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2012 J. Phys.: Conf. Ser. 402 012006

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# Investigating robustness of interatomic potentials with universal interface

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**Abstract.** We present a set of Python routines to perform basic tests of classical atomistic potentials and their example applications. These routines are implemented using universal Atomic Simulation Environment (ASE) and LAMMPS molecular dynamics code. ASE is utilized to create atomic configurations, to write input scripts for LAMMPS, and to read results from output files. Evaluated properties are formation energies and volumes of simple point defects (vacancies, substitutions, and interstitials), formation energies of basic surfaces, heats of formation of simple binary compounds, and elastic constants. The flexibility of LAMMPS allows easy switching between different semi-empirical potentials, while the universality of ASE allows to compare results with a variety of electronic structure codes.

## 1. Introduction

Molecular dynamics (MD) simulations provide a useful insight into phenomena between the scales of quantum and continuum level simulations. Interatomic potentials used in MD simulations require validation by comparison with available experimental properties, with high accuracy electronic structure calculations, and their quality is also assessed by comparison with other MD potentials. In order to perform validation tests of interatomic potentials, one needs to learn formats of input parameter files, atomic configuration files, and output files of classical MD code implementing MEAM method (LAMMPS [1]) and electronic structure code chosen for validation. Also, atomic configurations for single crystal structures, crystalline compounds, point defects (vacancies, interstitials, substitutions), planar defects (various surfaces and stacking faults), and strained structures needs to be created. Therefore, a tool applicable to quickly evaluate basic properties from classical MD potentials (and electronic structure methods) is desirable. Ideally, a single universal tool should be able to create basic atomic configurations and manipulate them, to serve these atomic configurations as inputs for a variety of methods/simulation codes, and to obtain their energies. In the present effort, we developed Python routines for basic tests of atomistic potentials using Atomic Simulation Environment (ASE) [2]. These routines were constructed to validate the Modified Embedded Atom Method (MEAM) potentials for Al, Si,

Mg, Cu, and Fe alloys. Testing routines, results of MEAM potential tests, and sample tests of other MD potential [3] are available for download from a public repository [7].

## 2. Atomic Simulation Environment (ASE)

Atomic Simulation Environment (ASE) [2] is a universal object-oriented Python interface to a variety of electronic structure codes (calculators). It creates atomic configurations, input scripts, and parse output files for a variety of electronic structure codes. Recently, an ASE calculator interface to classical MD code LAMMPS [1] was implemented at the Department of Theoretical Chemistry, Technical University of Munich by Jörg Meyer.

ASE provides simple graphical user interface and visualization tools with an extensive documentation and tutorials [4]. It facilitates creation and manipulation of molecules, nanotubes, basic surfaces, and arbitrary crystalline structures utilizing its database of spacegroups. It supports structure optimization, symmetry analysis, dissociation, diffusion, constrains, nudged elastic band (NEB) method, vibration analysis, phonon calculations, infrared intensities, MD with a broad selection of ensembles and dynamics, STM imaging, and electron transport. Electronic structure codes (calculators) working with ASE are listed in table 1.

**Table 1.** Calculators working with ASE, as listed in ASE online documentation. Broad range of calculator types is supported: density functional theory (DFT), linearized augmented planewave (LAPW), effective medium theory (EMT), Hartree-Fock (HF), and classical molecular dynamics (CMD) calculators.

Code	Description	Type
VASP	Planewave PAW code	DFT
ABINIT	Planewave pseudopotential code	DFT
Castep	Planewave pseudopotential code	DFT, HF
Siesta	Linear combination of atomic orbitals pseudopotential code	DFT
Exciting	Full potential LAPW code	DFT, LAPW
Jacapo	ASE interface to Dacapo, planewave ultrasoft pseudopotentials	DFT
DFTB+	DFT based tight binding code	DFT
TURBOMOLE	Fast atom orbital code	DFT, HF
FHI-aims	Numeric atom-centered basis functions, full potential code	DFT, HF
FLEUR	Full potential LAPW code	DFT, LAPW
EMT	Effective medium theory calculator (written in Python)	EMT
Asap	Highly efficient EMT code (written in C++)	EMT
GPAW	Grid-based real-space PAW code	DFT, HF
Dacapo	Old interface to Dacapo	DFT
LAMMPS	Classical molecular dynamics code	CMD

