, here, the yield surface confined to be on 2D plane stress space problem for the sake of simplicity.
  + Usual presentation in pi-space is not relevant in that pure plastic boundary condition, where deviatoric description is plausible, is not possible for EVPSC.
  + This mingled elasto-plastic boundary condition is more realistic in that in experiments it is impossible to only plastically load the metallic sample.
* Choice of yield criterion may significantly influence the results.
  + There are various yield criteria, and among others a few of them are focused in this study: a) strain offset, b) equivalent work dissipation, and c) onset of micro-yielding.

## Various benchmark studies

Flow stress behavior (follow the benchmark problems…)

1) Forward shear and reverse shear. With an increasing amount of pre-tension strain, observe the more pronounced Bauschinger effect and the plateau.

2) Erase of residual internal elastic strain by EVPSC-RGVB

# Reference

Rauch, E. F., Gracio, J. J., & Barlat, F. (2007). Work-hardening model for polycrystalline metals under strain reversal at large strains. *Acta Materialia, 55*(9), 2939 - 2948.

* Part IV: Incorporation of transformation-induced plasticity to the Elasto-Visco-Plastic Self-Consistent model

# Introduction

## Advanced High Strength Steels (AHSS)

TRIP (transformation-induced plasticity) and TWIP (twin-induced plasticity) steels show many excellent characteristics attributed to their complex microstructure.

Both steels have unconventional plasticity accommodation mechanisms: a) transformation-induced plastic deformation that is associated with the formation of martensitic phase within austenitic grain and b) twin-induced plasticity deformation in which mechanical micro-twins significantly contribute to total plastic accommodation in addition to the conventional dislocation slip.

## Accurate predictive tool on constitutive behavior

Although AHSS features with unconventional plastic accommodators in the micro-scale, cost-efficient constitutive model for such steels should be phenomenological continuum model. Such a continuum model, for AHSS, should account for the unconventional plasticity accommodators to some extent. Such a model should provide a phenomenological way of material characterization.

A well-defined crystal plasticity framework will serve as a suitable base framework to extend to TRIP/TWIP. In current study, EVPSC is extended to model TRIP.

## Crystalline nature associated with TRIP

As a matter of a fact, crystal plasticity is an appropriate frame to model TRIP phenomena. For instance, the phenomenological theory on martensitic transformation (WLR, Bhadeshia… ) explains complete behaviors associated with crystalline nature between the austenite and martensite in terms of simple matrix algebra. This theory can explain … (inhomogeneous strain [alternating martensitic domains], transformation strain (thus including dilatation), crystal relation only based on lattice parameters) that are adequate information for crystal plasticity models with the assumption of homogeneous intra-granular strain and stress fields.

## Crystal plasticity as a meso-scale tool

The crystal plasticity framework with the homogeneous grain assumption provides adequate physical insights for continuum constitutive modelers.

List some successful examples from literature…

Brief the current work based on EVPSC frame

The focus of the current study is to incorporate a thermo-mechanical constitutive model into an elasto-visco-plastic polycrystal framework. Some details on the targeted martensitic transformation kind are given in what follows.

# Brief characteristics of TRIP phenomena

Martensitic transformation is diffusionless and displacive thermo-mechanical solid phase transformation that occurs for various metallic materials. It has some distinctive characteristics such as the habit phenomenon ([Machlin & Cohen, 1951](#_ENREF_5_5)), inhomogeneous strain in martensite domain, and transformation shear and dilatation attributed to the displacive nature. Quenching, a sudden temperature drop, is a typical process in steel making to trigger the martensitic transformation. On the contrary, the type of martensitic transformation of TRIP steels is designed to occur when deformed into a desire shape. This is due to the fact that some meta-stable austenite transforms by the help of mechanical stimuli. It is well known that such mechanical stimuli are either plastic deformation-driven ([Olson & Cohen, 1975](#_ENREF_5_7)) or assistive stress-driven.([Olson & Cohen, 1982](#_ENREF_5_8)). The main focus of the current study is on modeling of the latter.

