pylastic Documentation

Release 0.1

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Contents: Get DEFORMATION MATRIX for given spacegroup number and Lagranian strain.

Methods: get_eta : returns Lagrangian strain

get_sgn : returns spacegroup number

get_strainType : returns current strain (deformation) type

get_defMatrix : returns deformation matrix

get_strainList : returns list of deformation types for specific crystal symmetry

get_V0

set_eta : set Lagrangian strain

set_sgn : set spacegroup number

set_strainType : set current strain(deformation) type

set_defMatrix : calculates deformation matrix

set_strainList : finds list of deformation types for specific crystal symmetry

set_V0

Example:

```
import distort

dist = distort.Distort()                  # generate instance of distortion object
dist.sgn = sgn                            # set spacegroup number (int)
dist.set_strainList()                     # set strain list according to space group number

strainType = next(dist.strainList_iter)   # when using the iterator property --> get first distortion
dist.eta = eta                            # define lagrangian strain (float)
dist.set_strainType(strainType)           # set strain type (string)
dist.set_defMatrix()                      # ste deformation matrix
dist.get_defMatrix()                      # get deformation matrix
```

class distort.**Distort**(*volumeconserving=False*, *mthd='Energy'*, *order=2*)

Generate DEFORMATION MATRIX for given spacegroup number and Lagranian strain. arguments:

volumecoserving: (True/False) mthd: ('Energy'/'Stress') method of calculation order: (2/3) specify order of elastic constants

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class elatoms.**ElAtoms**

classdocs: ASE Atoms like object.

Methods: set_cell set_natom set_scale set_species set_workdir set_poscar set_poscarnew distort poscarToAtoms atomsToPoscar

get_cell get_natom get_scale get_species get_workdir get_poscar get_poscarnew

Example:

```
poscar = POS('POSCAR').read_pos()
structures = Structures()
```

Generate distortion:

```
atom1 = ElAtoms()
atom1.poscarToAtoms(poscar)
atom1.distort(eta=0.01, strainType_index = 0)
structures.append_structure(atom1)
```

Generate another distortion:

```
atom2 = ElAtoms()
atom2.poscarToAtoms(poscar)
atom2.distort(eta=0.01, strainType_index = 1)
structures.append_structure(atom2)

structures.write_structures()
```

class elatoms.**Structures**
Generate a series of distorted structures.

Methods: set_fname write_structures append_structure get_structures

class analyze.**Energy**(*strain*, *energy*, *V0*)

CHAPTER

ONE

INDICES AND TABLES

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