## 3. Bulk properties

### 3.1. Equilibrium atomic volume, energy, and bulk modulus

The equilibrium atomic volume  $V_0$  for a given structure is the volume per atom at which the structure has minimal energy. Equilibrium bulk modulus is defined as

$$B_0 = -V \left. \frac{\partial p}{\partial V} \right|_{V=V_0} \quad (1)$$

ASE provides a command line tool to calculate bulk properties by fitting values of energy at varying volumes to the stabilized jellium equation of state (SJEOS) [5]. Properties obtained from fit are equilibrium atomic volume  $V_0$ , corresponding equilibrium energy  $E_0$ , and bulk modulus  $B_0$ .

## 4. Point defects

### 4.1. Monovacancies

The formation energy of a single vacancy  $E_f^{\text{vac}}$  is defined as the energy cost to create a vacancy:

$$E_f^{\text{vac}} = E_{\text{tot}}[N - 1] - (N - 1)\varepsilon_0, \quad (2)$$

where  $E_{\text{tot}}[N - 1]$  is the total energy of a system with  $N - 1$  atoms containing a vacancy and  $\varepsilon_0 = E_0/N_0$  is the equilibrium energy per atom in the bulk (section 3). Python script that calculates monovacancy formation energy takes the atomic specie, crystal structure, and equilibrium lattice constant(s) as input parameters. First, energy without vacancy at equilibrium lattice parameter is calculated. Then, one atom is removed and energy without relaxation is obtained. After relaxation of atomic positions and cell volume optimization, relaxed vacancy formation energy and volume are evaluated.

### 4.2. Interstitials

The formation energy of an interstitial point defect  $E_f^{\text{int}}$  is given by

$$E_f^{\text{int}} = E_{\text{tot}}[N + 1] - N\varepsilon_X - \varepsilon_Y \quad (3)$$

where  $E_{\text{tot}}[N + 1]$  is the total energy of a system with  $N$  type-X bulk atoms plus one impurity atom of type-Y inserted at the interstitial site, and  $\varepsilon_X$  ( $\varepsilon_Y$ ) is the total energy per atom of type-X (type-Y) in its most stable bulk structure. The inserted atom Y can be of the same type as the bulk, in which case the point defect is called a self-interstitial defect. Self-interstitial formation energies are calculated at the octahedral, tetrahedral, and dumbbell sites. Dumbbell orientations are [100] for fcc, [0001] for hcp, and [110] for bcc and diamond structures. Systems sizes are  $5 \times 5 \times 5$  primitive fcc and bcc cells,  $3 \times 3 \times 3$  primitive diamond cells, and  $8 \times 4 \times 4$  orthogonal hcp cells. Script that calculates energy of an interstitial takes atomic specie, crystal structure, equilibrium lattice constant, and interstitial type as parameters. Evaluated properties are interstitial formation energy and volume.

### 4.3. Substitutions

The formation energy of a substitutional point defect  $E_f^{\text{sub}}$ , in the case of the substitution of a type-X atom of the host with a type-Y atom, is defined by

$$E_f^{\text{sub}} = E_{\text{tot}}[(N - 1) + 1] - (N - 1)\varepsilon_X - \varepsilon_Y \quad (4)$$

where  $E_{\text{tot}}[(N - 1) + 1]$  is the total energy of a system of  $N - 1$  host type-X atoms and one type-Y atom that replaced type-X atom in the original bulk position,  $\varepsilon_X$  and  $\varepsilon_Y$  are the total energies per atom for type-X and type-Y atoms in their ground state bulk structures. Parameters of the script that calculates formation energy of a substitution are host element type, structure, and lattice constant, substitutional element type, and the equilibrium energy  $\varepsilon_Y$  of a substituting atom. Evaluated properties are energy without substitution, unrelaxed and relaxed energy with substitution, and formation volume of substitution.