## Greenwood and Jonson, and Magee effects

Transformation induced-plasticity (TRIP) is often being as the term referring to the additional macroscopic plastic accommodation due to micro stress and strain fields induced due to the interaction of existing soft austenite and newly formed hard martensite. There are two well-known sources of TRIP: 1) [Greenwood and Johnson (1965](#_ENREF_5_2)) claimed that the specific volume differential between the two co-existing phases induces the softer phase to accommodate the internal micro stresses; 2) [Magee (1966](#_ENREF_5_6)) found that the stress-dependency of the variant selection results in preferred orientation distributions of the martensites that manifests as macroscopic shape change. Strictly speaking, Greenwood and Johnson’s TRIP is not a kind that is particularly associated with phase transformation per se. Greenwood Johnson effect refers to the plasticity caused by the interaction between ‘existing’ phases with dissimilar hardness or strength {cite Lebond}. On contrary, Magee’s TRIP occurs where existing stress influences the variant selection over the course of transformation. Due to anisotropic nature of associated transformation strain, biased variant selection results in macroscopic shape change.

## Meta-stable austenitic stainless steel

The chosen material for the current study is a 304 austenitic stainless steel. The 304 austenitic stainless steel (304-STS) is initially full austenitic and designed to phase-transform in the room temperature when plastically deformed. TRIP steels that are widely used for automotive components is not single austenitic. It is usually consisted of ferrite, bainite and some residual metastable austenite. Development of a model that accounts for a material with that many phases should be followed by the verification for the simple case where only austenite initially presents. For this reason, the chosen 304-STS sample is more suitable for verification of the model. The texture is represented as below: …

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Elements | C | N | Cr | Ni | Al | Mn | Mo | Si |
| Amount (wt%) | 0.06126 | 0.04386 | 19.13 | 8.85 | 0.013 | 1.04 | 0.090 | 0.40 |

# Literature survey

* + Continuum scale modeling
  + Micro-scale modeling
  + Meso-scale modeling
  + Polycrystal modeling

# Modeling strategy

The EVPSC framework is imposed a macroscopic boundary condition based on which microscopic responses are estimated self-consistently. Such boundary condition is given as a incremental form for each of increment all micro state variables are determined. Martensitic transformation is explicitly incorporated into the EVPSC framework in that based on the last self-consistent state variables, martensitic transformation associated evolution is determined for the next self-consistent solution seeking process.

## Variants and the selection criterion

The precise description on the crystal orientation relations between martensite and austenite is of prime important when investigation variant selection. The Kurdjumov-Sachs (KS) and Nishiyama-Wasserman (NW) relations have been widely used in many works [citation needed]. The work of Wechsler, Lieberman and Read (WLR) [citation needed] also provides orientation relationship that is determined by the lattice parameters. Bhadeshia claimed that WLR is more appropriate than KS or NW, since it can explain a complete set of phenomenological characteristics such as … . In fact, KS and NW are based on experimental observations within varying degrees of reliability (Cite Bhadeshia Scripta criticizing one work …). In fact, there is a varying degree of misorientaion within the experimentally observed orientation-relations [cite habit planes for many different steels from Bhadeshia’s worked examples book].

Often, the crystal orientation relation is expressed by providing habit plane normal (PN) and invariant line (IL) directions given in the crystal axes of both austenite and martensite. Such notation is quite commonly found in the literature. Table 1 contains orientation relations of KS and NW.

Table The Kurdjumov-Sachs and Nishiyama-Wasserman orientation relations are given. and b are a habit plane normal and an invariant line direction, respectively. The superscripts and refer to the parent austenite and child martensite.

|  |  |  |
| --- | --- | --- |
|  | Kurdjumov-Sachs | Nishiyama-Wasserman |
| Habit plane normal | //: // | //: // |
| Invariant direction | //: // | //: // |

Figure The schematic two-dimensional view on crystal orientation relation and its associated axes is given. The black solid axes represent the crystal orientations of the two phases. The two gray coincident axes are composed of habit plane normal and invariant line direction . Based on the directions of the bases vectors referred in their crystal axes, and , the orientation between the two solid axes can be determined.

