



Peierls-Nabarro Analyzer for DISlocation core structure and slip resistance

MANUAL

Version 1.0.0, March 16, 2018

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<https://sites.google.com/site/zrfbuaa/softwares/pnadis>

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DESIGN AND SIMULATIONS OF ADVANCED STRUCTURAL MATERIALS

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1. Features and history of PNADIS

1.1 Overview

PNADIS is a MATLAB program (only internal), which is designed and organized by Dr. S. H. Zhang and Prof. R. F. Zhang, for calculating the dislocation core structure, Peierls stress, pressure field around dislocation core and solid solution strengthening of a crystal based on the Peierls-Nabarro model and its derived ones. The name of the software comes from the name of the two famous scientist Peierls and Nabarro. To respect their great contribution to the plasticity model of dislocation slip, we name this software as “Peierls-Nabarro Analyzer” for dislocation core structure and slip resistance. PNADIS runs on WINDOWS, LINUX and MAC operating systems with MATLAB installed. Its running needs commercial MATLAB compiler. It is contributed free of charge for non-commercial users who must possess the license of MATLAB software. More details can be found at:

<https://sites.google.com/site/zrfbuaa/software/pnadis>

1.2 Features of PNADIS

The program has implemented the following methods

- 1D Peierls-Nabarro model
- 2D Peierls-Nabarro model
- Dislocation energetic minimization approach
- Force balance approach
- Classical Peierls-Nabarro model
- Semidiscrete Variational Peierls-Nabarro model
- Peierls stress

- Pressure field around dislocation core
- Solid solution strengthening
- etc.

1.3 Version history

v_1.0.0

(2018.3.16)

- 1D Peierls-Nabarro model
- 2D Peierls-Nabarro model
- Dislocation energetic minimization approach
- Force balance approach
- Classical Peierls-Nabarro model
- Semidiscrete Variational Peierls-Nabarro model
- Peierls stress
- Pressure field around dislocation core
- Solid solution strengthening
- etc.

Further development

- Modified SVPN model considering gradient energy
- Nonlocal SVPN model
- etc.

2. Getting started

2.1 How to obtain PNADIS

PNADIS is an open source code and can be downloaded at:

<https://sites.google.com/site/zrfbuaa/software/pnadis>

2.2 Necessary citations

Whenever using PNADIS in all publications and reports, you must cite the original papers, for example, in the following way:

Dislocation core structure, Peierls stress, pressure field around dislocation core and solid solution strengthening were calculated using the PNADIS code [1], based on the Semidiscrete Variational Peierls-Nabarro model and Nabarro-Labusch-Leyson solid solution strengthening model.

2.3. How to install PNADIS

Before install and run PNADIS code, MATLAB version 2015a or later is required. After you download the archive with PNADIS, you need to unpack it and the current directory is PROJECT_SOURCE_DIR. Run the following command in the MATLAB to install PNADIS:

```
>> run PROJECT_SOURCE_DIR/PNADIS_x.x.x/src/install.m
```

Note that the installer may require root privileges.

2.3 How to run PNADIS

To set up your calculation, find an example in the folder PROJECT_SOURCE_DIR/PNADIS_x.x.x/example (see Appendix 7.1 for a list

of example), which is similar to what you want to do, and start by editing the input file `infile.m`. Then move the `infile.m` file to the folder `INFILE_DIR` and run the PNADIS as follows:

- Run PNADIS in the MATLAB on the Windows/Linux/Mac

```
>> cd INFILE_DIR
```

```
>> PNADIS
```

- Run PNADIS on the cluster

```
$ cd INFILE_DIR
```

```
$ nohup matlab -r PNADIS > output.log &
```

3. Theoretical background

For this section, one may refer to our publication: S. H. Zhang, D. Legut and R. F. Zhang, PNADIS: automatic Peierls-Nabarro Analyzer for DISlocation core structure and slip resistance, in preparation.

4. Overview of input and output files

4.1 Input files

- *script* **infile.m**

Meaning: thoroughly described in Section 5.

4.2 Output files

>>> For both 1D and 2D P-N models

- *data* **pnadis.mat**

Meaning: all the input and output parameters. The input and output parameters are thoroughly described in Sections 5 and 6, respectively.

- *figure* **fitgamma.fig**

Variable: U_x , (U_z) , SFE and SFEfit

Meaning: the result of fitting γ -surface or generalized stacking fault energy (GSFE).

- *figure* **pressurefield.fig**

Variable: pressure_latxz_mis, pressure_latyy_mis and pressfld

Meaning: the result of position-dependent pressure field around dislocation core, only for `Pressure_Field='TRUE'`.

- *figure* **pnstress.fig**

Variable: upn, Epn, and strpn

Meaning: the result of Peierls energy barrier (Epn) and Peierls stress (strpn) as a function of the position (upn), only for `pnstrmethod=2`.

>>> Only for 1D P-N model○ *figure* **restoring_force.fig**

Variable: Uxdata, RestoringForce

Meaning: the result of restoring force, which is obtained by deriving the GSFE calculated *ab initio*.