## 5. Planar defects

### 5.1. Surfaces

The surface formation energy per unit surface area  $E_{\text{surf}}$  is defined as

$$E_f^{\text{surf}} = \frac{E_{\text{tot}}[N] - N\varepsilon_0}{A}, \quad (5)$$

where  $E_{\text{tot}}[N]$  is the total energy of the structure with two surfaces,  $N$  is the number of atoms in the structure,  $\varepsilon_0$  is the equilibrium energy per atom in the bulk, and  $A$  is the total area of both surfaces. Surface formation energy of the fcc (111), (110), (100), diamond (111), (100), hcp (0001), (10 $\bar{1}$ 0), bcc (111), (110), (100) surfaces are evaluated. Input parameters for the script are atomic specie, crystal structure of the surface and its orientation, lattice parameter, equilibrium energy per atom in the bulk structure, number of repetitions of the base cell in the surface structure, and the vacuum thickness. Surface formation energy is evaluated for both unrelaxed and relaxed surfaces.

## 6. Heats of formation for binary compounds

The heat of formation per atom,  $\Delta H$ , is defined as

$$\Delta H = \frac{E_{\text{tot}}[N_X + N_Y] - N_X\varepsilon_X - N_Y\varepsilon_Y}{N_X + N_Y}, \quad (6)$$

$E_{\text{tot}}$  is the equilibrium energy of the compound structure,  $N_X$  and  $N_Y$  are the numbers of type-X and type-Y atoms,  $\varepsilon_X$  and  $\varepsilon_Y$  are the equilibrium energies per atom for type-X and type-Y in their ground state bulk structures, respectively. Equilibrium volume and bulk modulus are obtained by fitting energy to SJEOS with lattice parameter varying by -2%, -1%, 1% and 2% as described in section 3. The heats of formation at equilibrium atomic volumes for B1, B2, B3, C1, C15, D0<sub>3</sub>, A15, L1<sub>2</sub> binary compounds are evaluated following equation (6), along with their equilibrium volumes and bulk moduli.

## 7. Elastic constants

### 7.1. Trigonal and tetragonal shear modulus

Starting from an unstrained equilibrium configuration, the change of energy density due to small strain can be expressed as

$$\Delta E_V = \frac{1}{2} \sum_{i=1}^6 \sum_{j=1}^6 C_{ij} \epsilon_i \epsilon_j \quad \text{with} \quad C_{ij} = C_{ji}, \quad (7)$$

where  $\epsilon_i$  are strains in modified Voigt notation. For small deformations of a cubic crystal, the change of energy density due to small strain is

$$\begin{aligned} \Delta E_V &= \frac{1}{2} C_{11} (\epsilon_1^2 + \epsilon_2^2 + \epsilon_3^2) + C_{12} (\epsilon_1 \epsilon_2 + \epsilon_2 \epsilon_3 + \epsilon_3 \epsilon_1) \\ &+ \frac{1}{2} C_{44} (\epsilon_4^2 + \epsilon_5^2 + \epsilon_6^2) + O(\epsilon_i^3). \end{aligned} \quad (8)$$

The trigonal shear modulus  $C_{44}$  was determined from rhombohedral deformation given by  $\epsilon_1 = \epsilon_2 = \epsilon_3 = 0$  and  $\epsilon_4 = \epsilon_5 = \epsilon_6 = \delta$  in equation (8), leading to

$$\Delta E_V(\delta) = \frac{3}{2} C_{44} \delta^2 + O(\delta^3). \quad (9)$$

The tetragonal shear modulus  $(C_{11} - C_{12})/2$  was determined from the deformation given by  $\epsilon_1 = \delta$ ,  $\epsilon_2 = \frac{1}{1+\delta} - 1$  in equation (8), leading to

$$\Delta E_V(\delta) = (C_{11} - C_{12}) \delta^2 + O(\delta^3). \quad (10)$$

Input parameters of the script are element specie(s), crystal structure, and equilibrium lattice parameter. Equilibrium volume is first validated as described in section 3. Evaluated properties are tetragonal and trigonal shear moduli.

## 8. Conclusions

We developed Python routines for basic tests of classical atomistic potentials using universal Atomic Simulation Environment [2]. These scripts, together with example application to validate MEAM potential for Al, Si, Mg, Cu, and Fe alloys [6], and resulting evaluated properties are available for download from a public Subversion repository [7] under the LGPL license.

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