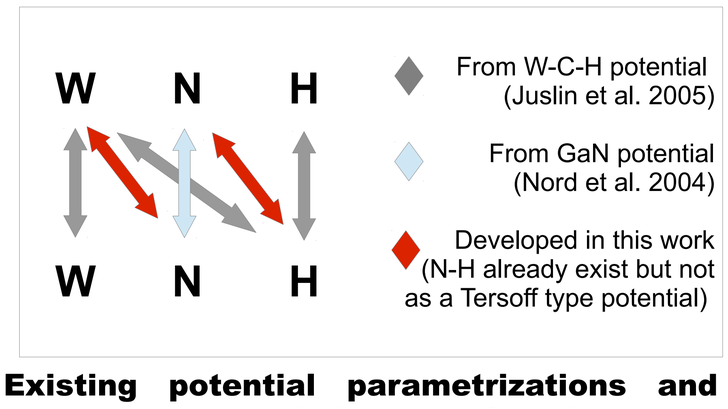
HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI
MATEMAATTIS-LUONNONTIETEELLINEN TIEDEKUNTA
MATEMATISK-NATURVETENSKAPLIGA FAKULTETEN
FACULTY OF SCIENCE

DEVELOPMENT OF AN INTERATOMIC POTENTIAL FOR W-N-H SYSTEM

Authors:
Jussi Polvi and Kai Nordlund
Department of Physics
Division of Materials Physics
P.O. Box 43
00014 University of Helsinki
Finland
Email: *jussi.polvi@helsinki.fi*

MOTIVATION

Tungsten monocarbide (WC) and mononitride (WN) are getting more attention from physicists and material scientists due to their unique physical and chemical properties such as extreme hardness and chemical inertness. These compounds belong to the most promising engineering materials with wide range of industrial applications.



Existing potential parametrizations and the parameters being developed in this work. N-H parameters already exist but not in a Tersoff-like potential formalism.

N_2 or noble gases will most likely be used as seeding species to reduce the power loads on the tungsten divertor target of ITER in relevant heated scenarios. The seeding species will interact with the plasma-facing materials beryllium and tungsten, and, in the case of nitrogen, also form chemical bonds with the wall surfaces as well as with plasma hydrogen isotopes. This raises a special interest in for W-N and N-H interactions in the fusion community.

Since interatomic potentials for W-Be (Björkas et al. 2010) and W-C-H (Juslin et al. 2005) interactions have already been developed, the W-N-H potential is a new important piece of a potential puzzle, soon hopefully containing all possible interactions between the fusion reactor materials.

METHODS

Our goal is to produce a reactive interatomic potential for W-N-H interactions using functionals developed by Brenner and Tersoff.

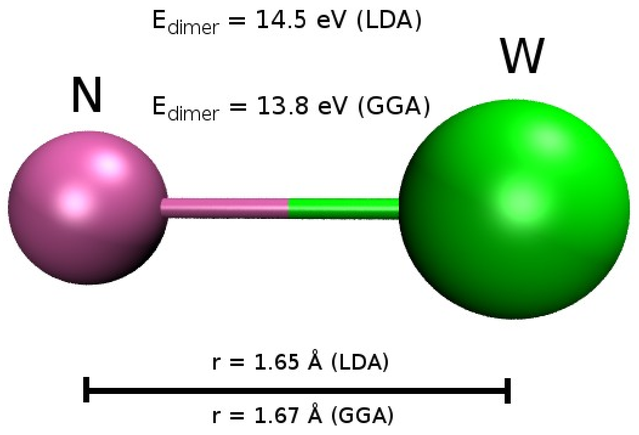
The development process is roughly as follows:

1) We start by obtaining information on as many coordination states (Z) as possible:
   - Z=1 (dimer)
   - Z=4 (zincblende, wurtzite)
   - Z=6 (NaCl, CsCl, NiAs)
   - Z=12 (WC)
2) Data from experiments or density functional theory (DFT) calculations:
   - Cohesive energy, lattice constant, bulk modulus for all Z
   - Elastic constants for most important structures
3) We use the gathered data to fit all 11 parameter of the potential functions
   - To aid in the fitting process a fitting code Pontifix (by Prof. K. Albe and Dr. P. Erhart) is used

In all *ab initio* simulations done for this work, the DFT code VASP was used. All structures were simulated using two different exchange correlation functionals: the local density approximation (LDA) and the generalized gradient approximation (GGA).