This presentation itself does not contain full orientation relation. It is required to have three independent relations to describe the orientation between the two axes. To this end, an auxiliary vector, **t**, is introduced as the cross product of and . The complete crystal orientation relationship is given based on the fact that // , // and //. Figure 1 schematically depicts the current problem. Details are given in what follows.

: Crystal axes of austenite and martensite, respectively.

where () indicates the single-row matrix.

The transformation matrix that rotates the austenite’s crystal axes, , to the one for martensite, , is as below:

Based on above lines the crystal relation for KS and NW are found and denoted as and , respectively.

On the contrary, WLR model provides the orientation relation in the form of an orthogonal rotation matrix. Their calculation is based on the lattice parameters of austenite and martensite. The lattice parameters being used in this study are given in the Table 2.

Table Lattice parameters of austenite and martensite

|  |  |  |
| --- | --- | --- |
|  | Austenite | Martensite |
| Lattice parameters [nm] | 0.3589 | 0.2873 |

Following Bhadeshia ([Bhadeshia, 2001](#_ENREF_5_1)), the crystal orientation relation and transformation strain are calculated based on the lattice parameters for a particular variant and denoted here as:

and .

The multiplication based on the cubic crystal symmetry operations, , of the above solution is performed as below:

As discussed earlier, variant selection is not random but influenced by the existing stress field. Variant selection is determined based on the interaction energy defined as below:

.

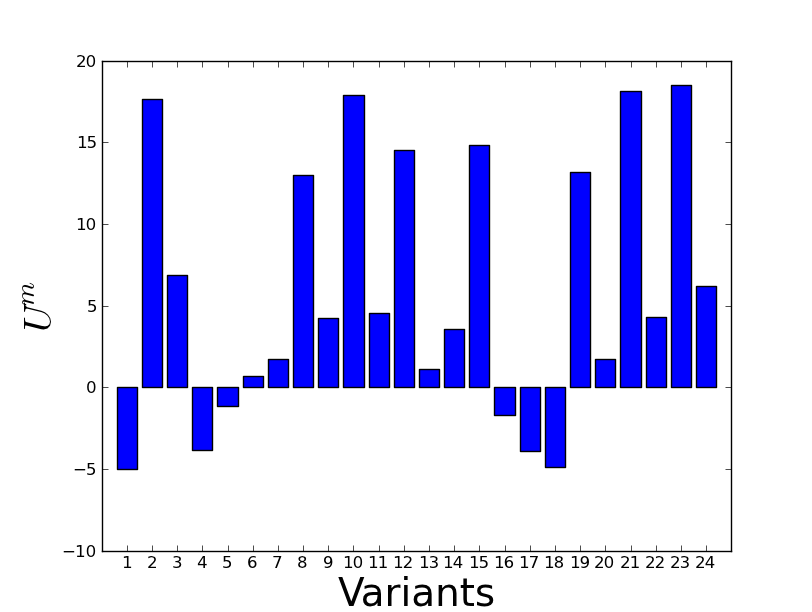


Figure . Exemplary interaction energy distribution for each of twenty-four variants of an austenitic parent grain

In Figure 2, about four variants show nearly equal interaction energies within 10% of difference. Likewise, Figure 3 depicts several clusters of poles indicating the minor difference in misorientaions between certain variants. In the current framework, for each of elasto-visco-plastic computational step, one variant is chosen when the criterion is met. Therefore, according to the interaction energy distribution in Figure 2, the variant 23 will be selected for the current parent austenitic grain. In reality, the previously created martensitic inclusion may have relaxed the surrounding matrix, so the variant selection will be perturbed to some extent. In order to statistically mimic this, a small window of variant selection pool is introduced for those variants whose interaction energy is within:

, where is an empirical parameter to determine.

