Saturation Moment Optimization of Electrical Steels: Slater-Pauling pattern repetition in multi-component alloys

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1. Introduction

Electrical steels, as Si-alloyed iron, are the most popular soft magnetic materials. Their specific uses widely vary from tiny motors in home appliances to huge transformers in power plants. As we are daily faced, high energy efficiencies are required in these power generating and consuming devices. In electrical steel design, hence, two creditable properties are pursued to achieve such requirement. One is high permeability and the other is low core loss. When we substitutionally introduce small amount of silicon into bcc iron, high permeability can be achieved via lowered magnetic anisotropy. Increased electrical resistivity by Si-addition lessens total energy dissipation via reduced eddy current. However, Si alloying detrimentally reduces the saturation magnetic flux density due to the nonmagnetic nature of Si. This causes energy inefficiency in application level. Therefore, while keeping Si as primary solute, searching for proper additional alloying elements which can restore lost flux density is urgently demanding in electrical steel design.

2. Computational Method

For the first principles total energy calculations, we have employed the full-potential linearized augmented plane-wave (FLAPW) method implemented in WIEN2k code. Generalized gradient approximation is used for exchange-correlation potential. Muffin-tin (MT) radius of each atomic species is chosen between 2.0~2.3 a.u. depending on atomic radius. Wave-functions inside MT-spheres are expanded in spherical harmonics up to l=10 and in interstitial regions with plane-waves up to K_{max}=4.0. Charge densities are described with plane-waves up to $G_{max}=16\sqrt{Ry}$. In all calculations, volume optimizations with atomic relaxations are performed until forces at every atomic site become less than 1.0 mRy/a.u.. For disorder effects, magnetic moments are averaged for selected 2~3 atomic configurations at each solute composition level.

3. Result and Discussion

In this work, we investigated the general features of magnetic saturations of Fe-rich alloys, Fe-X and Fe-Si-X, with a single parameter of average valency. The solute species is extended from 3*d* transition metals (TM) to late 4*d*-5*d* TM and late 3*sp*-6*sp* elements. For binary alloys of Fe-*X* (*X*=3*d*-5*d* TM and 3*sp*-6*sp* elements), the usual mountain-shape behavior of Slater-Pauling curve is produced even for late 4*d*-5*d* TM and the monotonically decreasing behavior for 3*sp*-5*sp* elements. Anomalously, a rise and fall pattern is found for 6*sp* element of *X*=Bi. For ternary alloys of Fe-Si-*X* (*X*=3*d*-5*d* TM and 3*sp*-6*sp* elements), the role of Si is shown to shift the starting point of moment variation and the magnetic flux density of Si-steel is found to repeat Si-absent binary alloy pattern at the shifted reference moment. Based on the calculated magnetic moments, we have described the alloying effects of new solute species beyond ternary alloys. As a feasible candidate for the magnetically optimized products of electrical steels, we have proposed the quaternary alloys of Fe-Si-X-*Y* (*X*=Co, Pd, Pt, and *Y*=Al, Sb, Bi). We expect that the results would lead to the promising applications in improving magnetic flux density of electrical steels.

4. References

[1] R. M. Bozorth, *Ferromagnetism*, Van Nostrand, New York (1953); Wiley-IEEE Press, New York (1993).

[2] M. F. Littmann, IEEE Trans. Magn. **7**, 48 (1971).

[3] J. W. Shilling and G. L. Houze, Jr., IEEE Trans. Magn. **10**, 195 (1974).

[4] G. Y. Chin, Science **208**, 888 (1980).

[5] A. J. Moses, IEE Proc. **137**, 233 (1990).

[6] J. S. Woo and C. S. Lee, J. of the Korean Inst. of Metals, **28** 179 (1990); J. T. Park and J. S. Woo, J. of the Korean Inst. of Met. & Mater. **30**, 561 (1992).

[7] J. B. Lorenzo, T. Ros-Yanez, M. De Wulf, and Y. Houbaert, IEEE Trans. Magn. **40**, 2739 (2004).

[8] G. B. Olson, Science **288**, 993 (2000).

[9] J. C. Slater, J. App. Phys. **8**, 385 (1937).

[10] L. Pauling, Phys. Rev. **54**, 899 (1938).

[11] N. F. Mott, Adv. Phys. **13**, 325 (1964).

[12] A. R. Williams, V. L. Moruzzi, A. P. Malozemoff, and K. Terakura, IEEE Trans. Magn. **19**, 1983 (1983).

[13] A. P. Malozemoff, A. R. Williams, and V. L. Moruzzi, Phys. Rev. B **29**, 1620 (1984).