Ab initio calculations of the lattice parameter and elastic stiffness coefficients of bcc Fe with solutes

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All DFT calculations were performed with VASP [1] version 5.3.3, using the PBE exchange-correlation functional [2] and PAW potentials [3] generated by Kresse and Joubert [4].

POTCAR versions

Fe: PAW_PBE Fe 06Sep2000
Al: PAW_PBE Al 04Jan2001
B: PAW_PBE B 06Sep2000
Cu: PAW_PBE Cu 22Jun2005
Mn: PAW_PBE Mn 06Sep2000
Si: PAW_PBE Si 05Jan2001
C: PAW_PBE C 08Apr2002
N: PAW_PBE N 08Apr2002

The VASP input files INCAR, KPOINTS, and CONTCAR, and the output files OSZICAR and OUTCAR are contained in BCC-LatticeParameter-Cij-data.tgz, along with the .csv files and scripts that compute the data in these files.

The PureFe.csv file contains computed properties of pure bcc Fe. The properties are labeled in the file using the following Tags:

Properties	Tags
lattice parameter, a	LatticeParameter
magnetic moment	MagneticMoment
elastic stiffness coefficients, Cij	C11, C12, C44
Cij derivatives wrt a, dCij/da	dC11da, dC12da, dC44da

The SoluteEffects.csv file contains computed properties of bcc Fe with solutes. The properties are labeled in the file using the following Tags:

Properties	Tags
solute strain misfit tensor components	eps11, eps33
average solute strain misfit tensor	epsAvg
Cij derivatives wrt solute concentration:	
volumetric contributions	dC11dcV, dC12dcV, dC44dcV
chemical contributions	dC11dcC, dC12dcC, dC44dcC
total contributions (volumetric + chemical)	dC11dcT, dC12dcT, dC44dcT
direct calculations	dC11dcD, dC12dcD, dC44dcD

The calculations in BCC-LatticeParameter-Cij-data.tgz are organized as follows:

The PureFe/ directory contains the data for the pure bcc Fe lattice parameter, magnetic moment, elastic stiffness coefficients Cij, and the Cij derivatives with respect to lattice parameter. These calculations were carried out using different k-point densities with standard Gamma-point-centered Monkhorst-Pack (M-P) meshes [5], and M-P meshes shifted off of the Gamma-point.

The Cij derivatives converge slowly with respect to k-points for these meshes, so we also compute all the properties using simple cubic k-point meshes [6] generated by combining the two individual M-P meshes. All properties converge faster with the combined meshes. The Polycrystalline.txt file contains the polycrystalline bulk modulus B, shear modulus G, and Young's modulus E for pure bcc Fe computed from our calculated single-crystal Cij.

The SoluteStrainMisfits/ directory contains the VASP calculations for the solute strain misfit tensor for each solute in 2x2x2 (16-atom), 3x3x3 (54-atom), and 4x4x4 (128-atom) supercells.

The Cij-WithSolutes/ directory contains the VASP calculations for the Cij derivatives with respect to solute concentration for 2x2x2, 3x3x3, and 4x4x4 supercells. We compute separate chemical and volumetric contributions to these derivatives, and sum them to get the total contribution for each solute. We also compute the derivatives directly using calculations that encompass both contributions. The separate calculations are more computationally efficient and provide more information than the direct calculations. Comparison with the direct calculations validates the accuracy of the separate calculations. The PolyModuliTOT-FeWithSolutes.txt and PolyModuliDIR-FeWithSolutes.txt files contain the computed polycrystalline elastic moduli for bcc Fe with solutes.

Running Extract-Data-script.sh in BCC-LatticeParameter-Cij-data/ will regenerate all the data in the .csv and .txt files from the VASP output files.

References:

[1] G. Kresse and J. Furthmuller, Phys. Rev. B 54, 11169 (1996).

[2] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).

[3] P. E. Blochl, Phys. Rev. B 50, 17953 (1994).

[4] G. Kresse and D. Joubert, Phys. Rev. B 59, 1758 (1999).

[5] H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5188 (1976).

[6] D. J. Singh and L. Nordstrom (eds.). "Planewaves, Pseudopotentials, and the LAPW Method", 2nd edition. Springer, New York, 2006.