A Theoretical Approach to Synthesize $L1_0$ type FeNi Alloy Powder

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$L1_0$ type FeNi alloy ($L1_0$ FeNi) is a potential candidate for a rare-earth free magnet. However its synthesis is very difficult as it shows an order-disorder transition temperature at 320°C. Various synthesis routes such as neutron irradiation[1)], alternate monoatomic layer deposition[2)] and chloride complex reduction[3)] have been investigated, but industrial synthesis has never been achieved. In this paper, a new route to synthesize $L1_0$ FeNi by nitriding and denitriding of the disordered alloy is presented.

The nitrogen in iron nitrides is interstitially located in the lattice and weakly interacts with metals. Nitrogen tends to coordinate around iron atoms since its affinity to iron is stronger than that to nickel. FeNiN, formed by the nitriding of disordered FeNi in a rapid stream of ammonia[4)], has an FeN/Ni alternation layer structure. The coordination of metal atoms to FeNiN is similar to that in $L1_0$ FeNi. Therefore it is expected that $L1_0$ FeNi can be synthesized by topotactic denitriding.

Dynamic simulations were performed by a combination of molecular dynamics (MD) and Monte Carlo (MC) methods. MD calculations were carried out using the free calculation code “LAMMPS”. The embedded atom model (EAM) potential was employed between metals, and the Lenard Jones (LJ) potential was applied between the metal and nitrogen. Results shown in Fig. 1. (a), (b) and (c) demonstrate nitriding, denitriding and the diffusion path of nitrogen, respectively. Iron and nickel were ordered in nitriding, and remained ordered in the denitriding process. In nitriding, the corner positions were ordered when the nitrogen/metal ratio was around 1/4. The face-center positions were ordered when the ratio was above 1/4. Nitrogen diffused randomly in nitriding, but it diffused along an iron layer during denitriding. This may be the reason why iron and nickel do not become disordered in the denitriding process.

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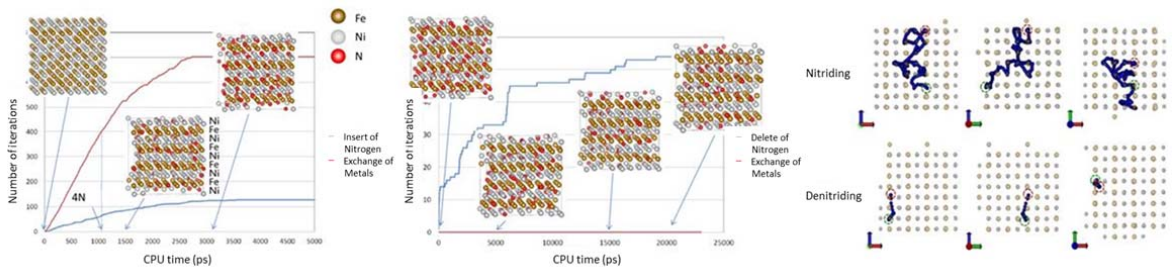
Reference

1) L. Neel et al., J. Appl. Phys., 35(1964) 873.
2) M. Mizuguchi et al., J. Magn. Soc. Jpn., 35(2011) 370.
3) Y. Hayashi et al., J. Magn. Soc. Jpn., 37(2013) 198.
4) R. J. Arnott et al., J. Phys. Chem. Solids Pergamon Press 15(1960) 152.



(a)Nitriding (b)Denitriding (c)Diffusion Path of Nitrogen

Fig. 1 Dynamic Simulations of Nitriding and Denitriding