LAMMPS Implementation of an interatomic potential for the simulation of systems containing Fe, Ti and C.

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(Dated: September 2, 2015)

I. INTRODUCTION

The present report describes the details of the implementation of the potential developed in reference[2] for the simulation of systems containing Fe, Ti, C into the MD software LAMMPS `http://lammps.sandia.gov/`.

II. IMPLEMENTATION PROCEDURE

The implementation of a ternary 2nn-MEAM potential for LAMMPS, two files need to be generated: first, the so called "library" file which has generic MEAM settings for the elements, and, second, the "parameter" file which contains settings that override or complement the library file settings.

A. The library file

The generation of the library file can be done using the first sheet of the program "kissmd-to-lammps.xlsx" available in `https://cmse.postech.ac.kr/lammps/3707`. In the case of the present Fe-Ti-C potential, this file will be named FeTiClibrary.meam.

B. The parameters file

Similarly to the library file, the generation of the parameters file is partially done via the third sheet of the program "kissmd-to-lammps.xlsx". This sheet allows to generate the parameters required for the single-element and for the binary interactions. Nevertheless, the parameters corresponding to the ternary interactions need to be input in the parameter file manually. This parameters can be obtained from reference[2]. It is important to notice that the sequence of i, j, k is different in reference[2] and LAMMPS. In the reference, Cmin(i,j,k) means that the i-k pair is screened by j, while in LAMMPS, it means that the i-j pair is screened by k.

In the case of the present Fe-Ti-C potential, this file will be named FeTiC.meam.

III. TESTS

A. Single-Element and Binary systems

TABLE I. Calculated values of the Nearest neighbour distance.

Nearest neighbour distance[Å]		
	Current	Literature
Fe	2.48	2.48
Ti	2.92	2.92
C	1.54	1.54
Fe-Ti	2.58	2.58
Ti-C	2.21	2.21

TABLE II. Calculated values of the cohesive energy.

Cohesive Energy[eV/*Atom*]		
	Current	Literature
Fe	4.29	4.29
Ti	4.87	4.87
C	7.37	7.37
Fe-Ti	4.80	4.80
Ti-C	6.90	6.90

TABLE III. Dilute heat of solution of a single C atom in a BCC matrix. Results for two different cut-off radius values (rc).

Dilute heat of solution[eV]		
Current		Literature
rc 4.8	rc 3.6	rc 3.6
1.31	1.22	1.22

B. Ternary systems

The testing of the ternary systems was done by the developers of the potential at Postech CMSE lab (`https://cmse.postech.ac.kr/home_2nnmeam`). The tests where done by comparing the results obtained using KISSMD and LAMMPS for the interfacial energies -as calculated in[2]- of three different systems containing an interface between Fe and TiC. The difference between the three systems is the ratio X_{Fe} between the number of Fe and TiC atoms.

TABLE IV. Comparison between the interfacial energies of the interface Fe-TiC calculated using KISSMD and LAMMPS.

	KISSMD			LAMMPS		
X_{Fe}	0.67	0.75	0.80	0.67	0.75	0.80
$\sigma[\mathrm{J\,m^{-2}}]$	0.2504	0.2138	0.1855	0.2492	0.2132	0.1852

The reason for making a comparison between these two software is that the interatomic potential in question was developed and thoroughly tested in KISSMD (`https://cmse.postech.ac.kr/home_2nnmeam`).

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