The variant is randomly picked among those within this statistical range. When is unity, the most strict variant selection criterion is applied while with a lower more relaxed selection is rendered. Determination of is …

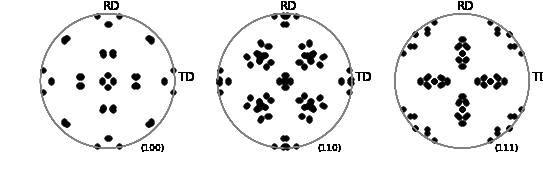


Figure Pole figures of 24 variants of a cube-oriented grain based on WLR orientation relation

## Martensitic transformation kinetics

In the current framework, the polycrystalline aggregate firstly deforms only with austenitic grains, and martensitic grains are created on the fly. For each computational increment, each and every austenitic grain is checked if transformation-starting criterion is met. Currently, when the accumulative total slip shear, , reaches austenitic grain is eligible to transit a part of its volume to a new martensitic grain. The volume of martensite is determined following Olson and Cohen ([Olson & Cohen, 1975](#_ENREF_5_7)). Olson and Cohen (OC) model is in a form of double exponential equation. The volume fraction of martensite, , is expressed as a function of macroscopic strain as shown in, originally designed to reproduce the macroscopic volume evolution of martensite:

|  |  |
| --- | --- |
|  | eq. |

, where and are fitting parameters and is an exponent associated with shear band formation.

OC model is adapted onto the grain level. Instead of the macroscopic strain, total sum of accumulative slip shear, , is used to account for the inhomogeneous activity of each austenitic grain:

For each computational step time, , the volume of newly created martensite should be:

.

In the current framework, only one martensitic grain for each incremental step is inherited from a parent grain. The boundary condition, as of mixed boundary condition of macroscopic velocity gradient and stress, is given incrementally. The computation incremental step is set as axial strain. Therefore, in order to achieve 0.3 macroscopic axial strain, total incremental steps will be: steps. If we generate new martensitic grains for each of steps, the computation will be too much costly.

## Characteristics of newly formed martensitic grain

Newly created martensite in the EVPSC framework should be assigned relevant properties. Some of them are fairly straightforward to obtain based on some models available from the literature: martensitic starting temperature, ; 2) Gibbs free energy where martensite transformation may spontaneously start, ; 3) temperature at which Gibbs free energy of the two phases becomes equivalent, Some of them are subject to estimate based on comparison between simulation results and experimental observations such as the crystal relation option or the statistical window, . On the contrary, there are characteristics that are difficult to figure out, some of which are beyond author’s scope of knowledge. In such cases, determination of the unknown parameters is subject to educative guess. Moreover, considering computational, cost-effective approach is necessary. Especially, in the current case new grains, that were initially not present, are created which significantly consumes a lot of computation resources. In the current section, these issues are discussed and decisions are given.

### Crystal orientation relationship

Crystal orientation of the martensite is dependent on the habit plane and invariant line direction for the case of KS and NW. On the other hand, WLR model, as explained in Bhadeshia, provides a full rotation matrix.

### Morphology of martensitic inclusion

Shape of martensite is either plate-like or lath-like. In the current model, the morphology is assumed to be thin plate-like disc with dictating the three lengths of principal axes. The morphological orientation is determined such that the thinnest axis is parallel to the normal direction of the habit plane.

### Thermo-mechanical characteristics

Thermo-mechanical characteristics associated with the kinetics of martensitic transformation are obtained based on chemical compositions. Use of … models

### Determination of

Determination of p is based on literature survey and its influence on the average number of variants that are activated.

### Transformation strain

There are many different suggestions available in the literature when determining the transformation strain associated with the martensite formation. Among others, Wechsler-Lieberman-Read ([1953](#_ENREF_5_9)) model’s transformation strain as suggested in Bhadeshia ([2001](#_ENREF_5_1)) is used for all considered orientation relationships. Following Bhadeshia ([2001](#_ENREF_5_1)), the transformation strain[[1]](#footnote-2) is calculated based on the lattice parameters in Table 2.

# Benchmark studies

## Cube texture benchmark

Humbert et al. ([2007](#_ENREF_5_3)) showed that there is a evident variant selection mechanism in martensitic transformation using the Kurdjumov-Sachs type variant mechanisms. The same was proved by Kundu and Bhadeshia ([2006](#_ENREF_5_4)) with WLR model. For this reason, EVPSC-TRIP is tested for a cube-textured polycrystal. The cube texture was created by rotation of the ideal cube component with respect to randomly generated reference axis. The created texture is shown in Figure 4.