○ *figure* **fitrestoringforce.fig**

Variable: Uxdata, RestoringForce and RestoringForcefit

Meaning: the result of the least square minimization of the difference between the elastic resistance F_{EL} and restoring force $\tau[u(x)]$ to determine the dislocation core structure via 1D P-N model.

○ *figure* **misdens.fig**

Variable: xmis, misfit and misdens

Meaning: the results of dislocation core structure, including disregistry (misfit) and misfit density (misdens).

>>> Only for 2D P-N model○ *figure* **gammafiterror.fig**

Variable: Ux, Uz and gammafiterror

Meaning: the difference (gammafiterror) between the fitting and initial GSFE data vs. Ux and Uz.

○ *figure* **misfit.fig**

Variable: xmis, misfit_x_axis and misfit_z_axis

Meaning: the results of dislocation core structure including the components of disregistry along x and z axes.

- *figure* **misdens.fig**

Variable: xmis, misdens_x_axis and misdens_z_axis

Meaning: the results of dislocation core structure including the components of misfit density along x and z axes.

- *figure* **Einteraction_[eb]_[es].fig**

Variable: pressfld_latxz, pressfld_latyy and Einact_plot

Meaning: the result of position-dependent solute/dislocation interaction energy as the volumetric and slip misfit parameters are equal to [eb] and [es] respectively, only for `Einteraction_Plot='TRUE'`.

5. Input options: The `input.m` file

5.1 All input parameters (or at least most)

Here is a short overview of all input parameters currently supported in PNADIS code, together with a short description and the default value.

Name	Description	Default Value
system	System name	-
filepath	The absolute path to save the result files	pwd
misdim	The dimension of P-N model: 1D or 2D	-
Dislocation_Core_Structure	Calculating the dislocation core structure or NOT	TRUE
Ux, Uz, SFE	The data of GSFE and normalized disregistry vector	-
Nmis	Which trial function of disregistry vector to employ	1D P-N model: 3 2D P-N model: 0
mis_1st	Considering the first-order approximation in the trial function of disregistry vector or NOT	FALSE
BurVect	The value of Burgers vector	-
shear_modulus, poisson_ratio	The values of shear modulus and Poisson's ratio	-
mistype	The dislocation type: edge or screw	e
fitcut	Which GSFE fitting function to employ	0
pnmode	Mode of P-N models: CCPN or SVPN	1
Inpas	Interplanar distance Δx	-
dax	The reference position x_m is defined as $x_m = m\Delta x + dax$ for SVPN model ($m=0, \pm 1, \pm 2, \dots, \pm \infty$)	-
Xcoef_range, Xdist_range, Xwid_range, Xalpha_range, dx_range	Matrix of the lower and upper bounds, and initial values of each unknown variable	-
minimethod	The minimization method for 2D P-N model: PSO or GA	2d_PSO
fitmethod	The method for fitting the restoring force	1d_lsq_curvefit
PopulationSize, MaxIterations	Size of the population and maximum number of iteration for PSO and GA	1000
Peierls_Stress	Calculating the Peierls stress or NOT	FALSE
pnstrmethod	The method to calculate the Peierls stress	2
Pressure_Field	Calculating the pressure field or NOT	FALSE
pressfld_latxz, pressfld_latyy	The lattice matrix for pressure field	-
dis_component_xz	Which component of the dislocation to calculate: x or z	x
Solution_Strengthening	Calculating the solid solution strengthening or NOT	FALSE
Einteraction_Plot	Plotting the position-dependent solute/dislocation interaction energy or NOT	FALSE
eb_input, es_input	The input volumetric misfit and slip misfit parameters	-
LatC_spacing	The interlayer spacing along FCC [111] or HCP [0001] direction	-
coefV	The coefficient to calculate the extra volume	-

<code>wc_range</code>	Matrix of the lower and upper bounds to search the characteristic bow-out distance w_c	[0, 50]
<code>solute_concentration</code>	Concentration of solute atom	1.0000

5.2 Type of run and system

○ variable **system**

Meaning: System name. (STRING) The **system** variable is for the user only and should help the user to identify what he wants to do with this specific input file. Help yourself and be as verbose as you can.

Default: no default.

Format: `system='PNADIS'`

○ variable **filepath**

Meaning: The absolute path to save the result files. (STRING)

Default: `pwd`

Format: `filepath='INFILE_DIR'`

○ variable **misdim**

Meaning: the dimension of P-N model. (INT)

Possible values:

- 1 ----- 1D Peierls-Nabarro model
- 2 ----- 2D Peierls-Nabarro model

Default: no default.

Format: `misdim=1`

5.3 The calculation of dislocation core structure

○ variable **Dislocation_Core_Structure**

Meaning: Calculating the dislocation core structure or NOT. (STRING)

Possible values

- TRUE ----- calculate the dislocation core structure
- FALSE ----- NOT calculate the dislocation core structure, and it is also able to continue calculating the Peierls stress, pressure field and solid solution strengthening on the basis of the previous results of dislocation core structure by loading the `pnadis.mat` file, instead of calculating the dislocation core structure once again.

