Homework Assignment Number Two

The Embedded Atom Method(EAM) potential has been extensively used to simulate metals. Consider the following article:

Title: Development of new interatomic potentials appropriate for crystalline and liquid iron
Authors: M. I. Mendelev , S. Han , D. J. Srolovitz , G. J. Ackland , D. Y. Sun & M. Asta
Journal: Philosophical Magazine
Volume: 83 Issue: 35 Pages: 3977-3994 Published: 2003
DOI: http://dx.doi.org/10.1080/14786430310001613264

There are three tasks in this homework.

Task 1. Implement a 0 K minimization and a finite temperature simulation of bcc Fe using the EAM potential. Compare your results with Table 1 of the reference above with respect to

- lattice constant at 0 K
- cohesive energy at 0 K
- elastic constants, C_{11}, C_{12} and C_{44} at 0 K
- lattice constant at finite temperature
- cohesive energy at finite temperature

Task 2. Provide some justification that your finite temperature simulation is reasonable in terms of

- the number of atoms
- the size of the time step
- the duration of the simulation

Task 3. Repeat Task 1 for an fcc metal. You can use, for example, the following paper for a list of lattice constants, cohesive energies and elastic constants.

Title: Tight-binding potentials for transition metals and alloys
Authors: Fabrizio Cleri and Vittorio Rosato
Journal: Physical Review B
Volume: 48 Issue: 1 Pages: 22-33 Published: 1993
DOI: http://dx.doi.org/10.1103/PhysRevB.48.22

Append your LAMMPS input files for Tasks 1 and 3 to your homework.

There is no need to attach lengthy output.

Submit the homework as a pdf file electronically through the course website system.

Please do not submit a paper copy of this homework.