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Data Article

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

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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).

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*

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	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
How data was acquired	*Density functional theory calculations performed using VASP*
Data format	*Raw and analyzed data*
Data source location	*Urbana, IL, USA and Warren, MI, USA*
Data accessibility	*Data are available in the NIST dSpace repository* (http://hdl.handle.net/11256/671)

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/11256/67), 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

Table 1
Computed properties of pure Fe in PureFe.csv and their associated tags and units. The data type of each entry is numeric.

Properties	Tags	Units
Lattice parameter	LatticeParameter	Å
Magnetic moment	MagneticMoment	μ_B
Elastic stiffness coefficients C_{ij}	C11, C12, C44	GPa
C_{ij} derivatives with respect to lattice parameter	dC11da, dC12da, dC44da	GPa/Å

Table 2
Computed solute effects on bcc Fe in SoluteEffects.csv and their associated tags and units. The data type of each entry is numeric. The solute strain misfit tensor and elastic stiffness coefficient derivative values in the CSV file are for atomic concentrations. For atomic percent, the values must be divided by 100.

Properties	Tags	Units
Solute strain misfit tensor components	eps11, eps33, epsAvg	unitless
Volumetric contributions to C_{ij} derivatives with respect to solute concentration	dC11dcV, dC12dcV, dC44dcV	GPa
Chemical contributions to C_{ij} derivatives with respect to solute concentration	dC11dcC, dC12dcC, dC44dcC	GPa
Sum of volumetric and chemical contributions	dC11dcT, dC12dcT, dC44dcT	GPa
Direct calculations of C_{ij} derivatives with respect to solute concentration	dC11dcD, dC12dcD, dC44dcD	GPa

stiffness coefficients from derivatives of stress with respect to strain, approximated using a standard four-point central finite-difference formula [3]. Tables 1 and 2 list the properties contained in the PureFe.csv and SoluteEffects.csv files, respectively, along with identifying tags that label the properties in the files and their units.

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.11.092.

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