# Mechanomagneto effects in Fe-Si system

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Abstract

Silicon steel (Si dilute Fe-Si alloys) is widely used as transformers, motors, magnetic coils, and structural materials due to the variety of magnetic and mechanical properties. Typical silicon steels in the practical applications contain Si from 2 up to 6.5wt.%. It is well known that the increase of Si to 5-6wt.% achieves excellent magnetic properties such as high permeability and nearly zero magnetostriction, also improves yield stress. However, beyond 4.5wt.% (8.6at.%), an obvious decrease in ductility has been reported [1]. In order to understand the microscopic mechanism of the effects of Si on various properties in Fe-Si alloys, the first-principles calculation on elastic properties of dilute Si in bcc-Fe has been performed at 0, 2.4, 5.6, 8.3, 10.9 and 12.5 at.%Si. Main results [2 and 3] are summarized below.

The calculated elastic constants including $c_{11}$, $c_{12}$, $c_{44}$, bulk modulus ($B$), shear modulus ($G$), and Young's modulus ($E$) at different Si concentrations indicate a steady change with the increase of Si up to 8.3at.%Si. Then, drastic drops of those constants are realized followed by recoveries at 12.5 at%Si. This trend of Si dependence is well consistent with experiment up to 10.9 at.%Si [4]. The further investigation of the ratio of bulk modulus (B) to shear modulus (G) indicates the dropping of B/G from 2.0 to 1.5 between at 8.3-10.9 at.%Si. According to Puge's empirical rule [5], 1.75 of B/G value is regarded as a critical value of ductile to brittle transition. The origin of such dependence on Si concentration motivated the present work.

Up to 8.3at%Si, the calculated density of states (DOS) distributions share similar characteristics, while a noticeable change at 10.9at.%Si is found. In both 8.3 and 10.9 at.%Si, Fermi levels are located in the majority-spin. But for minority-spin, the Fermi level is at the dip between two peaks at 8.3%at Si, while it just falls on the peak at the 10.9%at Si. The increase of minority-spin leads to an obvious increase of the total DOS, which results in a significant drop of magnetic moment. Furthermore, the change in total DOS at 8.3 and 10.9at.%Si suggests a different bonding characteristic between these two concentrations.

In the course of the analyses of the relation between the change in magnetic moment and elastic properties, it is found that the average magnetic moment decreases with Si concentration, which leads to a reduction of equilibrium volume as a consequence of negative magnetic pressure. Such a volume change which is induced by the change of magnetic moment has been known as Magnetovolume effects. Based on Stoner's Itinerant model, the non-monotonous behavior of elastic properties found in the present study up to 8.3at.%Si can be explained by the magnetovolume effect.

The present calculations imply that the precursor to ductile to brittle transition is closely related to magnetovolume effects, and the authors propose to call it as mechanomagneto effects. It is, however, noted that the non-monotonic behavior of B/G across 10.9at.%Si is not explained solely by the magnetic effects. The additional mechanism should be sought in the peculiar ordering behavior in the Fe-rich region of Fe-Si. In the presentation, we discuss mechanomagneto effects as a precursor to

ductile to brittle transition and the interplay between magnetic effects and ordering effects.

Acknowledgement
This research was supported by Japan Science and Technology Agency (JST) under Collaborative Research Based on Industrial Demand "Heterogeneous Structure Control”. The authors sincerely thanks to the crew of Center for Computational Materials Science of the Institute for Materials Research, Tohoku University for their continuous support of the SR11000/SR16000 supercomputing facilities.

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