Symposium | A. Advances in Materials Theory for Multiscale Modeling

## [SY-A2]Symposium A-2

Chair: Kenjiro Sugio(Hiroshima Univ., Japan)

Mon. Oct 29, 2018 3:45 PM - 5:30 PM Room6

# [SY-A2]Electronic structure analysis of Fermi level instability in Fe-rich Si alloy

○Chen Ying[1], Arkapol Saengdeejing[1], Tetsuo Mohri[2] (1.School of Engineering, Tohoku University, Japan, 2.Institute for Materials Research, Tohoku University, Japan)

Fe-Si binary alloy has a variety of applications due to its excellent magnetic and mechanical properties. Some drastic change in mechanical properties as Si concentration increasing to 9-10at.% has been intriguing since a long time ago. We have conducted an integrated study on elastic properties in Fe-rich Si alloy based on the electronic structure calculations incorporated with phonon vibration effect and thermal electrons excitation for a Si-doped bcc-Fe alloy up to 12.5at.%Si [1,2], as a part of a multiscale simulation of the mechanical properties of Fe-Si [3]. Our calculations reproduced a non-monotonic change of the elastic properties with Si concentration, showed a ductile to brittle transition behavior as the Si content increases beyond 9.4at.%, which is agree with the well know experimental results, The calculation further revealed that the Si concentration dependence of the elastic properties is originated from a combination of magnetovolume effect at a low Si concentration up to 8.0 at.%, $D0_3$ ordering on the recovery of elastic properties at Si concentration’s being over 10.9at.%, and the instability of density of states at the Fermi energy right at the Si concentration with drastic degradation of elastic properties. The present work aims at a thorough understanding on this Fermi level instability. We calculated the Fermi surfaces at 9.4, 10.9 and 12.5at.%Si, and found that at 10.9 at.%Si, the Fermi surface just touches the boundary of the Brillouin zone which leads to a decrease of the energy of the electrons, further deceases the elastic properties. This founding suggests that the Fermi lever stability/instability is related to the local atomic configuration of doped atoms, then the re-distribution of band structure and furthermore the relative position of Fermi surface to the Brillouin zone, which might be the electronic structural origin of the drastic change of the mechanical properties at some subtle Si concentrations in Fe-rich Si alloy.

References

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[3] T. Mohri, Y. Chen, A. Saengdeejing, et al., npj Computational Materials - Nature 3, 10 (2017)