# Fundamental magnetic and elastic properties of Fe-Si alloys: A first-principles study

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## 1. Introduction

Silicon steels, especially with 3 wt.% Si, are widely used as energy converting materials for transformers, motors, etc. Silicon steels with 6.5 wt.% Si may be promising future electrical steels, due to their zero magnetostriction, reduced magnetocrystalline anisotropy, higher permeability, and lower coercivity [1]. However, it is known that the body centered cubic (bcc) Fe with Si content higher than 4 wt.% become significantly brittle and consequently their rolling process is hardly applicable. For this reason, the studies for relationship between magnetic and elastic properties have been strongly required. Here, we investigated fundamental magnetic and elastic properties of ferrites with the various Si concentrations (0−12.5 at.% of Si) and its D03 structure (25 at.% of Si) using the highly precise all-electron full-potential linearized augmented plane wave (FLAPW) method [2] based on density functional theory.

## 2. Computational Method and Models

The Perdew-Burke-Ernzerhof form of the generalized gradient approximation (GGA) [3] for the exchange correlation potential was used. An energy cutoff of 5.0 ($2\pi/a$), where a is the lattice parameter, was employed for expanding the linearized augmented plane wave basis set. An 18 ($2\pi/a$) star function cutoff was used for depicting the charge density and potential in the interstitial regions. Lattice harmonics with $l \leq 12$ were employed to expand the charge density, potential, and wave functions inside each muffin-tin sphere, with radii of 2.2 and 2.0 a.u. for Fe and Si atoms, respectively. Integrations inside the Brillouin zone (BZ) were performed using the improved tetrahedron method over a 13×13×13 mesh within the three-dimensional (3D) BZ. We considered the models as $Fe_{26}Si$, $Fe_{15}Si$, and $Fe_7Si$ which are corresponding to 3.7, 6.25, and 12.5 at.% of Si in bcc Fe, respectively. We also considered $D0_3$ structured $Fe_3Si$ (25 at.% of Si) of ordered phase.

## 3. Results and Discussions

From the total energy calculations, we determined that the equilibrium lattice constants are 2.83, 2.83, 2.82, and 2.80 Å for $Fe_{26}Si$, $Fe_{15}Si$, $Fe_7Si$, and $D0_3$ $Fe_3Si$ in ferromagnetic states, respectively; the lattice constant of ferrite slightly decreases with increasing Si concentration. We also calculated spin magnetic moments ($m_{Fe}$, in units of $\mu_B$) of the nearest neighbor Fe to Si atoms. The local magnetic moments of Fe atoms decrease as the Si concentration increase. Among the considered systems, magnetic moment of the Fe atom for $D0_3$ $Fe_3Si$ is smallest

which is consistent with theoretical and experimental values (1.35 $\mu_B$) [4].

In a cubic system, there are only three independent elastic constants, such as C11, C12, and C44, and they can be calculated by solving coupled quadratic energy equations with respect to volume conserving lattice distortions and equation of states for the bulk modulus (B). Furthermore, tetragonal shear constant (C'), shear modulus (G), Young's modulus (E), Posisson's ratio (v), and Cauchy pressure (CP) can be estimated from those elastic constants. The calculational results are listed in Table I.

To elucidate whether Fe-Si alloys are ductile or brittle, we used Pugh's relation [5] and $C_P$ [6]. Both the calculated $C_P$ and $G/B$ show the same tendency with the Si concentration in the range of 0−12.5 at.% Si. However, these brittle/ductile tendency deviate in ordered $D0_3$ $Fe_3Si$ (25 at.% of Si). The calculated values imply that D03 Fe3Si is more ductile than bcc Fe. Thus, the question on the origin of the observed embrittlements of the high Si content Fe-Si alloys steels remains to be open.

Table I. The calculated bulk modulus (GPa), tetragonal shear constant (GPa), shear modulus (GPa), Young's modulus (GPa), Poisson's ratio, Cauchy pressure (GPa), and the ratio of shear modulus to bulk modulus for Fe-Si alloys.

| Systems | Si (at.%) | *B* | *C'* | *G* | *E* | *v* | *CP* | *G/B* |
|---|---|---|---|---|---|---|---|---|
| bcc Fe | 0 | 189 | 68 | 96 | 246 | 0.28 | 30 | 0.51 |
| $Fe_{26}Si$ | 3.7 | 187 | 62 | 97 | 247 | 0.28 | 26 | 0.52 |
| $Fe_{15}Si$ | 6.25 | 174 | 57 | 98 | 248 | 0.26 | 10 | 0.56 |
| $Fe_7Si$ | 12.5 | 149 | 36 | 87 | 217 | 0.26 | 5 | 0.58 |
| $D0_3$ Fe3Si | 25 | 213 | 42 | 108 | 274 | 0.29 | 35 | 0.50 |

## 4. Summary

In this study, the magnetism and the elastic properties of Fe-Si alloys have been investigated using the all-electron FLAPW method based on the GGA. The local magnetic moment of Fe atoms decreases gradually. From the Pugh's relation and $C_P$, in the ordered $D0_3$ $Fe_3Si$, we predict that it presents intrinsic ductility.

## 5. References


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