Default: TRUE

Format: `Dislocation_Core_Structure='TRUE'`

○ variable **Ux, Uz** and **SFE**

Meaning: The data of generalized stacking fault energy (unit: J/m^2) and normalized disregistry vector (unit: 1). (MATRIX)

Default: no default

○ variable **Nmis**

Meaning: Which trial function of disregistry vector to employ. (INT)

Possible values:

- -1 ----- the trial function of

$$u_x(x) = \frac{b}{2\pi} \left(\alpha_1 \tan^{-1} \frac{x-(d_x/2-\Delta d_x)}{\omega_x} + \alpha_2 \tan^{-1} \frac{x-d_x/2}{\omega_x} + \alpha_3 \tan^{-1} \frac{x-(d_x/2+\Delta d_x)}{\omega_x} \right. \\ \left. + \alpha_4 \tan^{-1} \frac{x+(d_x/2-\Delta d_x)}{\omega_x} + \alpha_5 \tan^{-1} \frac{x+d_x/2}{\omega_x} + \alpha_6 \tan^{-1} \frac{x+(d_x/2+\Delta d_x)}{\omega_x} \right) + \frac{b}{2},$$

$$u_z(x) = \frac{\sqrt{3}b}{6\pi} \left(\beta_1 \tan^{-1} \frac{x-(d_z/2-\Delta d_z)}{\omega_z} + \beta_2 \tan^{-1} \frac{x-d_z/2}{\omega_z} + \beta_3 \tan^{-1} \frac{x-(d_z/2+\Delta d_z)}{\omega_z} \right. \\ \left. + \beta_4 \tan^{-1} \frac{x+(d_z/2-\Delta d_z)}{\omega_z} + \beta_5 \tan^{-1} \frac{x+d_z/2}{\omega_z} + \beta_6 \tan^{-1} \frac{x+(d_z/2+\Delta d_z)}{\omega_z} \right)$$

including only two triplet partial dislocations, will be employed. $u_x(x)$ and $u_z(x)$ are the components of the partial dislocations along the x and z axes, respectively. The amplitudes α_i and β_i must satisfy the conditions $\sum_{i=1}^3 \alpha_i = \sum_{i=4}^6 \alpha_i = 1$ and $\sum_{i=1}^3 \beta_i = -\sum_{i=4}^6 \beta_i = 1$, respectively. It is able to obtain only for 2D Peierls-Nabarro model.

- 0 ----- the trial function of

$$u_x(x) = \frac{b}{2\pi} \left(\tan^{-1} \frac{x-d_x/2}{\omega_x} + \tan^{-1} \frac{x+d_x/2}{\omega_x} \right) + \frac{b}{2},$$

$$u_z(x) = \frac{\sqrt{3}b}{6\pi} \left(\tan^{-1} \frac{x-d_z/2}{\omega_z} - \tan^{-1} \frac{x+d_z/2}{\omega_z} \right),$$

including only two single partial dislocations, will be employed. It is able to obtain only for 2D Peierls-Nabarro model.

- ≥ 1 ----- the generalized trial function of

$$u(x) = \frac{b}{\pi} \sum_{i=1}^N \alpha_i \tan^{-1} \frac{x-d_i}{\omega_i},$$

will be employed with N partial dislocations. It is able to obtain for both 1D and 2D Peierls-Nabarro models. α_i , d_i and ω_i are variational constants, and b is the Burgers vector. The normalization of $u(x)$ requires that $\sum_{i=1}^N \alpha_i = 1$ and

$\sum_{i=1}^N \alpha_i = 0$ for the directions along the Burgers vector (x axis) and perpendicular

to the Burgers vector within the slip plane (z axis), respectively.

Default: 3 for 1D Peierls-Nabarro model; 0 for 2D Peierls-Nabarro model

Format: `Nmis=0`

○ variable **mis_1st**

Meaning: Considering the first-order approximation in the trial function of disregistry vector or NOT, only for 1D Peierls-Nabarro model. (STRING)

Possible values:

- TRUE ----- consider the first-order approximation in the trial function of disregistry vector, *i.e.* the trial function of

$$u(x) = \frac{b}{\pi} \sum_{i=1}^N \alpha_i \left[\tan^{-1} \frac{x-d_i}{c_i \omega_i} + (1-c_i) \frac{\omega_i (x-d_i)}{(x-d_i)^2 + (c_i \omega_i)^2} \right],$$

will be employed with **Nmis**=N partial dislocations.

- FALSE ----- NOT consider the first-order approximation in the trial function of disregistry vector.

