Non-collinear spin structures of Fe, Co, and Ni

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To explore excited magnetic states of 3d transition metals, non-collinear spin structures for bcc Fe, fcc Fe, fcc Co, and fcc Ni are studied by employing the real space spin-polarized tight-binding linearized-muffin-tin-orbital recursion band method[1] in the local spin density approximation. We simulated the excited magnetic states by adopting two spin configurations: the spiral-spin (SS) and canted (CT) spin configurations.

We have found that the ground state of fcc Fe is antiferromagnetic, while the ground states of other systems (bcc Fe, fcc Co, and fcc Ni) are ferromagnetic. We have also found an indication of possible spiral-spin state occurring at high q for fcc Fe. In general, magnetic excitation of smoothly varying SS spin configuration is found to be energetically more favorable than that of canted (CT) spin configuration We have obtained a set of Heisenberg exchange parameters, J, waves for bcc and fcc Fe, fcc Co, and fcc Ni utilizing the impurity calculation technique [1]. Using the obtained exchange parameters, the spin-wave stiffness constant D and the Curie temperature Tc are determined. The calculated Curie temperature Tc for bcc Fe agrees well with the experimental value, while that of fcc Ni is underestimated by about 20 %.

References

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