



ELSEVIER

Contents lists available at ScienceDirect

## Data in Brief

journal homepage: [www.elsevier.com/locate/dib](http://www.elsevier.com/locate/dib)

## Data Article

## Data files for ab initio calculations of the lattice parameter and elastic stiffness coefficients of bcc Fe with solutes

Michael R. Fellinger<sup>a,\*</sup>, Louis G. Hector Jr.<sup>b</sup>, Dallas R. Trinkle<sup>a</sup><sup>a</sup> Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA<sup>b</sup> General Motors R&D Center, 30500 Mound Road, Warren, MI 48092, USA

## ARTICLE INFO

## Article history:

Received 3 October 2016

Received in revised form

18 November 2016

Accepted 23 November 2016

Available online 29 November 2016

## Keywords:

Lattice parameters

Elastic constants

Solute

Iron

Steel

Ferrite

Ab initio

## ABSTRACT

We present computed datasets on changes in the lattice parameter and elastic stiffness coefficients of bcc Fe due to substitutional Al, B, Cu, Mn, and Si solutes, and octahedral interstitial C and N solutes. The data is calculated using the methodology based on density functional theory (DFT) presented in Ref. (M.R. Fellinger, L. G. Hector Jr., D.R. Trinkle, 2017) [1]. All the DFT calculations were performed using the Vienna Ab initio Simulations Package (VASP) (G. Kresse, J. Furthmüller, 1996) [2]. The data is stored in the NIST dSpace repository (<http://hdl.handle.net/11256/671>).

© 2016 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

## Specifications Table

Subject area	Materials science
More specific subject area	Computational materials science
Type of data	1. VASP input and output text files 2. PureFe.csv file containing computed data for pure bcc Fe 3. SoluteEffects.csv file containing computed solute effects on the

DOI of original article: <http://dx.doi.org/10.1016/j.commat.2016.09.040>

\* Corresponding author.

E-mail address: [mfelling@illinois.edu](mailto:mfelling@illinois.edu) (M.R. Fellinger).<http://dx.doi.org/10.1016/j.dib.2016.11.092>2352-3409/© 2016 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

	<i>lattice parameter and elastic stiffness coefficients of bcc Fe 4. Text files containing UNIX shell scripts that compute the data from the VASP output files</i>
How data was acquired	<i>Density functional theory calculations performed using VASP</i>
Data format	<i>Raw and analyzed data</i>
Data source location	<i>Urbana, IL, USA and Warren, MI, USA</i>
Data accessibility	<i>Data are available in the NIST dSpace repository (<a href="http://hdl.handle.net/11256/671">http://hdl.handle.net/11256/671</a>)</i>

---

### Value of the data

---

- The data gives the strain and chemical effects of Al, B, Cu, Mn, Si, C, and N solutes on the lattice parameter and single-crystal elastic stiffness coefficients  $C_{ij}$  of bcc Fe.
  - The data can be used to estimate solute-induced changes in mechanical properties like strength and ductility of the ferrite phase of steel.
  - The data can be directly incorporated into mesoscale methods used in integrated computational materials engineering (ICME) of multiphase steels, including crystal plasticity simulations for predicting stress-strain curves and plastic flow.
  - The data alleviates other researchers from performing the large number of computationally intensive DFT calculations required to compute the effects of these solutes on bcc Fe.
- 

### 1. Data

We use density functional theory (DFT) to compute the effects of substitutional Al, B, Cu, Mn, and Si solutes, and octahedral interstitial C and N solutes on the lattice parameters and elastic stiffness coefficients  $C_{ij}$  of bcc Fe. The PureFe.csv file contains the computed lattice parameter, magnetic moment,  $C_{ij}$ , and the derivatives of the  $C_{ij}$  with respect to lattice parameter for pure Fe. The computational methodology we developed in Ref. [1] calculates a strain-misfit tensor for each solute which determines changes in the lattice parameter and volumetric contributions to the derivatives of the  $C_{ij}$  with respect to solute concentration. We also compute chemical contributions from each solute to the derivatives of the  $C_{ij}$  with respect to solute concentration. The sum of the volumetric and the chemical contributions gives the total derivatives of the  $C_{ij}$  with respect to solute concentration. The SoluteEffects.csv file contains the diagonal components of the solute strain-misfit tensors and their average values, the volumetric and chemical contributions to the  $C_{ij}$  derivatives, the sum of the two contributions, and direct calculations of the total derivatives that encompass both contributions. We compute the solute data using  $2 \times 2 \times 2$  (16 atoms),  $3 \times 3 \times 3$  (54 atoms), and  $4 \times 4 \times 4$  (128-atom) supercells.

### 2. Computational methods

We use the VASP code [2] to perform the DFT calculations. The calculation details, including the exchange-correlation functional, pseudopotentials, and all numerical convergence parameters used in generating the data, are given in Ref. [1]. The VASP input files INCAR and KPOINTS, and output files CONTCAR, OUTCAR, and OSZICAR for all the calculations are stored in the NIST dSpace repository (<http://hdl.handle.net/11256/671>), along with the analyzed data stored in the PureFe.csv and SoluteEffects.csv files. The repository also stores Unix shell scripts we developed for calculating the data in the CSV files from the raw VASP output files. The fundamental quantities necessary for computing strain misfit tensors and elastic stiffness coefficients are the numbers of atoms in the computational supercells, lattice parameters, applied strain magnitudes, and stresses. The scripts compute the elastic

Download English Version:

<https://daneshyari.com/en/article/4765283>

Download Persian Version:

<https://daneshyari.com/article/4765283>

[Daneshyari.com](https://daneshyari.com)