Default: FALSE

Format: `mis_1st='FALSE'`

○ variable **BurVect**

Meaning: the value of Burgers vector (unit: Å). (FLOAT)

Default: no default

○ variable **shear_modulus** and **poisson_ratio**

Meaning: The values of shear modulus (unit: GPa) and Poisson's ratio (unit: 1).
(FLOAT)

Default: no default

○ variable **mistype**

Meaning: the dislocation type, *i.e.* edge or screw dislocation. (CHAR)

Possible values:

- e ----- edge dislocation
- s ----- screw dislocation

Default: e

Format: `mistype='e'`

○ variable **fitcut**

Meaning: Which GSFE fitting function to employ. (INT)

Possible values:

- -1 ----- The GSFE fitting function of

$$\begin{aligned} \gamma(u_x, u_z) = & c_0 + c_1 [\cos(2qu_z) + \cos(pu_x + qu_z) + \cos(-pu_x + qu_z)] \\ & + c_2 [\cos(2pu_x) + \cos(pu_x + 3qu_z) + \cos(-pu_x + 3qu_z)] \\ & + c_3 [\cos(4qu_z) + \cos(2pu_x + 2qu_z) + \cos(pu_x - 2qu_z)], \\ & + a_1 [\sin(pu_x - qu_z) - \sin(pu_x + qu_z) + \sin(2qu_z)] \\ & + a_2 [\sin(2pu_x - 2qu_z) - \sin(2pu_x + 2qu_z) + \sin(4qu_z)] \end{aligned}$$

will be employed. $p=2\pi/a_x$ and $q=2\pi/a_z$. It is able to obtain only for 2D Peierls-Nabarro model.

- 0 ----- The GSFE fitting function of

$$\begin{aligned}
\gamma(u_x, u_z) = & c_0 + c_1 [\cos(2qu_z) + \cos(pu_x + qu_z) + \cos(-pu_x + qu_z)] \\
& + c_2 [\cos(2pu_x) + \cos(pu_x + 3qu_z) + \cos(-pu_x + 3qu_z)] \\
& + c_3 [\cos(4qu_z) + \cos(2pu_x + 2qu_z) + \cos(pu_x - 2qu_z)] \\
& + c_4 \left[\begin{aligned} & \cos(3pu_x + qu_z) + \cos(3pu_x - qu_z) + \cos(2pu_x + 4qu_z) \\ & + \cos(2pu_x - 4qu_z) + \cos(pu_x + 5qu_z) + \cos(-pu_x + 5qu_z) \end{aligned} \right], \\
& + a_1 [\sin(pu_x - qu_z) - \sin(pu_x + qu_z) + \sin(2qu_z)] \\
& + a_2 [\sin(2pu_x - 2qu_z) - \sin(2pu_x + 2qu_z) + \sin(4qu_z)]
\end{aligned}$$

will be employed for 2D Peierls-Nabarro model, and the GSFE fitting function of

$$\begin{aligned}
\gamma(u_x) = & c_0 + c_1 \cos(pu_x) + a_1 \sin(pu_x) + c_2 \cos(2pu_x) + a_2 \sin(2pu_x) \\
& + c_3 \cos(3pu_x) + a_3 \sin(3pu_x) + c_4 \cos(4pu_x) + a_4 \sin(4pu_x), \\
& + c_5 \cos(5pu_x) + a_5 \sin(5pu_x)
\end{aligned}$$

will be employed for 1D Peierls-Nabarro model. It is able to obtain for both 1D and 2D Peierls-Nabarro model

- ≥ 1 ----- The generalized fitting function of

$$\gamma(u) = \sum_G c_G \exp[iGu],$$

will be employed with a plane-wave cutoff $k=\text{fitcut}$. $G = m \frac{2\pi}{a_x}$ and

$G = (m \frac{2\pi}{a_x}, n \frac{2\pi}{a_z})$ for 1D and 2D γ -surface, respectively, $m, n = 0, \pm 1, \pm 2, \dots, \pm \infty$,

and a_x and a_z are the lengths of one period along x and z axes, respectively. It is

able to obtain for both 1D and 2D Peierls-Nabarro model

Default: 0

Format: `fitcut=0`

- variable **pnmode**

Meaning: Mode of Peierls-Nabarro models, only for 2D Peierls-Nabarro model. (INT)

Possible values:

- 1 ----- Classical continuum Peierls-Nabarro model
- 2 ----- Semidiscrete variational Peierls-Nabarro model

Default: 1

Format: `pnmode=1`

○ variable **Inpas**

Meaning: Interplanar distance Δx (unit: Å), only for the Semidiscrete Variational Peierls-Nabarro model and the calculation of Peierls stress. (FLOAT)

Default: no default

○ variable **dax**

Meaning: The reference position x_m will be defined as $x_m = m\Delta x + dax$ ($m=0, \pm 1, \pm 2, \dots, \pm\infty$) (unit: Å), only for Semidiscrete Variational P-N model. (FLOAT)

Default: no default

○ variable **Xcoef_range, Xdist_range, Xwid_range, Xalpha_range, dx_range**

Meaning: Matrix of the lower and upper bounds, and initial values of each unknown variable. (1×3 MATRIX). The parameter of **Xalpha_range** is necessary only for `mis_1st='TRUE'`, and the parameter of **dx_range** is necessary only for `Nmis=-1`.