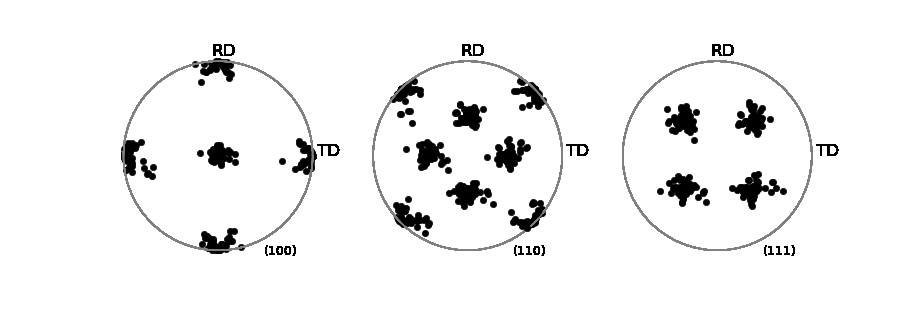


Figure (100), (110) and (111) pole figures of the cube texture based on the Gaussian distribution

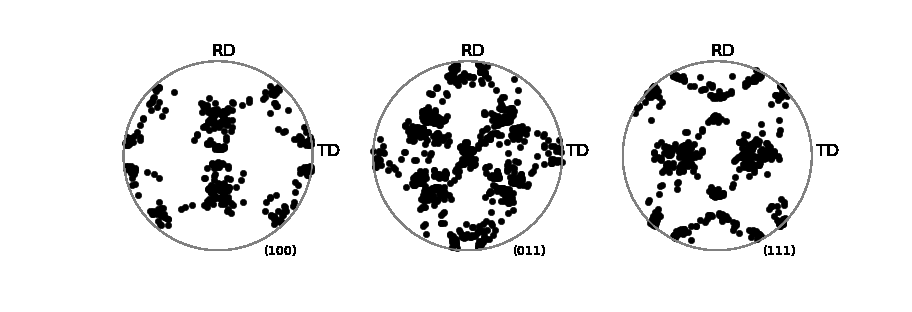


Figure Pole figures of the formed martensite from the cube texture by WLR theory.

## Transformation strain accommodation

When phase transform occurs, austenite undergoes a significant amount of characteristic shear on a characteristic crystallographic plane known as the habit plane. In addition, the dilatation with originated from difference in specific volume of the two phases gives invokes local micro-stress field to the surrounding soft austenitic phase. The characteristic shear together with the dilatation can be expressed in the full tensorial strain. Following Bhadeshia (worked example citation needed), the macroscopic shape strain is calculated based on the lattice parameters of the two phases.

## Stress and strain partitioning

Stress and strain partitioning is discussed.

Parameters that influence the partitioning:

* Slip system hardening parameters
* Transformation strain is taken as ‘additional plastic strain given in martensite’- thus martensite may accommodate a significant amount of plastic strain in total

It should be mentioned here that quantitative analysis is not appropriate in the given framework.

## Internal lattice strain measure (missing experimental data)

* Display only the ‘compact’ figures on the internal strain results
  + May consider putting exhaustive figures in appendix
* May need to compare the cases with or without non-deviatoric transformation strain. (May be in appendix)

# Discussion

# Reference

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* Summary and discussions

# Potentials benefits

## Multi-scale approach and expected role of crystal plasticity for metal forming simulations

## Future applications of crystal plasticity

### Diffraction based internal strain measurement

### Interaction between crystal plasticity and atomic simulations

### Macroscopic manifestation of granular scale mechanisms

# Discussion

* Acknowledgement
* Appendix

1. In the original book of Bhadeshia used the term, *macroscopic* shape strain. In it, the *shape* strain of martensitic grain is referred as the macroscopic strain in comparison to the invariant *lattice* strain. In the current manuscript, the macroscopic scale refers to a bigger scale, i.e., the aggregative one spanning constituting grains collectively. [↑](#footnote-ref-2)