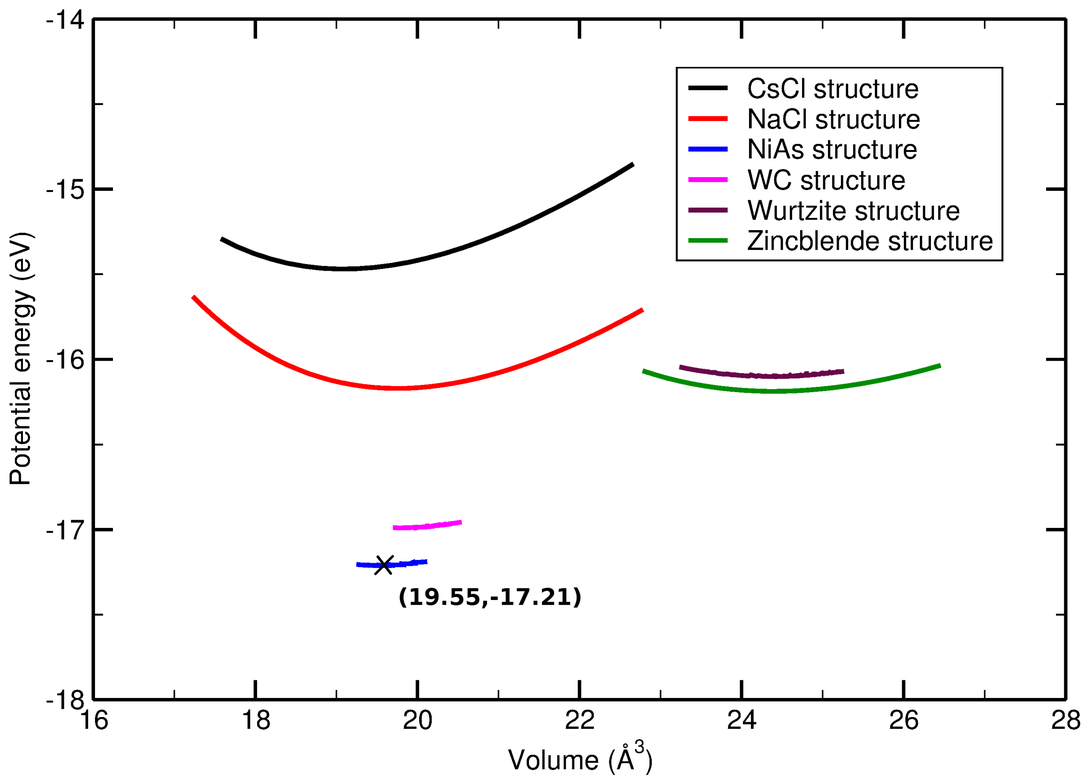
FUTURE WORK

We have gathered most of the necessary reference data for W-N, so we can start the fitting process. After that comes the task of generating the N-H part; and then finally we need to combine these new parts with previously developed pieces of the potential.



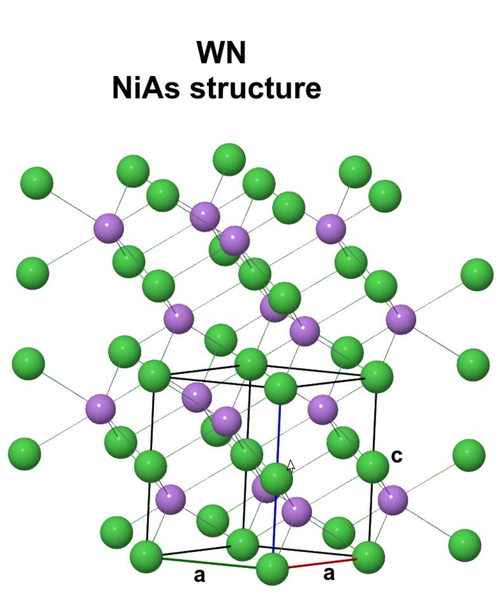
The potential energy of N-W dimer and the bond lenght from DFT calculations. The experimental bond lenght is 1.69 Å.

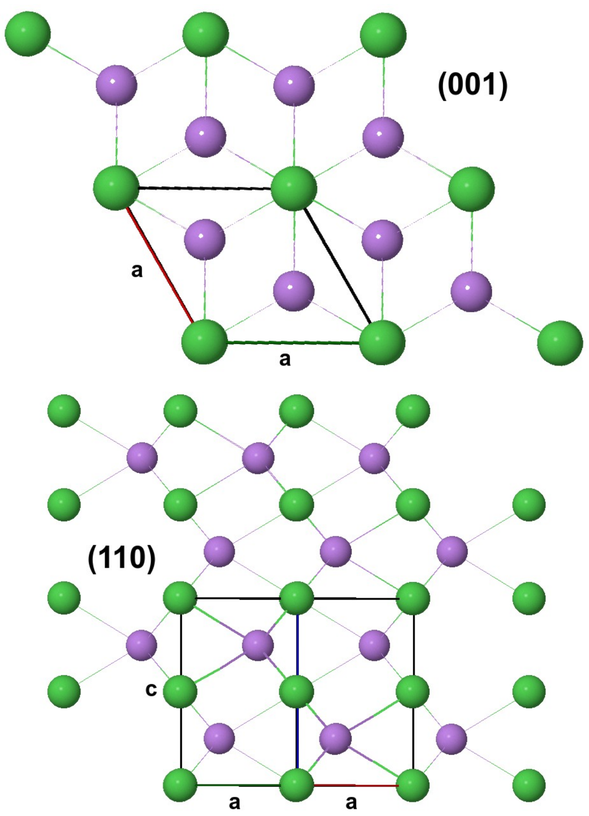
RESULTS FROM DFT CALCULATIONS



Potential energy vs. Volume per WN pair from DFT with LDA. NiAs type structure has clearly the lowest potential energy and appears to be the ground state structure. (DFT calculation with GGA gives the same ground state structure.)

WN
NiAs structure





Visualization of the NiAs type crystal structure. It is a hexagonal lattice with a=2.81 Å and c=5.71 Å. Green tungsten atoms form flattened hcp lattice and violet nitrogen atoms located at every other gap between them.

Acknowledgements This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.