Default:

- For 1D Peierls-Nabarro model

`Xcoef_range=[0.0000, 1.0000, 1/Nmis];`

`Xdist_range=[-50.0000, 50.0000, 0.0000];`

`Xwid_range=[0.0000, 10.0000, 5.0000];`

```
Xalpha_range=[ 0.0000, 2.0000, 1.0000];
```

- For 2D Peierls-Nabarro model

```
Xcoef_range=[ 0.0000, 1.0000, 0.5000];
```

```
Xdist_range=[-50.0000, 50.0000, 0.0000];
```

```
Xwid_range=[ 0.0000, 5.0000, 1.0000];
```

```
dx_range=[ -5.0000, 5.0000, 0.0000];
```

Format: `Xcoef_range`=[Lower bound, Upper bound, StartPoint]

NOTE: The lower and upper bounds, and the initial values of these variational constants are very crucial for whether the global minimum could be found.

○ variable **minimethod**

Meaning: The minimization method only for 2D Peierls-Nabarro model. (STRING)

Possible values:

- 2d_PSO ----- Particle swarm optimization method
- 2d_GA ----- Genetic algorithm method

Default: 2d_PSO

Format: `minimethod`=' 2d_PSO'

○ variable **fitmethod**

Meaning: The method for fitting the restoring force via least square minimization, only for 1D Peierls-Nabarro model. (STRING)

Possible values:

- 1d_fitting_toolbox ----- The fitting toolbox of MATLAB
- 1d_lsqr_curvefit ----- The `lsqrcurvefit` function of MATLAB

Default: 1d_lsqr_curvefit

Format: `fitmethod='1d_lsq_curvefit'`

○ variable **PopulationSize, MaxIterations**

- *Meaning:* Size of the population and maximum number of iterations before the algorithm halts in the particle swarm optimization and genetic algorithm methods only for 2D Peierls-Nabarro model. (INT)

Default: 1000 for both PopulationSize and MaxIterations

5.4 The calculation of Peierls stress

○ variable **Peierls_Stress**

Meaning: Calculating the Peierls stress or NOT. (STRING)

Possible values:

- TRUE ----- calculate the Peierls stress
- FALSE ----- NOT calculate the Peierls stress

Default: FALSE

Format: `Peierls_Stress='FALSE'`

○ variable **pnstrmethod**

Meaning: The method to calculate the Peierls stress, only for

`Peierls_Stress='TRUE'`. (INT)

Possible values:

- 1 ----- Analytical formula

- 2 ----- Discrete dislocation energy approach

Default: 2

Format: pnstrmethod=2

5.5 The calculation of pressure field around dislocation core

- variable **Pressure_Field**

Meaning: Calculating the pressure field around dislocation core or NOT. (STRING)

Possible values:

- TRUE ----- calculate the pressure field around dislocation core
- FALSE ----- NOT calculate the pressure field around dislocation core

Default: FALSE

Format: Pressure_Field='FALSE'

- variable **pressfld_latxz, pressfld_latyy**

Meaning: The lattice matrix (unit: Å) for calculating the pressure field around dislocation core, only for Pressure_Field='TRUE' or Solution_Strengthening='TRUE'. (MATRIX)

Default: no default

NOTE: several examples of **pressfld_latxz** and **pressfld_latyy** are provided for FCC (111)[1-10] dislocation and HCP (0001)[11-20] dislocation.

- For edge dislocation of FCC and HCP structures

```
[pressfld_latxz,pressfld_latyy]=meshgrid(-(7+1/4)*BurVect:(1/2*BurVect):(7+1/4)*BurVect,...
                                          -(14+1/2)*LatC_spacing:LatC_spacing:(14+1/2)*LatC_spacing);
```

- For screw dislocation of FCC structure

```

pressfld_latxz=sqrt(3)*repmat([- (7+1/4)*BurVect:(1/2*BurVect):(7+1/4)*BurVect;...
                                - (7+7/12)*BurVect:(1/2*BurVect):(6+11/12)*BurVect;...
                                - (7+5/12)*BurVect:(1/2*BurVect):(7+1/12)*BurVect],10,1);
pressfld_latyy=repmat([- (14+1/2)*LatC_spacing:LatC_spacing:(14+1/2)*LatC_spacing]',1,30);

```

- For screw dislocation of HCP structure

```

pressfld_latxz=sqrt(3)*repmat([- (7+1/4)*BurVect:(1/2*BurVect):(7+1/4)*BurVect;...
                                - (7+5/12)*BurVect:(1/2*BurVect):(7+1/12)*BurVect],15,1);
pressfld_latyy=repmat([- (14+1/2)*LatC_spacing:LatC_spacing:(14+1/2)*LatC_spacing]',1,30);

```

- variable **dis_component_xz**

Meaning: Which component of the dislocation to calculate the pressure field around dislocation core, only for 2D Peierls-Nabarro model and Pressure_Field='TRUE'. (CHAR)

Possible values:

- x ----- the component along x axis
- z ----- the component along z axis

Default: x

Format: dis_component_xz='x'

5.6 The calculation of solid solution strengthening

- variable **Solution_Strengthening**

Meaning: Calculating the solid solution strengthening or NOT. (STRING)

Possible values:

- TRUE ----- calculate the solid solution strengthening
- FALSE ----- NOT calculate the solid solution strengthening

Default: FALSE

Format: Solution_Strengthening='FALSE'

NOTE: only FCC (111)[1-10] dislocation and HCP (0001)[11-20] dislocation are supported in the present version.

