Electronic structures and non-collinear magnetic properties of structurally disordered Fe

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To explore the magnetic properties of amorphous Fe, we have studied electronic structures of structurally disordered Fe systems generated from crystalline bcc and fcc Fe by using the Monte-Carlo scheme. As a first principles band method, we have used the real space spin-polarized tight-binding linearized-muffin-tin-orbital recursion method[1] in the local spin density approximation.

We have studied electronic structures with varying the disorderness of cluster and also with allowing the noncollinear polarized direction of magnetic moment of each atom. To simulate an amorphous system, we have considered 54-atom cluster generated from bcc Fe and 64-atom cluster generated from fcc Fe, where all the atoms up to the third near neighbors from the central atom are included in the cluster.

Electronic structures of disordered systems are characterized by broadened band width, smoothened local density of states, and reduced local magnetic moment, as compared to the crystalline system.
In disordered systems, the nearest neighbor hopping strengths are not uniform, and so yield the inhomogeneous local magnetic moment distribution.

Noncollinear magnetic structures of disordered systems depend on the short range configurations: the antiferromagnetic structure is the most stable for the bcc-based disordered system, while the non-collinear spin spiral structure becomes more stable for the fcc-based disordered system.

References

[1] J. H. Park, S. K. Kwon, and B. I. Min, J. Korean Phys. Soc. **37**, 109 (2000)