○ variable **Einteraction_Plot**

Meaning: Plotting the position-dependent solute/dislocation interaction energy or NOT, only for `Solution_Strengthening='TRUE'`. The plotted figures will be save to `Einteraction_[eb]_[es].fig.` (STRING)

Possible values:

- TRUE ----- plot the position-dependent solute/dislocation interaction energy
- FALSE ----- NOT plot the position-dependent solute/dislocation interaction energy

Default: FALSE

Format: `Einteraction_Plot='FALSE'`

○ variable **eb_input, es_input**

Meaning: The input volumetric misfit (`eb_input`, unit: 1) and slip misfit (`es_input`, unit: 1) parameters, only for `Solution_Strengthening='TRUE'`. (FLOAT or MATRIX)

Default: no default

○ variable **LatC_spacing**

Meaning: The interlayer spacing along FCC [111] or HCP [0001] direction (unit: Å), only for `Solution_Strengthening='TRUE'`. (FLOAT)

Default: no default

- variable **coefV**

Meaning: The coefficient to calculate the extra volume introduced by the solute atom, i.e. $\Delta V = \text{coefV} \cdot \varepsilon_b$ (unit: \AA^3), only for `Solution_Strengthening='TRUE'`. (FLOAT)

Default: no default

- variable **wc_range**

Meaning: Matrix of the lower and upper bounds to search the characteristic bow-out distance w_c (unit: \AA), only for `Solution_Strengthening='TRUE'`. (1×2 MATRIX)

Format: `wc_range=[Lower bound, Upper bound]`

Default: [0, 50]

- variable **solute_concentration**

Meaning: Concentration of solute atom (unit: 1), only for `Solution_Strengthening='TRUE'`. (FLOAT)

Default: 1.0000

6. Output options: The `pnadis.mat` file

6.1 All output parameters (or at least most)

Here is a short overview of all output parameters currently supported in PNADIS code, together with a short description.

Name	Description
SFEfit	The fitting data of γ -surface or GSFE
gammafitresult	The result of fitting γ -surface or GSFE (MATLAB FUNCTION)
gammafiterror	The difference between the fitting and initial GSFE data
Uxdata, RestoringForce, RestoringForcefit	The data of restoring force and its fitting value
xmis, misfit, misdens	The normalized disregistry and misfit density
lb, ub, InitialPopulationMatrix	The lower bound, upper bound and initial population for PSO and GA
xmis, misfit_x_axis, misfit_z_axis	The components of normalized disregistry along x and z axes
misdens_x_axis, misdens_z_axis	The components of misfit density along x and z axes
str_is, half_width, str_pn_narrow, str_pn_wide	The ideal slide stress, half width of dislocation, and the Peierls stress of narrow and wide dislocation
upn, Epn, strpn	The Peierls energy barrier and Peierls stress
pressure_latxz_mis, pressure_latyy_mis, pressfld	The position-dependent pressure field around dislocation core
Einact_plot	The position-dependent solute/dislocation interaction energy
wc, Ebarrier, crss0	The characteristic bow-out distance, the predicted energy barrier and corresponding CRSS at 0K for solid solution strengthening

6.2 The output parameters

- variable **SFEfit**:

Meaning: the fitting data of γ -surface or GSFE (unit: J/m²).

- variable **gammafitresult**

Meaning: the result of fitting γ -surface or GSFE. (MATLAB FUNCTION)

- variable **gammafiterror**

Meaning: The difference between the fitting and initial GSFE data (unit: J/m²).

- variable **Uxdata**, **RestoringForce**, **RestoringForcefit**

Meaning: the data of restoring force and its fitting value (unit: GPa).

- variable **xmis**, **misfit**, **misdens**

Meaning: the calculated normalized disregistry (unit: 1) and misfit density (unit: 1), only for 1D Peierls-Nabarro model.

- variable **lb**, **ub**, **InitialPopulationMatrix**

Meaning: the lower bound, upper bound and initial population used to seed for the particle swarm optimization and genetic algorithm, only for 2D Peierls-Nabarro model. It is generated based on the values of **Xcoef_range**, **Xdist_range**, **Xwid_range**, **Xalpha_range** and **dx_range**.

- variable **xmis**, **misfit_x_axis**, **misfit_z_axis**

Meaning: the calculated components of normalized disregistry along x and z axes (unit: 1), only for 2D Peierls-Nabarro model.

- variable **misdens_x_axis**, **misdens_z_axis**

Meaning: the calculated components of misfit density along x and z axes (unit: 1), only for 2D Peierls-Nabarro model.

- variable **str_is**, **half_width**, **str_pn_narrow**, **str_pn_wide**

Meaning: the calculated ideal slide stress (unit: GPa), half width of dislocation (unit: Å) and the Peierls stress of narrow and wide dislocation (unit: MPa), only for `pnstrmethod=1`.

- variable **upn**, **Epn**, **strpn**

Meaning: the calculated Peierls energy barrier (unit: $\times 10^{-10}$ J/m) and Peierls stress (unit: MPa), only for `pnstrmethod=2`.

- variable **pressure_latxz_mis**, **pressure_latyy_mis**, **pressfld**

Meaning: the calculated position-dependent pressure field around dislocation core (unit: GPa).

- variable **Einact_plot**

Meaning: the calculated position-dependent solute/dislocation interaction energy (unit: eV), only for `Einteraction_Plot='TRUE'`.

- variable **wc**, **Ebarrier**, **crss0**

Meaning: the characteristic bow-out distance (**wc**, unit: Å), the predicted energy barrier (**Ebarrier**, unit: eV) and corresponding CRSS (**crss0**, unit: MPa) at 0K for solid solution strengthening.

7. Appendices

7.1 List of Examples

>>> 1d_PN_model

- infile_1d_Al
- infile_1d_Pd
- infile_1d_Pd_pnmethod=1
- infile_1d_Mg2SiO4_110_001
- infile_1d_Mg2SiO4_110_111
- infile_1d_MgSiO3
- infile_1d_Si_Glide
- infile_1d_Si_Shuffle
- infile_1d_SrTiO3_100_011
- infile_1d_SrTiO3_110_001
- infile_1d_SrTiO3_110_-110

>>> 2d_PN_model

- infile_2d_Ag
- infile_2d_Al
- infile_2d_Cu
- infile_2d_Mg
- infile_2d_Ti
- infile_2d_Zn

>>> Pressure Field

- infile_2d_Al_edge_x

- infile_2d_Al_edge_z
- infile_2d_Al_screw_x
- infile_2d_Al_screw_z

>>> Solution strengthening

- infile_2d_Al_edge
- infile_2d_Al_screw
- infile_2d_Mg_conf.1
- infile_2d_Mg_conf.2

7.2 Sample infile.m files

>>> For the 1D Peierls-Nabarro model

```
% -----
% Script: infile_1d
% -----
% Aim:
% one example of infile.m file for 1D P-N model
% -----

% % System name

system='1D P-N model';

% % The absolute path to save the result files

filepath=pwd;

% % The dimension of P-N model: 1 or 2

misdim=1;

%% -----
%% The Parameters for the calculation of dislocation core structure
%% -----

% % Calculating the dislocation core structure ('TRUE') or NOT ('FALSE')

Dislocation_Core_Structure='TRUE';

% % The data of GSFE (unit: J/m2) and normalized disregistry vector (unit:1)

Ux=[];
SFE=[];

% % Which trial function of disregistry vector to employ (>=1)

Nmis=6;

% % Considering the first-order approximation in the trial function of disregistry
% vector (1) or NOT (0)
```

```

mis_1st=0;

% % The value of Burgers Vector (unit: A)

BurVect=[];

% % The values of shear modulus (unit: GPa) and Poisson's ratio (unit: 1)

shear_modulus=[];
poisson_ratio=[];

% % The dislocation type: edge ('e') or screw ('s')

mistype='e';

% % Which GSFE fitting function to employ (>=0)

fitcut=0;

% % Matrix of the lower and upper bounds, and initial values of each unknown
%   variable ([Lower bound, Upper bound, StartPoint])

Xcoef_range=[ 0.0000, 1.0000, 1/Nmis];
Xdist_range=[-50.0000, 50.0000, 0.0000];
Xwid_range =[ 0.0000, 10.0000, 5.0000];
Xalpha_range=[ 0.0000, 2.0000, 1.0000];

% % The method for fitting the restoring force: "ld_fitting_toolbox" or "ld_lsq_curvefit"

fitmethod='ld_fitting_toolbox';

%% -----
% The Parameters for the calculation of Peierls stress
% -----

% % Calculating the Peierls stress ('TRUE') or NOT ('FALSE')

Peierls_Stress='TRUE';

% % The method to calculate the Peierls stress: 1 or 2

pnstrmethod=1;

% % Interplanar distance  $\Delta x$  (unit: A)

Inpas=BurVect;

%% -----
% The Parameters for the calculation of pressure field around dislocation core
% -----

% % Calculating the pressure field around dislocation core ('TRUE') or NOT ('FALSE')

Pressure_Field='TRUE';

% % The lattice matrix for pressure field

% pressfld_latxz=[];
% pressfld_latyy=[];

```

>>> For the 2D Peierls-Nabarro model

```

% -----
% Script: infile_2d
% -----
% Aim:
% one example of infile.m file for 2D P-N model
% -----

% System name

```

```

system='2d P-N model';

% The absolute path to save the result files

filepath=pwd;

% The dimension of P-N model: 1 or 2

misdim=2;

%% -----
% The Parameters for the calculation of dislocation core structure
% -----

% % Calculating the dislocation core structure ('TRUE') or NOT ('FALSE')

Dislocation_Core_Structure='TRUE';

% % the data of GSFE (unit: J/m2) and normalized disregistry vector (unit: 1)

[Ux,Uz]=meshgrid(0:0.1:1,0:0.0666:1);
SFE=[];

% % Which trial function of disregistry vector to employ (>=-1)

Nmis=0;

% % The value of Burgers vector (unit: A)

BurVect=[];

% % The values of shear modulus (unit: GPa) and Poisson's ratio (unit: 1)

shear_modulus=[];
poisson_ratio=[];

% % The dislocation type: edge ('e') or screw ('s')

mistype='e';

% % Which GSFE fitting function to employ (>=-1)

fitcut=0;

% % Mode of P-N models: CCPN (1) or SVPN (2)

pnmode=1;

% % Interplanar distance  $\Delta x$  (unit: A)

Inpas=[];

% % The reference position  $x_m$  is defined as  $x_m=m\Delta x+dax$  for SVPN model
% (m=0,  $\pm 1$ ,  $\pm 2$ , ...,  $\pm \infty$ )

dax=0.5;

% % Matrix of the lower and upper bounds, and initial values of each unknown
% variable ([Lower bound, Upper bound, StartPoint])

Xcoef_range=[ 0.0000, 1.0000, 0.5000];
Xdist_range=[-50.0000, 50.0000, 0.0000];
Xwid_range=[ 0.0000, 5.0000, 1.0000];
dx_range=[ -5.0000, 5.0000, 0.0000];

% % The minimization method for 2D P-N model: PSO ('2d_PSO') or GA ('2d_GA')

minimethod='2d_PSO';

% % PSO or GA Parameters

% % % Size of the population and maximum number of iteration

PopulationSize=100;
MaxIterations=1000;

```

```

%% -----
% The Parameters for the calculation of Peierls stress
% -----

    % % Calculating the Peierls stress ('TRUE') or NOT ('FALSE')

    Peierls_Stress='TRUE';

    % % The method to calculate the Peierls stress: 1 or 2

    pnstrmethod=2;

    % % Interplanar distance  $\Delta x$  (unit: A)

    % Inpas=BurVect;

%% -----
% The Parameters for the calculation of pressure field around dislocation core
% -----

    % % Calculating the pressure field around dislocation core ('TRUE') or NOT ('FALSE')

    Pressure_Field='TRUE';

    % % The lattice matrix for pressure field

    pressfld_latxz=[];
    pressfld_latyy=[];

    % % % >>> For edge dislocation of FCC and HCP structures

    % LatC_spacing=sqrt(2/3)/2*BurVect;
    % [pressfld_latxz,pressfld_latyy]=meshgrid(-(7+1/4)*BurVect:(1/2*BurVect):(7+1/4)*BurVect,...
    %                                     -(14+1/2)*LatC_spacing:LatC_spacing:(14+1/2)*LatC_spacing);

    % % % >>> For screw dislocation of FCC structure

    % pressfld_latxz=sqrt(3)*repmat(-(7+1/4)*BurVect:(1/2*BurVect):(7+1/4)*BurVect;...
    %                               -(7+7/12)*BurVect:(1/2*BurVect):(6+11/12)*BurVect;...
    %                               -(7+5/12)*BurVect:(1/2*BurVect):(7+1/12)*BurVect],10,1);
    % pressfld_latyy=repmat(-(14+1/2)*LatC_spacing:LatC_spacing:(14+1/2)*LatC_spacing]',1,30);

    % % % >>> For screw dislocation of HCP structure

    % pressfld_latxz=sqrt(3)*repmat(-(7+1/4)*BurVect:(1/2*BurVect):(7+1/4)*BurVect;...
    %                               -(7+5/12)*BurVect:(1/2*BurVect):(7+1/12)*BurVect],15,1);
    % pressfld_latyy=repmat(-(14+1/2)*LatC_spacing:LatC_spacing:(14+1/2)*LatC_spacing]',1,30);

    % % Which component of the dislocation to calculate: x or z

    dis_component_xz='x';

%% -----
% The Parameters for the calculation of solid solution strengthening
% -----

    % % Calculating the solid solution strengthening ('TRUE') or NOT ('FALSE')

    Solution_Strengthening='TRUE';

    % % Plotting the position-dependent solute/dislocation interaction energy
    % ('TRUE') or NOT ('FALSE')

    Einteraction_Plot='TRUE';

    % % The input volumetric misfit (eb_input) and slip misfit (es_input) parameters

    eb_input=[];
    es_input=[];

    % % The interlayer spacing along FCC [111] or HCP [0001] direction

    LatC_spacing=[];

    % % % >>> for FCC structure

```

```
% LatC_spacing=sqrt(2/3)/2*BurVect;

% % The coefficient to calculate the extra volume, i.e. dV=coefV*eb

coefV=[];

% % % >>> for FCC structure

% coefV=3/4*(sqrt(2)*BurVect)^3;

% % Matrix of the lower and upper bounds to search the characteristic bow-out distance wc (unit:
A)

wc_range=[];

% % Concentration of solute atom

solute_concentration=1;
```

References

- [1] S. H. Zhang, D. Legut and R. F. Zhang, PNADIS: automatic Peierls-Nabarro Analyzer for DISlocation core structure and slip resistance, in preparation.